

Benchmarking Quantum Algorithms with Neural Networks

CSRI Summer Proceedings 2021

Presented by: Collin Frink

SAND2021-XXXX



Sandia
National
Laboratories



U.S. DEPARTMENT OF
ENERGY

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

This work describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Benchmarking Quantum Algorithms with Neural Networks

Intern: Collin Frink, University of Wisconsin, Madison, **Virtual at:** Shoreview, MN

Mentor: Andrew Baczewski, 1425 Department of Quantum Computing

Abstract Quantum computers are an exciting technology that promises to revolutionize fields in physics, computer science, biology, etc. Thus there is motivation to develop and benchmark algorithms for quantum computers as the physical technology develops. In order to do so, it is useful to understand the capabilities of classical computers to perform similar tasks in which quantum algorithms are theorized to be effective. Recently, some of these classical methods have adopted neural networks to increase computational efficiency. The goal of this project, then, is to determine the effectiveness and efficiency of a variety of neural networks. More specifically, the performance of simpler network structures (Restricted Boltzmann machines) is compared to that of more complex network structures (such as Paulinet and Ferminet) in solving classical physics problems such as dissociation energies.

Problem Domain

Quantum Chemistry

Technical Approach

Neural Networks

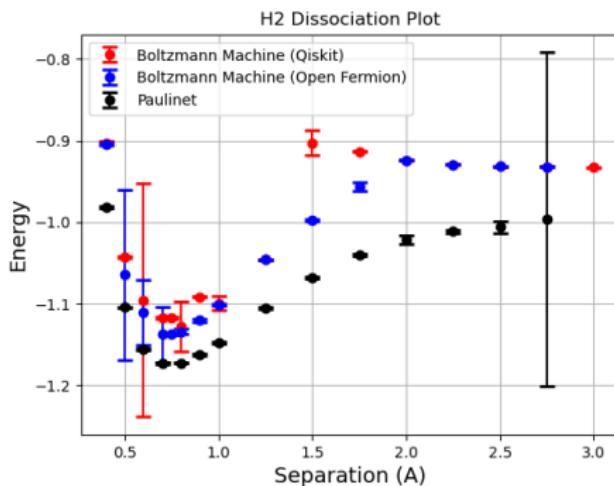
Mission Application

Quantum Technology

H2 Dissociation Energy

Intern: Collin Frink, University of Wisconsin, Madison, **Virtual at:** Shoreview, MN

Mentor: Andrew Baczewski, 1425 Department of Quantum Computing



Above: solutions to the H2 dissociation energy found by two Restricted Boltzmann machines (5 mins) and a CNN based network; Paulinet (3 hrs).

Next, we will further our investigations into the efficiency and effectiveness of all of the previously listed neural networks through hyper-parameter tuning, and deeper examinations of computational efficiency.

Computationally harder problems, such as dissociation energies of larger molecules, can also be used to benchmark each network. Other network structures (including deeper artificial neural networks with more layers than a Boltzmann machine) are another point of interest.