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White P. 1

Journal 0

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Please note that this project is joint work with Emily Ye in your second period.

Give a three sentence overview of your project.

Research and development of new drugs is hindered by costly computation of quantum chemical properties, which is typically done by approximating molecular wavefunctions using density functional theory. However, graph convolutional networks can efficiently identity key features from graphical input, and multitask learning increases accuracy and reduces training time by sharing layers between tasks. Our project is training multitask graph convolutional networks on small drug-like molecules in order efficiently predict chemical properties.

What obstacles will you face in completing this project?

In order for our project to have a fair basis for comparison, we will judge the success of our network based on looking at how the error margins compare to density functional theory rather than just giving raw errors. However, density functional theory calculations include multiple human-set parameters, so over the course of the coming weeks, we will have to manually test different settings in order to get accurate results from density functional theory. Beyond this, because there are only a few implementations of graph convolutional networks floating around, it is likely that we will have to code close to the metal.

What materials do you need for your project?

We need Syslab resources to train our network.

What will your first mark of progress on this project?

Our first mark of progress is making sure that we are, in fact, capable of using computational chemistry software in order to predict the properties we are studying on the molecules that we are studying.