

Journal Report 17

2/17/20 - 2/23/20

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Period 2, White

Daily Log

Tuesday February 18

Continued trying to increase accuracy for HOMO and LUMO GCN models, focusing on HOMO specifically

Thursday February 20

Continued trying to increase accuracy for HOMO and LUMO GCN models, focusing on LUMO specifically

Timeline

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	Some progress, but I want to continue trying to improve accuracy
March 1	Continue improving accuracy for HOMO and LUMO models	
March 8	Test different convolutions to improve accuracy	

Reflection

My main goal for this week was to continue improving accuracy for the HOMO and LUMO models. I have made some progress, but I am still looking to improve the accuracy a little more through a few more tweaks to the GCN layers. Like I mentioned in my last journal, this has been slow because of the time needed to retrain each time. I have started using a smaller training size for testing the GCNs because it does not take as long and should still allow for comparing accuracies.

This week, I plan to continue working on HOMO and LUMO, potentially working on some of the other underperforming properties if I have extra time towards the end of the week. Once I finish, I am planning to look into other convolutions and possible ways to continue improving the accuracy of the multitask GCN.