Machine learning a highly accurate exchange and correlation functional of the electronic density

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In recent years a lot of progress has been made in the study of water and its different phases. Empirical methods are progressing to the point of being better than first principle methods, thanks to the unlimited degrees of freedom allowed in more and more complex force fields and the availability of better accurate data. These methods are however limited in their scope, and completely incapable of being generalized or of treating reactive environments. At the ab-initio level, to reach chemical accuracy, one often has to rely on hybrid functionals, thereby limiting the size of systems for which simulations are feasible. Several attempts have been made in the past to solve this problem. Most approaches try to re-parametrize the exchange part of the generalized gradient approximation (GGA) functional. However, it turns out that one of the main deficiencies of GGA, namely its self-interaction error, places an upper bound on the accuracy of these techniques. Here, we propose a new framework to create density functionals for electronic structure calculations by using supervised machine learning. These machine learned functionals are built on top of well-established and physically motivated density functionals and are designed to correct their shortcomings. We show that our functional can lift generalized gradient methods to the accuracy of coupled cluster calculations for small organic molecules, all while being highly data-efficient and somewhat transferable across chemical systems. We further test our method on water, where it accurately reproduces results for both gaseous and condensed systems.