Journal Report 11

11/25/19-12/8/19
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Daily Log

Tuesday November 26

Updated GitHub by editing readme and uploading my journals and papers that I read
Continued working on saving and loading weights

Monday December 2

Successfully saved weights from edge-conditioned GCN model to load in file for demo
Began reviewing Spektral methods for reading in data from the QM9 dataset (for comparison to Sohom's code for reading in specific molecules from the QM9 dataset)

Tuesday December 3

Added code in for training on each molecular property separately to edge-conditioned model
Played around with training edge-conditioned model on larger dataset and with different numbers of epochs to see how I could get the highest accuracy
Continued reviewing Spektral methods for reading in data from the QM9 dataset (for comparison to Sohom's code for reading in specific molecules from the QM9 dataset) while training models

Thursday December 5

Continued playing around with training edge-conditioned model on larger dataset and with different numbers of epochs to continue trying to improve accuracy
Retrained edge-conditioned model on a larger dataset and resaved weights in preparation for working more on the demo file next week

Timeline

November 25	Determine which kind of GCN to use for final project after comparing TAGCN with previously-implemented edge-conditioned GCN	Decided to use edge-conditioned GCN
December 2	Figure out how to save and load model weights for the edge-conditioned GCN using EdgeConditionedLayers from Spektral	Worked mostly on updating GitHub with a readme and journals/useful papers instead
December 9	Figure out how to save and load model weights for the edge-conditioned GCN using EdgeConditionedLayers from Spektral, in addition to retraining edge-conditioned GCN	Successfully saved and loaded model weights for the edge-conditioned GCN and retrained edge-conditioned model
December 16	Merge code for reading in molecules with code for model with loaded-in weights and test demo	
December 23	Continue testing demo and have it ready by December 20 (before winter break)	
Winter Goal	Create a demo that can take a molecule and calculate the relevant properties using density functional theory (DFT) or the edge-conditioned GCN, so a user can see the relative accuracy and speed	

Reflection

My main goal this week was to make sure everything with the edge-conditioned model was trained and ready so I can focus on the winter goal demo itself for the next two weeks. Originally, I thought this involved both making sure I could save the weights of the trained edge-conditioned model to load into a different file (the file for the winter goal demo) and improving the accuracy of the edge-conditioned model. However, I also needed to train separate models for each property I wanted to predict rather than a single model as I had used before.

This is because there is a difference in how my winter demo code will read in data and how my edge-conditioned model read in data. I need to read in a single molecule at a time from QM9 for the winter demo, unlike Spektral's method for reading in data from QM9, which randomly selects a given number of molecules to form training, validation, and testing sets. For the next week, my goal is to reconcile reading in single, specific molecules with the edge-conditioned GCN model, which was designed and written using Spektral methods. I hope that I will be able to finish the code for the demo by the end of this week or early next week, so I can use the extra time to test.