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August 27, 2019

1 Three Sentence Introduction

Currently, drug researchers use computationally expensive methods such as density functional theory to predict quantum mechanical (QM) properties of hypothetical molecules prior to synthesis. Recent breakthroughs in machine learning have resulted in two new kinds of neural networks, multitask neural networks and graph convolution networks (GCNs), which have achieved success in work with computational chemistry. My project will apply multitask techniques to a GCN in order to provide more accurate and efficient prediction of QM properties.

2 Summer Work

Over the summer, my partner and I downloaded the QM9 dataset, which contains information about various molecules and their QM properties. In addition, we downloaded Psi4, a software that can perform traditional QM property prediction through density functional theory, which we plan to use as a speed benchmark for our network.

3 Potential Obstacles

Unfortunately, my partner and I have not yet worked with QM9, so one foreseeable obstacle is converting the data into a usable format for training our neural network. In addition, we still need to do more research on multitask neural networks and GCNs in order to implement them effectively. Furthermore, we have not worked with Psi4 in the past, so we need to figure out which functions are applicable to our project and how to use them.

4 First Marker of Success

The first marker of success is being able to implement a GCN using TensorFlow. From there, we can begin comparing the accuracy and speed of our GCN to Psi4's density functional theory and to past work done with GCNs. We can also start integrating multitask features with our GCN.

5 Materials

Since we were able to find a free database and open-source software for our project, we do not require any additional materials.