Journal Report 1

9/2/19-9/9/19
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Daily Log

Tuesday September 3

Tested Psi4 installation. Read Psi4's manual to better understand theory and code for density functional theory.

Searched online for premade implementations of graph convolutional networks or multitask neural networks. Found Spektral, a Keras-based library for graph deep learning, which includes a method for reading in data from the QM9 dataset.

Thursday September 12

Installed Graphviz and Pygraphviz, two required libraries for Spektral usage.

Installed Spektral and tested installation. Found an error in an import statement in Spektral's source code for method to load data from the QM9 dataset and corrected it (though this requires further testing because it seems to be a consistent error across Spektral's source code).

Loaded QM9 dataset and worked with it to better understand how Spektral loaded in the data and how to use it in a graph convolutional network.

Timeline

Date	Goal	Met
August 26	N/A	N/A
September 2	N/A	N/A
September 9	Read in data from QM9 dataset	Used Spektral library to load QM9 data
September 16	Create a basic graph convolutional network using Spektral	
September 23	Create a specialized graph convolutional network for QM9	

Reflection

This week, my main goal was to be able to load the QM9 data. While researching the QM9 dataset in order to better understand the format of the data, I stumbled upon Spektral, a library which has a convenient method to load data from QM9 and also has methods to support graph neural networks. Not only did Spektral allow me to fulfill my weekly goal, but it will also make writing a graph convolutional network (GCN) easier in future weeks.

Unfortunately, I struggled with connecting my laptop to TJ wifi early on this week, so downloading Spektral and its required dependencies was difficult. On Tuesday, I was only able to use my phone's hot spot, so I spent a portion of class testing my Psi4 installation and reading up on density functional theory (DFT), even though my partner is working with the DFT calculations. I feel that I have a slightly better understanding of DFT and how to use Psi4 now, but I will definitely need to learn more as we move further through our project.

After resolving my wifi issues, I was able to download Spektral on Thursday. I tested my installation by attempting to load in the QM9 data, but there was an error in an import statement that said `from keras.backend import tf`. I changed this to `import tensorflow as tf`, which allowed me to load the QM9 data. However, this import statement is used widely throughout Spektral's source code, so I need to ensure that this change works with all of the Spektral methods we plan on using.

For this upcoming week, I hope to implement a GCN using Spektral's graph convolution layers. Once that is accomplished, I will begin fine-tuning it to work with the QM9 dataset. Meanwhile, my partner will work on the DFT calculations and looking into multitask learning.