Machine Learning of Quantum Forces: building accurate force fields via "covariant" kernels

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Abstract

In recent years, the construction of data-driven force fields via Machine Learning methods proved to be a promising route in order to bridge the gap between accurate (but slow) quantum calculations and fast (but unreliable) classical potentials [1,2,3].
I will present a new scheme [4] that accurately predicts forces as vector quantities, rather than sets of scalar components, by Gaussian Process (GP) Regression. This is based on matrix-valued kernel functions, to which we impose that the predicted force rotates with the target configuration and is independent of any rotations applied to the configuration database entries. We show that such "covariant" GP kernels can be obtained by integration over the elements of the rotation group *SO(n)*. Remarkably, in specific cases the integration can be carried out analytically and yields a conservative force field that can be recast into a pair interaction form. The accuracy of our kernels in predicting quantum-mechanical forces in real systems is investigated by tests on pure and defective crystalline systems.

I will further discuss how such learning algorithm can be used to build a measure of complexity of physical systems. Indeed, this can be defined as the number of canonically sampled configurations needed to achieve low generalization error with high probability.

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