Machine Learning: Bayesian Machine Learning

Master of Science thesis project

Nov 28, 2019

Machine Learning and the Quantum Many-body Problem

Solving quantum mechanical problems for atoms, molecules, materials, and interfaces is of fundamental importance to a large number of disciplines including physics, chemistry, and materials science. Since the early development of quantum mechanics, it has been noted, by Dirac among others, that *...approximate, practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.*

Historically, this has meant invoking approximate forms of the underlying interactions (mean field, tight binding, etc.) or relying on phenomenological fits to a limited number of either experimental observations or theoretical results (e.g., force fields).

The development of feature-based models is not new in the scientific literature. Indeed, prior even to the acceptance of the atomic hypothesis, van der Waals argued for an equation of state based on two physical features. Machine learning (i.e., fitting parameters within a model) has been used in physics and chemistry since the dawn of the computer age. The term machine learning is new; the approach is not.

More recently, high-level ab initio calculations have been used to train artificial neural networks to fit high-dimensional interaction models and to make informed predictions about material properties.

Machine learning can also be used to accelerate or bypass some of the heavy machinery of the ab initio method itself. In the work of Snyder et al, the authors replaced the kinetic energy functional within density-functional theory with a machine-learned one, *learned* the mappings from potential to electron density and from charge density to kinetic energy, respectively.

Thesis Projects

Specific tasks and milestones. The specific task here is to implement and study the recently developed deep learning algorithms for solving quantum

mechanical many-particle problems. The results can be easily compared with exisiting standard many-particle codes developed by former students at the Computational Physics group. These codes will serve as useful comparisons in order to gauge the appropriateness of recent Machine Learning approaches to quantum mechanical problems. The aim here is to use recurrent neural networks to study quantum mechanical many-body methods like the family of similarity renormalization group methods. This method is a rewrite of many-body equations in terms of coupled ordinary differential equations, see chapter 10 of Lecture Notes in Physics vol. 936.

The projects can easily be split into several parts and form the basis for collaborations among several students. The milestones are as follows

1. Spring 2020:
2. Fall 2020:
3. Spring 2021:

The thesis is expected to be handed in May/June 2021.

References. Highly relevant articles for possible thesis projects are: