Machine Learning in Natural Sciences: from Quantum Physics to Nanoscience and Structural Biology

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## Quantum flows neural network for variational solutions of the Schrödinger equation

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The computational technology of highly expressive parametric neural-network-functions has allowed machine learning to make a major foray into disciplines of natural sciences. The neural network functions may be effectively "fitted" to a loss function, given in the form of a variational principle or virial theorem, to provide solutions to quantum mechanical problems. Recently, a few deep neural network models for solving the electronic Schrödinger equation were developed [1-3], demonstrating both outstanding computing efficiency and accurate results.

Here, we present a new quantum-flow-neural-network approach for obtaining variational solutions of the Schrödinger equation. At the core of the method is an invertible neural network composed with the general basis of orthogonal functions [4], which provides a more stable framework for simultaneous optimization of the ground state and a lot of excited states. We apply our approach to calculations of the vibrational energy levels of polyatomic molecules as well as of electronic energies in a single-active-electron approximation. The results show a considerable improvement of variational convergence for the ground and the excited states.

[1] M. T. Entwistle, Z. Schäzle, P. A. Erdman, J. Hermann, F. Noé, arXiv:2203.09472 (2022)

[2] D. Pfau, J. S. Spencer, A. G. D. G. Matthews, W. M. C. Foulkes, Phys. Rev. Research 2, 033429 (2020), arXiv:1909.02487v3

[3] J. Hermann, Z. Schäzle, F. Noé, Nat. Chem. 12, 891 (2020), arXiv:1909.08423v5

[4] K. Cranmer, S. Golkar, and D. Pappadopulor, arXiv:1904.05903

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