Journal Report 11

12/2/19-12/6/19
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Daily Log

Tuesday, November 26

tried (and failed) to save information about custom classes when saving model

Monday, November 26

changed single task training to save weights instead of the model
tested training, saving, and loading of single task models
tested calculation of transfer coefficients from file

Tuesday, November 26

continued training single task models
continued mining for available values that can be pulled from Psi4; fixed minor bugs

Tuesday, November 26

completed training of single task models
completed calculation of cross-task transfer coefficients

Timeline

Date	Goal	Met
Nov 18	Finish performing neural clustering. Start implementing deep relationship networks.	Postponed, due to errors in last week's work.
Nov 25	Finish performing neural clustering. Generate 19x19 table of task relatedness. Start building demonstration program with DFT and single-task results.	Successful builds of DFT, partial completion of code to cluster tasks.
Dec 2	Continue building demonstration with preliminary multitask results.	Yes.
Dec 9	Cluster tasks. Train multitask network. Finish building demonstration with multitask and DFT methods.	
Dec 16	Final testing of my demonstration.	
Winter Goal	Have a program capable of taking an input molecule and predicting the relevant molecular properties, using a choice of density functional theory or multitask-learned networks. The demo will let the use see firsthand the relative accuracies and speeds of the methods.	

Reflection

I realized this week that, even though it's not easy to save that my models directly using Keras because of the custom classes used, it's trivial to save and load the weights. I was also able to finish training all of the single task networks and calculate the cross-task correlations. I haven't actually figured out how exactly I'm producing my clusters; somehow, I need to find large sets of tasks that mutually have low transfer coefficients. This would probably be a hard task in general, but because I'm only work with this specific graph of 19 nodes, I expect to be able to use some simple thresholding where two tasks are trained together when their transfer loss is low.

In other news, not all of the tasks that appear in our dataset can actually be calculated using Psi4, to the best of my knowledge. I do not know how to extract electronic spatial extent, polarizability, and the atomization energies. For this reason, I will not include those particular tasks in my DFT demo.

Included below are some of the calculated cross-task transfer coefficients; I did not include all 342 values because I didn't want to waste paper.

```
A B 0.13086552423238754
A C 0.04075440979003906
A mu 0.9960114765167236
A alpha 0.9690558757781983
A homo 1.0085037326812745
A lumo 1.0072671127319337
```

```
A gap 0.9788152894973755
A r2 0.9844315662384033
A zpve 0.985578049659729
A u0 0.9353220615386962
A u298 0.9660965385437011
A h298 0.9426877708435059
A g298 0.9355496406555176
A cv 0.9767080888748169
```

In earlier journals, I had hoped to start studying deep relationship networks. As of right now, I don't think it is important that I complete this investigation before winter break, and I will meet with my partner over the break to solidify our plans for the third quarter.