Benchmarking of Different Optimizers in the Variational Quantum Algorithms for Applications in Quantum Chemistry

Harshdeep Singh[a], Presenting Author[a], Sabyashachi Mishra[b], and Sonjoy Majumder[c]

[a]*Center of Computational and Data Sciences, Indian Institute of Technology, Kharagpur, India*

[b]*Department of Chemistry, Indian Institute of Technology, Kharagpur, India* [c]*Department of Physics, Indian Institute of Technology, Kharagpur, India*

Variational Quantum Algorithms (VQAs) are hybrid-classical-quantum algorithms, which use a classical optimizer to train a parameterized quantum circuit. The optimizers are incredibly important factors in the performance of these variational quantum algorithms, as it determines the overall efficiency of the employed algorithm, both in terms of accuracy and convergence speed. There are numerous optimizers available, each having different architectures based on that, we can broadly classify them into three categories: *(i) gradient-based optimizers* (as the name suggests, these optimizers involve finding the gradient of the objective function e.g. Gradient Descent, etc.), *(ii) gradient-free optimizers* (these optimizers do not require gradient evaluation, e.g. POWELL [1], etc.), and *(iii) quantum-hardware-specific optimizers* (these are a modern class of optimizers which involve quantum architecture for gradient evaluation, e.g. AQGD [2], etc.). VQAs are now being extensively used in for research in quantum chemistry, and therefore, a benchmarking of optimizers specific to quantum chemistry applications is necessary.

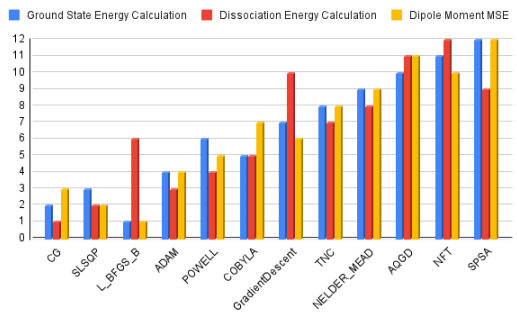

Figure 1: Performance Ranks of Different Optimizers in Quantum Chemistry Applications

Our benchmarking scheme involves using VQAs with the UCC ansatz and commonly-used optimizers to simulate molecules such as the Hydrogen molecule, Lithium Hydride, Beryllium Hydride, Water molecule, and Hydrogen Fluoride, and evaluating the errors across different properties like ground-state energy, dissociation energy, and the dipole moment. Figure 1 shows the performance ranking of different optimizers when used for different tasks where taller bars infer a higher error and hence, worse performance. The number of qubits varied from two, starting from the Hydrogen molecule to ten qubits, in Hydrogen Fluoride.

[1] Powell, M. (1964). An efficient method for finding the minimum of a function of several variables without calculating derivatives. The Computer Journal, 7(2), 155-162.

[2] Maria Schuld, Ville Bergholm, Christian Gogolin, Josh Izaac, & Nathan Killoran (2019). Evaluating analytic gradients on quantum hardware. Physical Review A, 99(3).