A powerful yet inadequate tool - ML for electronic structure

Isaac Tamblyn

Acting as a surrogate model, machine learning (ML) models such as deep neural networks have the ability to estimate the output of expensive electronic structure calculations at a fraction of the computational cost. When trained properly, they are capable of scaling to much larger system sizes, operating at length scales which were previously thought inaccessible. Unfortunately, these advantages have come at a high price - supervised ML models provide little intuition or explanation about *how* they arrived at a particular prediction. As a result, it is difficult for ML practitioners to obtain transferable insight. Each problem feels like a new one.

I will discuss some of the recent successes and failures of ML and provide examples which attempt to provide generalized insight.