Quantum Machine Learning: Some lessons learned

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Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Efficient exploration algorithms need to exploit all implicit redundancies present in chemical space. I will discuss our recently developed statistical learning approaches for the inference of quantum mechanical observables throughout chemical space. Numerical results indicate remarkable performance in terms of predicted property accuracy, speed, universality, and size scalability. General insights gained will be highlighted throughout.