

Daily Log

Monday, February 17

Investigated dimension mismatch in readout step of MPNN. (Bug not resolved, but I shifted attention to setting up Python2 environment to ensure errors were not caused by code deprecation in numpy.)

Tuesday, February 18

Found and installed binaries for necessary Python2 packages.
Resolved version conflicts.

Thursday, February 20

Found compatible version of deepchem in PyPI archives.
Allowed for link forwarding between my Ubuntu subsystem and Windows main OS.
Encountered error: Jupyter Notebook no longer using correct Python interpreter.

Timeline

Date	Goal	Met
Feb 10	Identify and start implementing alternative neural methods.	Yes; installed DeepChem to investigate MPNNs.
Feb 17	Understand code from MPNN tutorial. Start building neural fingerprinting.	No; this goal has been expanded to fill the next 2 weeks.
Feb 24	Build first example MPNN.	No; still in process of setting up testbed to use sample code.
Mar 2	Build first example MPNN (possibly in Python 3).	
Mar 9	Start molecular fingerprinting.	

Reflection

This week has been a continuation of some of the setup woes that I was encountering last week. For the most part, it looks like I have successfully built a conda environment for Python2 code execution without version conflicts (which was surprisingly hard to finagle). However, I have not yet tested whether the MPNN code that I pulled from Github now works or if there are outstanding errors. More annoyingly, I have not been able to force Jupyter notebook to use the Python installation of the current conda environment. It instead having it default to an installation located elsewhere. At the start of next class, I will try to see if I need to change my installation of the IPython kernel or otherwise change the settings of Jupyter itself. If does not resolve the error, then I will instead resort to running the file as a .py file instead of a .ipynb, which will unfortunately slow down my workflow.

For this reason, I think it will be for the best if I simply rebuild the providing code in Python3, using the Python2 environment so I can compare the output of the original and rebuilt code to ensure that I don't err in my building. After this, I will return to applying these technologies to our original problem in my first implementation of molecular fingerprinting.