Journal Report 2
9/9/19-9/16/19
Emily Ye
Computer Systems Research Lab
Period 2, White

Daily Log

Monday September 9

Worked through Spektral tutorial for writing a GCN using the Cora dataset.

Tuesday September 10

Found Spektral examples of GCNs using the QM9 dataset.

Read through Kipf & Welling's paper (2016) on graph convolutional layers, which the Spektral implementation of graph convolutional layers is based on.

Thursday September 12

Read through Spektral example code for GCNs in graph batch mode and using edge-conditioned convolutions.

Made changes to Spektral source code to make it compatible with current version of Keras.

Reviewed Spektral documentation for edge-conditioned layers and began implementing GCN based on Spektral example with edge-conditioned convolutions.

Timeline

Date	Goal	Met
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 GCN using Spektral	Created GCN with Cora dataset and began creating GCN using QM9 with edge-conditioned convolutions
September 23	Complete GCN with edge-conditioned convolutions	
September 30	Complete GCN in graph batch mode for comparison with edge-conditioned GCN	

Reflection

After working through a Spektral tutorial, I realized that there was a lot I still needed to understand about GCNs. Furthermore, the tutorial used the Cora dataset, which is vastly different from the QM9 dataset that we are using. Therefore, I spent most of the week gaining a better understanding of GCNs through reading a paper and some example code. Thus, even though I made a GCN using Cora, I was not able to finish a GCN using QM9.

Although I was able to find Spektral example code for two types of GCNs using QM9, there is a lot I do not understand in both examples, including the pros and cons of each kind of GCN. Therefore, I plan to implement both kinds and compare the results to determine which GCN we should use in our final project. I also plan to do more research into edge-conditioned convolutions next week, as those are used in one of the example GCNs I found.

Finally, one major issue I had last week and at the beginning of this week was that Spektral is incompatible with the current version of Keras. I was able to fix most of the problems (all of the ones I have found so far) by changing `from keras.backend import tf` to `import tensorflow as tf` and making sure any references to `keras.backend.tf` referred to just `tf` instead. This was also presented as a solution on the Spektral GitHub, so I hope it will work as a fix for now.