Simulating a Carbon-Free Future With a Hybrid-Quantum Neural Network

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1 The Carbon Fingerprint

It's safe to say that carbon is one of the most important elements we could possibly interact with. Besides being a key organic element, it's a fuel source. Now though, clean energy is the crisis of century, and in the push for cleaner energy, carbon alternatives have been proposed. Elements and compounds with similar properties to the life-giving element, but are less greenhouse-gas emitting. Carbon's chemical information is encoded in its chemical fingerprint, a characteristic topological description of every molecule. The chemical fingerprint is a unique identifier of the chemical properties of the compound. Similar fingerprints denote similar chemical properties. So, in the search for a cleaner carbon alternative, with similar properties to the element, a comparison of a chemical fingerprint. We attempt to find compounds closest in fingerprint to carbon using a Hybrid-Quantum Neural Network (QNN). Our dataset is composed of molecules and their unique chemical fingerprints.

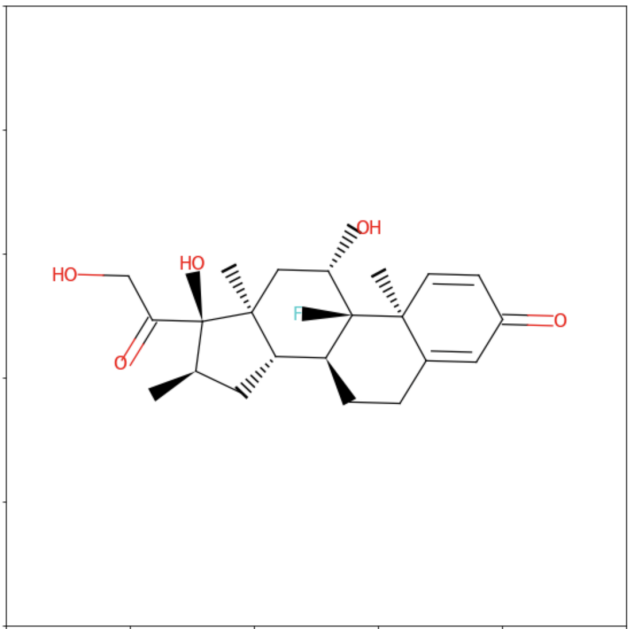

Figure 1: Dexamethasone Molecule Example.

Our QNN

We simulate such a dataset, and how they match up against our number one player, carbon, using Qiskit's Aer simulator. We encode this in our quantum circuit, shown on page 2. Now for the training. we compare 100 molecules from our dataset, subject them to gradient descent, and apply a loss function. The performance on test data yielded loss of -0.5069 with accuracy of 50.0%. For a first model, not terrible numbers. Nothing matches carbon perfectly, but we can get pretty close, and produce energy in a much cleaner manner.

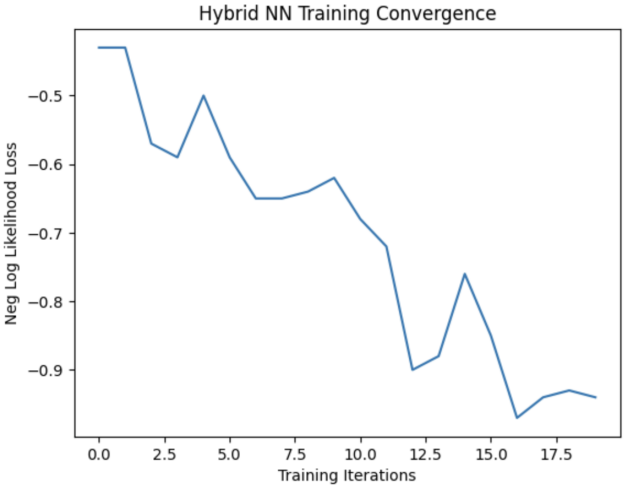

Figure 2: Hybrid QNN Loss Function.

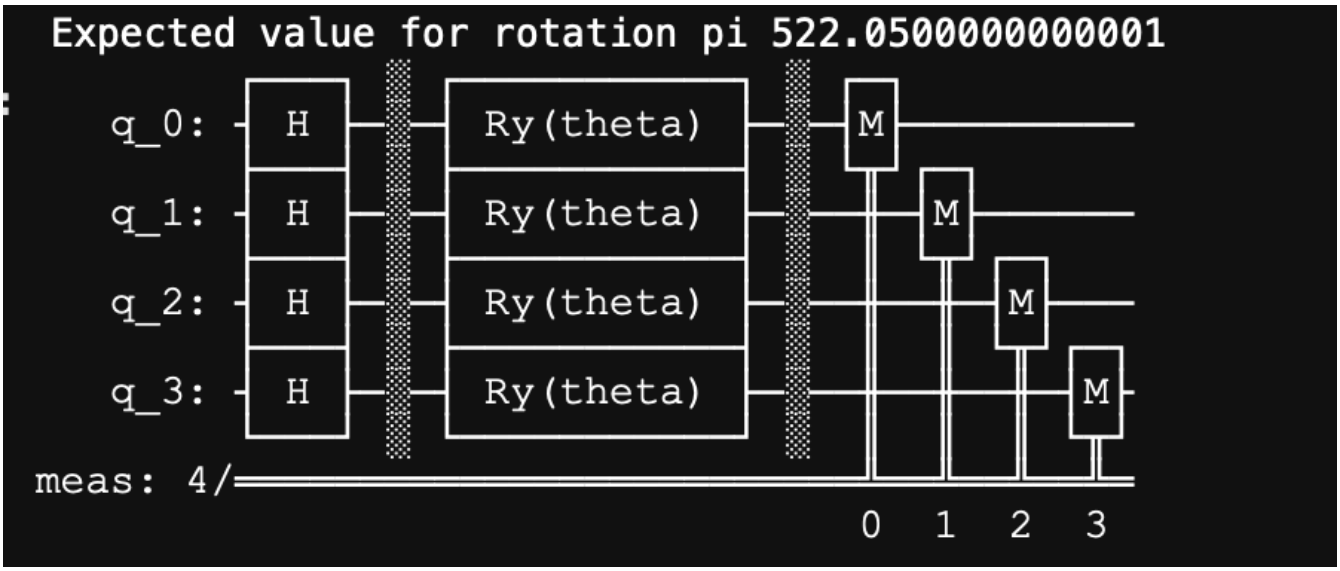

Figure 3: Quantum Circuit Using Qiskit Aer.