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Towards the Optimizer that NQS Deserves

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In this talk, I will be covering one of the newest methods for nuclear structure calculations, Neural Quantum States (NQS). While it is not specific to nuclear physics [1,2], since its first application for computing the deuteron bound state [3], its application to nuclear ground states has been consistently gaining momentum [4,5]. The claim of NQS is that, by introducing a highly-expressive neural-network ansatz in a Variational Monte Carlo (VMC) setting, we can obtain a system's wave function with only a polynomial cost in the number of particles. In the talk, I will briefly cover the optimization algorithms that power NQS nowadays, to then present our most novel optimizer, Decisional Gradient Descent (DGD) [6]. Whereas Stochastic Reconfiguration (SR) has been the preferred optimizer in VMC calculations, we have shown that it is not well-suited as a second-order optimization algorithm. Whereas SR performs poorly when used within Newton's method, DGD manages to reach the ground state of a variety of physical systems in a reduced number of iterations. Having been put to test in both continuous-coordinate and discrete-coordinate systems, this work paves the way for subsequent applications to the more complex nuclear systems.

[1] G. Carleo and M. Troyer, Science 355 602-606 (2017)
[2] D. Pfau, J. Spencer et al., Phys. Rev. Research 2, 033429 (2020)
[3] J. Keeble and A. Rios, Phys. Lett. B 135743 (2020)
[4] A. Gnech, B. Fore et al., Phys. Rev. Lett. 133, 142501 (2024)
[5] M. Rigo, B. Hall et al., Phys. Rev. E 107, 025310 (2023)
[6] M. Drissi, J. Keeble et al., Phil. Trans. R. Soc. A 38220240057 (2024)

Abstract

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