Reducing the approximations in density functional theory using machine learning

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Density functional theory (DFT) serves without doubt as the workhorse method for electronic structure simulations in materials science and physics. This is in no small part due to its favorable scaling, allowing users to study system with sizes out of reach for more accurate methods that rely on the computation of the many body electron wave function. However, inferences made from numerical simulations are only ever as good as their underlying approximations. This remains true for DFT, where these approximations are bundled somewhat opaquely in the elusive exchange-correlation (XC) functional. The Hohenberg-Kohn theorem guarantees that if this functional were known, ground-state properties of any interacting many-electron system could be described exactly. The question that is still open is whether an exact and universal functional can be obtained. In this talk I will introduce this topic and show how machine learning can help to answer this question. I will also show our approaches to obtaining such better functional approximations.