Machine Learning in Quantum Chemistry: Solving the Electronic Schrödinger Equation

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Abstract

Chosing the correct molecule in a certain application, e.g. materials science or drug discovery, can be a challenging task. To ease these processes, it is of vital importance to be able to predict molecular properties without the need of synthesizing said molecules. This talk focusses on the *electronic Schrödinger equation*, a partial differential equation originating from quantum chemistry that governs energetic properties of atoms and molecules. This equation, however, is notoriously difficult to solve because of its high dimensionality, scaling as $3N$ with the number of electrons N. Approximate numerical methods like *Hartree-Fock* and *density functional theory* exist, but they are slow at high accuracy levels making traversing the chemical compound space a tedious endeavour. Therefore this talk will showcase how modern machine learning models can be utilized to speed up this process significantly. Additionally, we will give a brief introduction to quantum physics to better understand the electronic Schrödinger equation with the focus on highlighting connections to *spectral theory* from functional analysis.