Journal Report 5
9/30/19-10/4/19
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Daily Log

Monday September 30

Tried running partner's code on my machine
Import matplotlib failed.
Uninstalled and re-installed matplotlib on all the locations where I knew I had Python. Error not yet resolved.

Tuesday October 1

Resolved error with matplotlib (included call to terminal from Jupyter notebook itself).
Failed to import sklearn because of a ImportError raised with in scipy. Apparent circular imports?

Thursday October 3

Import errors magically resolved.
Modified code to train for two features (heat capacity and zero point internal energy) simultaneously.

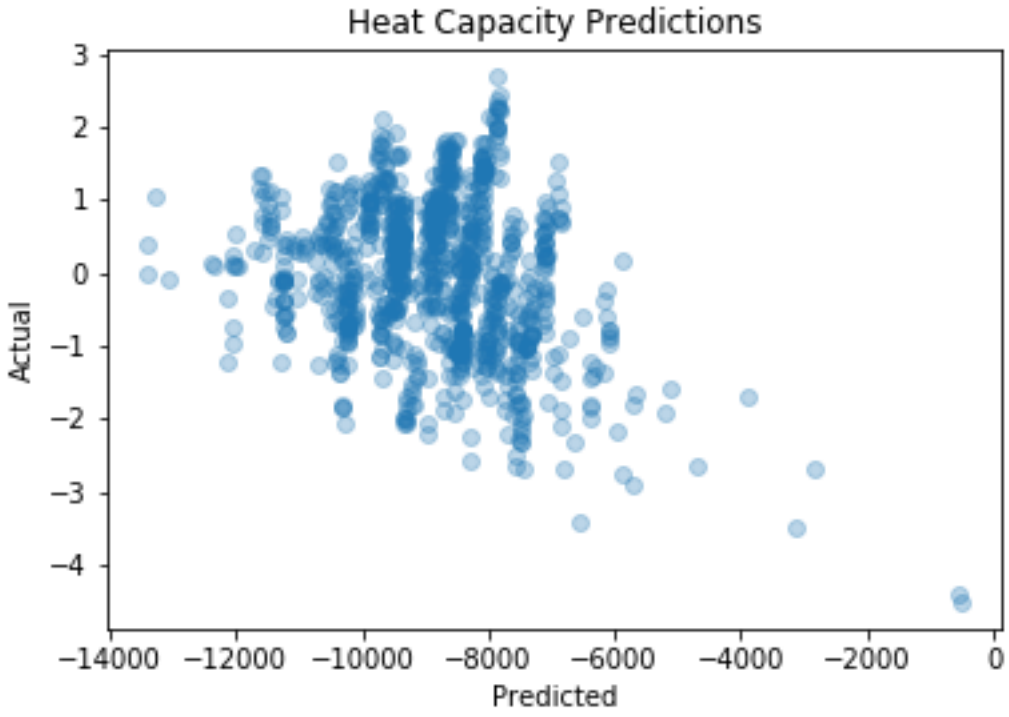
Timeline

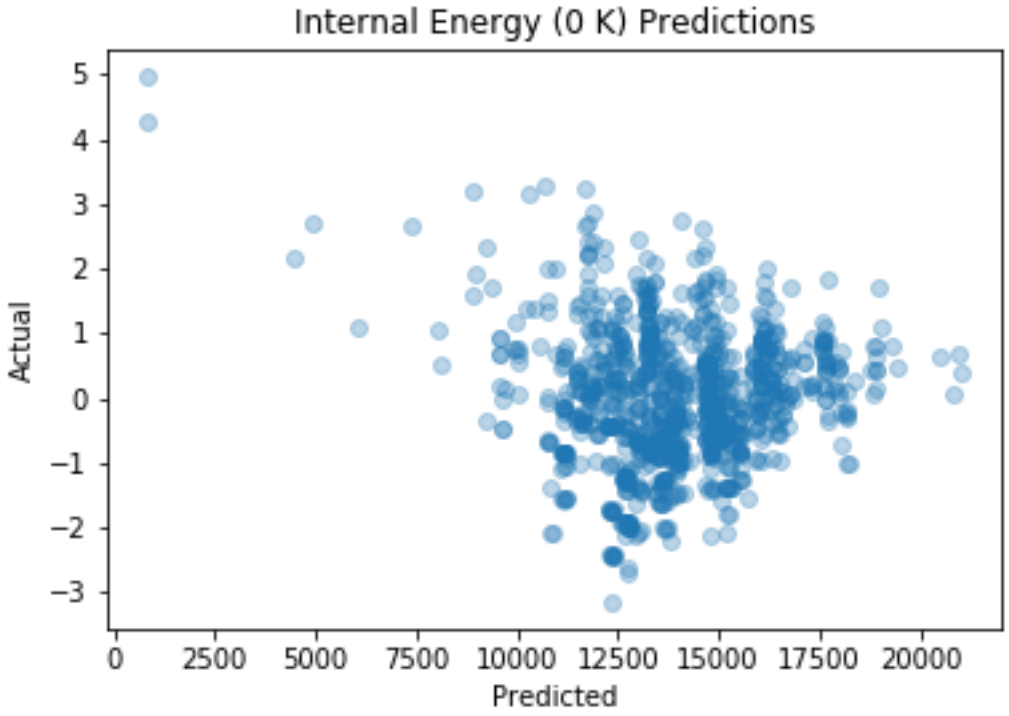
Date	Goal	Met
Sep 23	Write Python script to run DFT calculations and pull relevant features from our dataset.	Yes
Sep 30	Build toy networks with multitask learning	Abandoned; stole code from Github instead.
Oct 7	Integrate multitask learning (hard parameter sharing) into first GCNs	Partial; need to modify to include separate dense layers.
Oct 14	Train network and compare results to tasks done without multitask learning.	
Oct 21	Build network with soft parameter sharing; modify loss accordingly.	

Reflection

My work on Monday and Tuesday were both hampered by not being able to import the proper dependencies - which is really weird, considering that I've used by matplotlib and scipy in the past. For matplotlib, I was able to resolve the issue by issuing a terminal call from Jupyter itself. I don't know why running the same command from my actual terminal failed, especially because I verified that Jupyter was running Anaconda... but that is of no consequence. Similarly, on Tuesday, I was having some difficulty importing scipy. More specifically, an import statement to scikit-learn had an internal import statement to scipy.sparse.linalg.interface, which in turn imported a deprecated method from scipy.sparse.sputils. However, the method was still in the source code, so the fact that it was deprecated shouldn't have been the reason that Python was raising an ImportError. I tried all the reasonable changes - upgrading scipy, downgrading scipy, uninstalling and reinstalling scipy - none of which work. What fixed it was trying to show the problem to my friend, which caused my code to magically start working.

On Thursday, I started building modification to the GCN code to allow for multitask learning. I was not able to complete a true multitask network, mostly because of my inexperience with using Keras, but I experimented with just changing the output to a vector of multiple quantities. I'm getting horrifically bad results, which points to a bug in my code, but I haven't been able to find it yet. Otherwise, I think that I'll be back on track with hard parameter sharing and possibly a start on soft parameter sharing this coming week.


Heat Capacity Predictions
Actual
Predicted
3
2
1
0
−1
−2
−3
−4
−14000
−12000
−10000
−8000
−6000
−4000
−2000
0


Internal Energy (0 K) Predictions
Actual
Predicted
5
4
3
2
1
0
−1
−2
−3
0
2500
5000
7500
10000
12500
15000
17500
20000