Implementation of Neural Network using *TensorFlow* to solve quantum chemistry problems

Neural Networks in Quantum Chemistry

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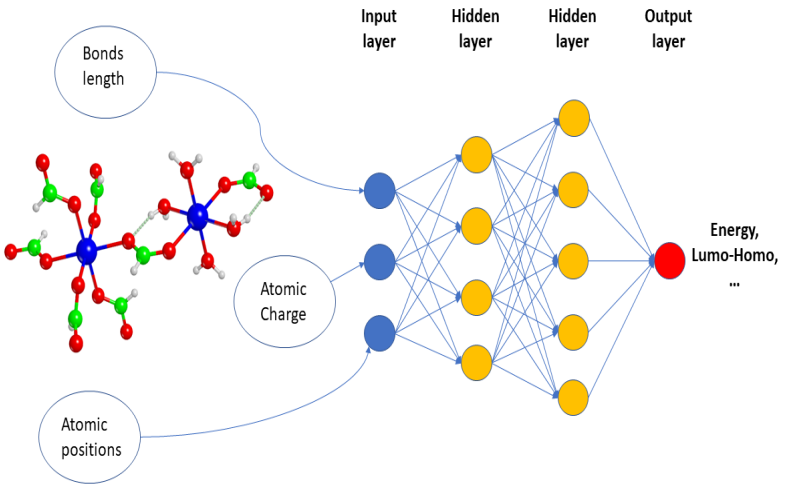

Application of Neural Networks on chemical data with Molecular Descriptors in order to model and predict Molecular properties such as energies, forces or evidence of hydrogen bonds.

Deep learning and Neural Networks (NN) have become an extremely useful machine learning tool in the recent history. They have been deployed on tasks such as Image recognition, Self Driving cars and automatic Text Generation and making huge advancements in these complex problems. Neural Networks are designed to mimic an the neuron activity in our own brains. Whilst the inner workings of our brain are still widely undiscovered so we can't say for sure this is how they are designed. However, one imagines a brain to work similarly to a Neural Network where information is passed from neuron to neuron updating the information at each step until it reaches the final computation where the NN can tell if its a cat or dog in a photo just like our brain. Quantum Chemistry provides powerful tools to understand and uncover information about molecular properties and their reactions. Rapid progress in High Performance Computing (HPC) has allowed chemists to utilise Quantum Chemistry in their research. It helps to understand, model and predict Molecular properties, materials properties at a nano scale and molecular interactions occurring inside many biological systems.

The main goal of the project is to investigate the ability of NN frameworks to simulate molecular dynamics. Our NN models will be implemented using the widely adopted Deep Learning Framework *TensorFlow* in Python. Using the molecular descriptors supplied by the Dscribe library [1] we can input the chemical structures and turn the information into data which a NN model can interpret. Our model will use the input data to predict certain molecular properties such as energies and forces. Finally we want to implement this model both using parralel CPU and GPGPU in order to benchmark and conclude which is the superior execution platforms for Deep Neural Networks.

Final Product

Implementation of a specific Neural Network model in Python applied to one or many Quantum Chemistry problems. We will benchmark our parallel code and compare it to implementation on GPU.

Final Product Presentation

Firstly we will breifly discuss the Quantum Chemistry problem and explain the data and molecular descriptors being used as inputs to our model. After this we will provide an overview of the NN topology. Finally we will show our results of our model and analyse the performance on both GPU and parallel implementation.

Project Timeline

Week 3 (5 July – 25 July)

We began by getting familiar with Neural Networks and their implementation in *Tensorflow*. From understanding the basics to choosing the best hyperparameters for different problems. This was done by following step through tutorials and applying our findings to our specific example problem.

Week 4: (26 July – 1 August)

Introduce ourselves to the molecular descriptors using the Dscribe library. Following the available tutorials for using the Dscribe library we will learn how to transfer chemical information of molecules into viable data formats. An example of the information that can be garnered is the coulomb interaction between atoms in a structure.

Week 5 (2 August – 08 August)

We will use the prepared data formats of the chemical information using Dscribe and begin building our Neural Network model which we will feed the input data through to solve problems.

Week 6 (08 August – 15 August)

Continue building and amending our model and hopefully using a custom Molecular descriptor which is better suited to solve a given problem.

Week 7 (16 August – 22 August)

This week we will look to benchmark both our parallel implementation of our model and also the GPU implementation. Using these we aim to compare the methods and claim that one method is better than the other.

Week 8 (23 August – 31 August)

This week we will be finalising our project. We will demonstrate our work in the video presentation and finish writing up our final report which will contain the in-depth information about our Neural Network Model and analysis of the final products performance.

PRACE SoHPCTitle

Neural Networks in Quantum Chemistry

PRACE SoHPCSite

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PRACE SoHPCSoftware applied

TensorFlow, Dscribe, Python

PRACE SoHPCMore Information

Github Repository

PRACE SoHPCAcknowledgement

Many thanks to Marián Gall for his guidance throughout the project, to everyone at PRACE for the opportunity and the team in ICHEC for the insightful training week.

PRACE SoHPCProject ID

2107

[1] Himanen, Lauri and Jäger, Marc O. J. and Morooka, Eiaki V. and Federici Canova, Filippo and Ranawat, Yashasvi S. and Gao, David Z. and Rinke, Patrick and Foster, Adam S. *DScribe: Library of descriptors for machine learning in materials science*, Computer Physics Communications vol. 247, 2020