Journal Report 1
8/26/19-9/6/19
Sohom Paul
Computer Systems Research Lab
Period 1, White

Daily Log

Thursday August 26

Gave myself a crash course in quantum mechanics.
Read tutorial for DFT.

Tuesday September 3

Followed tutorial for semi-supervised learning using graph convolutional networks
Built a classifier on the Zachary's Karate Club dataset.
Started reading the research of Kipf and Welling and spectral graph convolutions.

Thursday September 5

Tried (and failed) to install GPU acceleration for Tensorflow.
Installed graph deep learning library Spektral.
Continued building Zachary's Karate Club example using spectral graph convolutions.

Timeline

Date	Goal	Met
Aug 26	N/A	N/A
Sep 2	N/A	N/A
Sep 9	Build first graph convolutional network and install relevant libraries	Partially; No backpropagation.
Sep 16	Run relevant DFT calculations; find best parameters	
Sep 23	Build toy networks with multitask learning	

Reflection

Because we are still in the early stages of research, much of the work done so far has been preliminary forays into understanding the tools we plan to use. Because we will eventually will have to work on a shared code base, we agreed to both spend the first week learning about the inner machinery in graph convolutional networks. I've been builing a toy GCN so that I might experiment with different graph convolutions. However, my partner has found a deep learning library built to handle graphs, so now our goal is to learn and use this library. My partner has already discovered that we had to edit the source code from reading "`from keras.backend import tf`" to "`import tensorflow as tf`", which shows that we will need to run more strenuous testing to make sure that this library functions and will meet our needs. Thus, she has taken it upon herself to learn and possibly fix this library's code for the coming weeks.

I spent a significant amount of time in class trying to get an installation of `tensorflow-gpu` onto my computer so that when we start building our networks, I would be able to test on my own machine. However, I use the Windows subsystem for Linux (WSL) so I can emulate Ubuntu behavior without actually dual-booting. However, as I eventually learned from the WSL Issues page on Github, this makes hardware acceleration impossible.

Because my partner is focusing on building the graph convolutional network, I am shifting my focus to actually benchmarking our data set using DFT. Without going into too much detail, DFT relies on solving the Kohn-Sham equations for the wavefunction and electron density. The wavefunction has to be represented as a linear combination of a finite basis set of functions, which the user must choose. Secondly, the exchange-correlation potential, which appears as a term in the Kohn-Sham equations, is unknown, so one has to choose an method of approximating this potential. My goal for the next week is to find an appropriate basis set and approximation method.

Our ultimate goal is to have multitask learning incorporated into our graph convolutional network. In order to understand how to implement multitask learning, and to learn how to use Keras and Tensorflow, I intend to spend the week after next building toy examples using multitask learning so that I will eventually be able to incorporate it into my partner's GCNs.