ML-Density and energy optimized exchange and correlation functionals for density functional theory.

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Density Functional Theory (DFT) is the standard formalism to study the electronic structure of matter at the atomic scale. The balance between accuracy and computational cost that
DFT-based simulations provide allows researchers to understand the structural and dynamical properties of increasingly large and complex systems at the quantum mechanical level.
The fundamental theorems of density functional theory ensure that there exists an exact functional which provides the exact energy of a system from its exact density. This functional is minimized at a fixed electron number and a fixed external potential by the exact electron density, hence providing both the density and and energy. However, doing this exactly comes at a colossal computational cost.
It is, however, possible to approximate the exact functional, providing a balance between accuracy and computational cost.
I will show different approaches to use machine learning methods to
construct approximations of the exact functional.
I will also show how to implement general methods to facilitate their incorporation in available electronic structure codes.
In addition, inherent limitations to differentiable methods -which have shown to be necessary to increase accuracy- will be highlighted.

References

[1] Wills, A and Dick, S and Navarro-Rodriguez, S and Franklin, J and Fernandez-Serra, MV (in Prep).
[2] Dick, S and Fernandez-Serra, MV Phys Rev B, 104 (2021) page (Arial 10)