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Deep learning density functionals for gradient descent optimization

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Machine-learned regression models represent a promising tool to implement accurate and compu- tationally affordable energy-density functionals to solve quantum many-body problems via density functional theory. However, in continuous systems, while they can easily be trained to accurately map ground-state density profiles to the corresponding energies, their functional derivatives often turn out to be too noisy, leading to instabilities in self-consistent iterations and in gradient-based searches of the ground-state density profile. We investigate how these instabilities occur when standard deep neural networks are adopted as regression models, and we show how to avoid them using an ad-hoc convolutional archi- tecture featuring an inter-channel averaging layer. Furthermore we study how this methods can be extended to spin models relevant for quantum simulators, considering a 1d quantum transverse Ising model with nearest-neighbours interaction. We study the conditions for applying DFT in quantum discrete systems and we implement a different kind of architecture (U-NET) to map the magnetization per site to the functional per site. noninteracting atoms in optical speckle disorder. With the inter-channel average, accurate and sys- tematically improvable ground-state energies and density profiles are obtained via gradient-descent optimization, without instabilities nor violations of the variational principle.

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