iQuHack Team 10

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February 2020

1 Introduction

The fundamental problem in quantum chemistry is solving the many-electron Schrödinger equation. Quantum computing holds the promise to revolutionize chemistry and materials science by solving problems that are too complex to be solved classically. Two algorithms that have successfully been used to find the ground state of small molecular systems are the quantum phase estimation (QPE) algorithm and variational quantum eigensolver (VQE). Among these, VQE poses less strict requirements on the quantum hardware's coherence times, thus making it more prone to be used in near-term quantum computers.

Here, we use the IBM Qiskit software framework to estimate the ground-state energy of the hydrogen molecule. We are interested in studying the effect of noise on simulations with different basis sets. The performance of different basis sets is of interest since the number of qubits scales with basis set size.

We compare the sensitivity to noise of three basis which all have only one contracted Gaussian-Type-Orbitals (CGTO), but differ in the way that these CGTOs are given. The simplest basis set, STO-3G, is composed of three primitive basis functions for the 1-s atomic orbital of H. This means that there are three Gaussian-type functions describing the 1s-orbital, whose relative weight are fixed when running quantum-chemical simulations. The molecular orbitals are given as a linear combination of atomic orbitals. Thus, the hydrogen molecule contains two CGTOs (1 for each H), and each has one linear coefficient, which represents the contribution of that atomic orbital to the overall molecular orbital. In contrast, a slightly more sophisticated basis set, STO-6G, contains six primitive basis functions per CGTO and thus can provide a more accurate description of the 1-s orbital. These STO-nG basis sets are used routinely in quantum-chemical simulations. Finally, we also test the performance of a custom-made basis set, which was obtained by the authors through a different method, and contains four primitive basis functions. Given that the number of CGTOs is the same on all three types of basis sets, their computational cost does not differ much, thus making them equally realistic for use on quantum computers. However, they might exhibit different accuracy due to their differing number of primitives.

The simulations are performed as follows: First, the ground-state electronic structure is found based on the restricted Hartree-Fock method (RHF), using the

PySCF program on a classical computer. Second, the obtained fermionic states are mapped onto the qubit's Hilbert space using a Bravyi-Kitaev encoding. Finally, the VQE is employed. The paramterized states are prepared using a quantum computer. These states are then optimized using a classical algorithm, following the variational principle. This gives a new set of states and parameters, which are then fed into the quantum computer. The several gates act on these new states and finally measure the expectation value of the Hamiltonian. This hybrid classical-quantum cycle is repeated iteratively until convergence.

We ran this VQE simulation for a hydogen molecule with three different basis sets.

The results obtained from these simulations are rather intriguing. To start off, the reported exact energies for each basis set recovered from the *Qiskit ExactEigensolver*, for the Sto-3G, Sto-6G and the Custom basis set were -1.8573, -1.8659, -1.8640 respectively. The results from the VQE with introduced errors from the Qiskit AER library are reported in Figure 1. What is interesting is that if we strictly compare the mean values from these simulations, then the Sto-6G has produced the worst results, which would imply that the basis set with most primitives would have been the most prone to errors. Though if we compare the STD of the Sto-3g and Sto-6g, there is heavy overlap, thus making the results inconclusive, meaning, that we should do more statistical testing to determine if there is actual difference. A similar results can be noticed in the absolute errors (Figure 2).

What is more, is that the difference in the energies are very similar (below 1% difference), thus inferring any conclusions is rather complex. This could be circumvented by simulating larger systems, where there is larger variance, but this is rather impossible on the current state of the art quantum computing systems.

To conclude, we also simulated the Sto-3g and Sto-6g on the Ibmq-London backend, and achieved energy values -1.4082 and -1.0142 respectively, which could be another argument for having the basis set with most primitives, the most prone to errors. But as this was just a single simulation on the quantum computer, the statistical uncertainty is just too high to make any meaningful conclusions.

Overall, we came into this hackathon with little to no knowledge of quantum computing with the goal of educating ourselves about the world and generating some possibly interesting results in quantum chemistry. We definately achieved the former result, and to an extent the later as well.
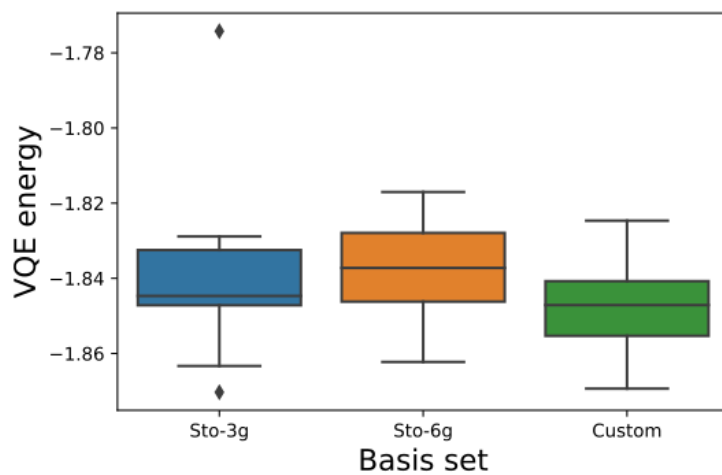
Figure 1: VQE calculated energy on the $qasm\_simulator$ with introduced errors
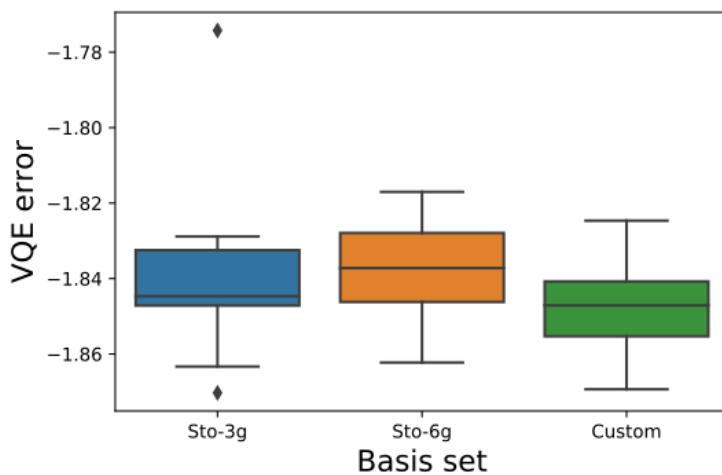

Figure 2: VQE error off of the exact solution calculated by the qiskit Eigensolver $((Exact - VQE_{err})/Exact)$