

Journal Report 14

1/13/20-1/19/20

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Period 2, White

Daily Log

Monday January 13

Retrained graph convolutional networks for each of the single-task properties as preparation to implement clustering

Tuesday January 14

Clustered single-task properties based on how the properties were clustered together in previous multitask code (from winter demo)

Attempted to revise code for training parameter sharing models to work with GCNs, but ran into several bugs

Thursday January 16

Revised layers of single-task GCN models after realizing inconsistencies with multitask clustering code

Continued debugging code for training parameter sharing models / clustering to work with GCNs

Timeline

December 22	Finalize demo and have it ready by December 20 (before winter break)	Successfully finished winter goal demo to show time/accuracy comparison of GCN with DFT
January 12	Review multitask papers and Sohom's multitask code in preparation for integrating the multitask and GCN networks	Reread multitask papers and read through Sohom's code
January 19	Implement clustering of single-task properties on GCN	Mostly finished, will continue debugging
January 26	Finish combining multitask and GCN networks	
February 2	Test and tweak multitask GCN to improve accuracy	

Reflection

My goal for this week was to implement clustering on the graph convolutional network based on the clusters used in the multitask winter demo. I started off by retraining the single-task networks based on each individual property since I had made a few edits to the layers of my GCN model since the winter demo. I was then able to modify code for parameter sharing models to work with both clustering and my previous GCN model. While there are still a few bugs to work through, I am fairly certain I will be able to have a functional multitask GCN by the end of this week, even though there may still be some tweaks needed to improve accuracy.

While working on code for the winter demo, I noticed that some of the single-task GCNs were significantly less accurate than the others. I plan to look into this next week and modify layer sizes in the multitask GCN to improve prediction of specific properties.