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Decisional Gradient Descent: A New Optimizer for Variational Monte Carlo

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The nuclear many-body problem is known to be computationally expensive to solve. Recently, with the advent of machine learning techniques in science, the method of Neural-Network Quantum States is being adopted by different groups to tackle nuclear systems, with the hope that it will be more efficient than the alternatives. Being a variational method, one of the inherent difficulties is to optimize the energy. Even for simple systems, the preferred optimization algorithm, Stochastic Reconfiguration, does not guarantee a smooth convergence towards the energy minimum. In this talk, I present our latest optimizer, Decisional Gradient Descent, from the point of view of second-order optimization theory. Not only does it consistently outperform the state-of-the-art Stochastic Reconfiguration (for our system of choice), but also the theoretical framework used to derive it is very wide. We believe this will allow for the development of several powerful optimizers within this decisional framework.

Abstract

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