CRUNCH Seminars at Brown, Division of Applied Mathematics

Friday – March 22, 2019

Paper Review: Deep Potential: a general representation of a many-body potential energy surface by Jiequn Han et al. Weinan E

Zhen Li

We present a simple, yet general, end-to-end deep neural network representation of the potential energy surface for atomic and molecular systems. This methodology, which we call Deep Potential, is "first-principle" based, in the sense that no ad hoc approximations or empirical fitting functions are required. The neural network structure naturally respects the underlying symmetries of the systems. When tested on a wide variety of examples, Deep Potential is able to reproduce the original model, whether empirical or quantum mechanics based, within chemical accuracy. The computational cost of this new model is not substantially larger than that of empirical force fields. In addition, the method has promising scalability properties. This brings us one step closer to being able to carry out molecular simulations with accuracy comparable to that of quantum mechanics models and computational cost comparable to that of empirical potentials.
arXiv Link: https://arxiv.org/abs/1707.01478