Representing complicated functionals through neural networks

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ABSTRACT

This research merges computational chemistry with artificial intelligence to refine the description of electron interactions, essential for chemical compound analysis [1]. By employing advanced mathematical methods and machine learning, particularly neural networks, we simplify complex Density Functional Theory equations, improving their software integration [2]. Our approach utilizes deep learning to represent complex relationships, offering enhancements over traditional methods [3]. Incorporating this approach offers significant advantages, facilitating the computation of derivatives of functionals to implement and calculate their self-consistent field. This work aims to provide new insights into electron interactions and improve computational modeling techniques, with broad implications in materials science, pharmacology, and energy.

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