Journal Report 16
2/10/20 - 2/16/20
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Daily Log

Monday February 10

Continued debugging combined multitask GCN code

Tuesday February 11

Finished debugging combined multitask GCN code

Played around with layer sizes on GCN to increase accuracy for specific features that performed poorly during testing for winter goal (specifically HOMO and LUMO – gap also did poorly, but since it is dependent on HOMO and LUMO, I decided to start with those two features)

Thursday February 13

Continued trying to increase accuracy for HOMO and LUMO GCN models

Timeline

February 2	Finish combining multitask and GCN networks, test and tweak multitask GCN to improve accuracy	Worked on presentation instead
February 9	Finish combining multitask and GCN networks, test and tweak multitask GCN to improve accuracy	Listened to presentations throughout the week
February 16	Finish combining multitask and GCN networks, test and tweak multitask GCN to improve accuracy	Finished combining multitask and GCN networks and began tweaking multitask GCN to improve accuracy
February 23	Improve accuracy for HOMO and LUMO models	
March 1	Test different convolutions to improve accuracy	

Reflection

My main goal for this week was to finish debugging the combined multitask GCN code, which I was able to do. I also started tweaking the layers of the individual GCNs trained for each property in order to increase accuracy. I started with HOMO and LUMO, since those two (along with gap) performed poorly when I was working on my winter goal. For the winter goal, I trained all of the GCNs using the same model, so this week, I started trying to use different layer counts for different properties. Progress on this was slow because the network takes a long time to train each time I retrain the GCNs.

Looking forward, I want to continue improving accuracy for the HOMO and LUMO models as well as some of the other properties that did not perform well for the winter goal, such as alpha. After that, I will continue testing different convolutions to look for continued improvement in the multitask GCN.