Journal Report 9
11/11/19-11/17/19
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Daily Log

Monday November 11

Continued testing TAGCN to lower loss, but with little success

Tuesday November 12

Reread TAGCN paper (Du, et al., 2017) to find ways to reduce loss for TAGCN, but found little information and moved on to coding accuracy graph

Began coding accuracy graph based on previous code used for edge-conditioned GCN

Thursday November 14

Continued debugging accuracy graph (see below for finished accuracy graph of predictions vs. actual values for the TAGCN)

Calculated R^2 value for accuracy graph to be around 0.597

Uploaded files to GitHub

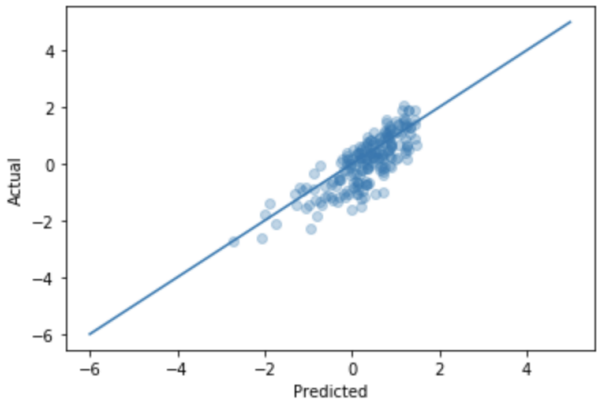

Figure 1: Accuracy of TAGCN on 2000 samples

Timeline

November 4	Finish implementing Du, et al.'s topology adaptive graph convolutional network with Spektral and QM9 dataset	No, didn't have enough time to finish due to presentations taking up part of the week
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	
December 2	Review Psi4 documentation and write code that can read in a molecule (so that its properties can be calculated by the selected GCN)	
Winter Goal	Create a demo that can take a molecule and calculate the relevant properties using density functional theory (DFT) or the selected GCN (i.e. TAGCN or edge-conditioned), so a user can see the relative accuracy and speed	

Reflection

This week, my main goal was to create an accuracy graph for the TAGCN code like I had done for the edge-conditioned GCN, which I was able to finish. Judging based on how the two graphs look and how their R^2 values compare, it is likely that we will go with the edge-conditioned GCN for our final project, but I will keep comparing the code and accuracies of the two GCNs this week. By the end of this week, I hope to discuss with my partner and choose either the edge-conditioned GCN or the TAGCN for use in our final project.

Looking forward, I will be able to start working on my winter goal once we select a GCN. My partner has already written code to calculate the properties of a molecule using DFT. Since I am unfamiliar with the Psi4 methods that we will need for our project, I plan to review the documentation this week and write my own code to read in a molecule so that its properties can be calculated. After I do this, I will compare my code with my partner's and get the DFT code from him while continuing to improve the selected GCN.