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TÉMA

Machine Learning for Interpolation of Electronic Structure Calculations

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Computational discovery, design and study of novel molecules and materials requires accurate electronic structure calculations, whose high computational cost is often a limiting factor. In high-throughput settings, machine learning can significantly reduce overall computational costs by rapidly and accurately interpolating between reference calculations. Effectively, the problem of solving a complex equation such as the electronic Schrödinger equation for many related poly-atomic systems is mapped onto a nonlinear statistical regression problem. [1]

I will introduce essential machine learning concepts, give a brief overview of machine learning for electronic structure calculations, and present our latest contribution, the many-body tensor representation [2] which enables predictions for both molecules and crystals, with state-of-the-art empirical performance on a variety of benchmark datasets.

[1] Matthias Rupp, Alexandre Tkatchenko, Klaus-Robert Müller, O. Anatole von Lilienfeld: Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning, Physical Review Letters 108: 058301, 2012.

[2] Haoyan Huo, Matthias Rupp: Unified Representation of Molecules and Crystals for Machine Learning, arXiv 1704.06439, 2017.

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