Journal Report 12
12/9/19-12/15/19
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Daily Log

Monday December 9

Began code to read in information about a specific molecule

Tuesday December 10

Finished code to read in information about a specific molecule and integrated it with code for the DFT calculation

Began code to put a specific molecule through the trained edge-conditioned models and gather output

Thursday December 12

Retrained edge-conditioned models after adjusting code to load in all data from QM9 instead of just the first 10000 molecules

Continued and debugged code to put a specific molecule through the trained edge-conditioned models and gather output

Timeline

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	Mostly done with demo, with a little debugging left to do
December 23	Finalize 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 finish the demo so I could use the last week before break to test my code and finalize it. I finished the demo for the most part, but there is still some debugging left to do. Furthermore, I noticed that I was only reading in the first 10000 molecules from the QM9 dataset (which are also the smallest molecules). I spent a large part of Thursday's class trying to figure out how to read in the data correctly, process it, and then retrain all of the networks for each molecular property.

Moving forward this week, I first want to make sure the networks were trained properly this time by reviewing all the code for training the edge-conditioned models, specifically reading in the data from the QM9 dataset. After that, I will work on debugging all my code for the winter demo, since there are a few issues left to smooth out.