INTERPRETABLE DEEP LEARNING FOR MOLECULES AND MATERIALS

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Deep learning has begun a renaissance in chemistry and materials. We can devise and fit models to predict molecular properties in a few hours and deploy them in a web browser. We can create novel generative models that were previously PhD theses in an afternoon. In my group, we're exploring deep learning in soft materials and molecules. We are focused on two major problems: interpretability and data scarcity. Now that we can make deep learning models to predict any molecular property ad naseum, what can we learn? I will discuss our recent efforts on interpreting deep learning models through symbolic regression and counterfactuals. Data scarcity is a common problem in chemistry: how can we learn new properties without significant expense of experiments? One method is in judicious choose of experiments, which can be done with active learning. Another approach is self-supervised learning and constraining symmetries, which both try to exploit structure in data. I will cover recent progress in these areas. Finally, one consequence of the state of deep learning is that you can just make cool things in chemistry with minimal effort. I'll review a few fun projects, including making molecules by banging on the keyboard, doing math with emojis, and doing molecular dynamics with ImageNet derived potentials.