Physics-Based Machine Learning for Atomistic Modelling

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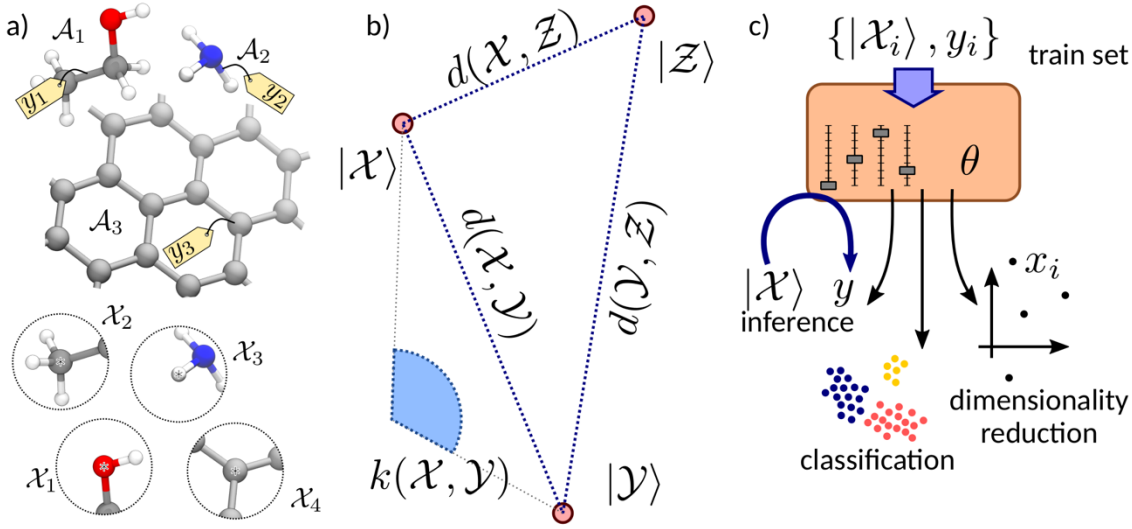
Statistical regression techniques have become very fashionable as a tool to predict the properties of systems at the atomic scale, sidestepping much of the computational cost of first-principles simulations and making it possible to perform simulations that require thorough statistical sampling without compromising on the accuracy of the electronic structure model.

In this talk I will argue how data-driven modelling can be rooted in a mathematically rigorous and physically-motivated framework, and how this is beneficial to the accuracy and the transferability of the model. I will also highlight how machine learning - despite amounting essentially at data interpolation - can provide important physical insights on the behavior of complex systems, on the synthesizability and on the structure-property relations of materials.

I will give examples concerning all sorts of atomistic systems, from semiconductors to molecular crystals, and properties as diverse as drug-protein interactions, dielectric response of aqueous systems and NMR chemical shielding in the solid state.



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