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Variational principle to regularize machine-learned density functionals

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Practical density functional theory (DFT) owes its success to the groundbreaking work of Kohn and Sham that introduced the exact calculation of the non-interacting kinetic energy of the electrons using an auxiliary mean-field system. However, the full power of DFT will not be unleashed until the exact relationship between the electron density and the non-interacting kinetic energy is found. Various attempts have been made to approximate this functional, similar to the exchange-correlation functional, with much less success due to the larger contribution of kinetic energy and its more non-local nature. In this work we propose a new and efficient regularization method to train density functionals based on deep neural networks, with particular interest in the kinetic-energy functional. The method is tested on (effectively) one-dimensional systems, including the hydrogen chain, non-interacting electrons, and atoms of the first two periods, with excellent results. For the atomic systems, the generalizability of the regularization method is demonstrated by training also an exchange-correlation functional, and the contrasting nature of the two functionals is discussed from a machine-learning perspective.

Primary author: DEL MAZO SEVILLANO, Pablo

Presenter: DEL MAZO SEVILLANO, Pablo

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