Journal Report 10
11/18/19-11/25/19
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Daily Log

Monday November 18

Compared code between edge-conditioned GCN and TAGCN

Reviewed Psi4 documentation for reading in molecules

Tuesday November 19

Attempted to write code for reading in molecules based on the Psi4 documentation

Referred to Sohom's code for reading in molecules after getting confused. Reviewed this code, as well as Sohom's code for calculating specific properties, while referring to the Psi4 documentation

Began to refamiliarize myself with code for the edge-condtioned GCN, which was written over a month ago

Created new file for winter goal demo

Thursday November 21

Set up model for loading weights in winter goal demo folder

Reviewed TensorFlow documentation for saving weights from a trained model (the edge-conditioned model) and loading them into a new file (file for winter goal demo)

Struggled to save and load weights because of how the edge-conditioned GCN model requires the EdgeConditionedLayer that is not present in TensorFlow and is instead used from Spektral

Began looking into how to make TensorFlow and Spektral more compatible

Updated GitHub files to include file for winter goal demo

Timeline

November 11	Finish implementing Du, et al.'s topology adaptive graph convolutional network with Spektral and QM9 dataset	Basically finished, but will continue testing and trying to reduce the loss value next week
November 18	Code accuracy graph (predictions v. true values) for TAGCN	Created accuracy graph and calculated R^2 value
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 Edge-ConditionedLayers from Spektral	
December 9	Merge code for reading in molecules with code for model with loaded-in weights	
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

This week, my main goal was to determine which kind of GCN to use for the final project. After reviewing both the edge-condtioned GCN and the TAGCN, it felt that the edge-conditioned GCN was more intuitive and easier to use. The edge-conditioned GCN also links to Spektral, which would facilitate further edits to the layers. Finally, the edge-conditioned GCN achieved a higher accuracy than the TAGCN did when both were initially written and modified slightly.

Looking ahead, I had planned to write code to read in a molecule using Psi4. However, after struggling to understand how to use it for about half a class, I looked at my partner's code for reading in molecules and decided to just use that instead of trying to rewrite it. At some point before winter break, I will revisit the Psi4 methods and discuss my partner's code with him to make sure I completely understand it.

This week, I also created a file for my winter goal demo. In order to make my demo quick and not need to retrain a model each time, I began looking into how to save a model or its weights and then quickly load it into a different file. While I found a few solutions, most of them were difficult to implement because Spektral is not entirely compatible with TensorFlow. This means that some of TensorFlow's built-in methods do not work. Thus, my goal for the next week is to work out these complications and find a way to save and load model weights for the GCN.