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Title: Explaining molecular properties with natural language

Abstract:
Chemists can be skeptical in using deep learning (DL) in decision making, due to the lack of interpretability in "black-box" models. Explainable artificial intelligence (XAI) is a branch of AI which addresses this drawback by providing tools to interpret DL models and their predictions. Molecular property prediction is an unusual space of XAI because the input features are graphs – which have poorly defined gradients. I will review the principles of XAI in the domain of chemistry and emerging methods for creating and evaluating explanations. Then describe its application to explaining solubility, blood-brain barrier permeability, and the scent of molecules. We show that XAI methods like counterfactuals and descriptor attributions can both explain DL predictions and give insight into structure-property relationships. Finally, we discuss how a two-step process of highly accurate black-box modeling and then creating explanations gives both highly accurate predictions and clear structure-property relationships.