LIMITATIONS AND OPPORTUNITIES FOR DEEP LEARNING BASED PDE SOLVERS

PHILIPP GROHS*

ABSTRACT

In recent years, deep learning based solvers for problems in numerical analysis and the computational sciences have emerged as a promising alternative to classical schemes. This promise is fueled by the ability of neural networks to approximate vast classes of complicated functions with only a moderate number of parameters. In the first part we discuss the extent to which these excellent approximation capabilities can be exploited by an actual algorithm. We find that the norm in which the accuracy is measured plays a crucial role: neural network training quickly becomes intractable if a small uniform error is needed while it may be tractable if only a small L^2-norm or accurate evaluation of a linear functional is desired. One important problem where the latter is the case is given by the computation of ground state energies of molecules via the multi electron Schrödinger equation. We demonstrate that deep learning methods are indeed emerging as a new state of the art in this problem.

References

[1] J. Berner, P. Grohs, F. Voigtlaender. *Training ReLU networks to high uniform accuracy is intractable.* Preprint available on https://arxiv.org/abs/2205.13531.

M. Scherbela, R. Reisenhofer, L. Gerard, P. Marquetand, P. Grohs. *Solving the electronic Schrödinger equation for multiple nuclear geometries with weight-sharing deep neural networks.* Nature Computational Science 2 (2022), pages 331–341.

L. Gerard, M. Scherbela, P. Marquetand, P. Grohs. *Gold-standard solutions to the Schrödinger equation using deep learning: How much physics do we need?.* Preprint available on https://arxiv.org/abs/2205.09438.

* University of Vienna, philipp.grohs@univie.ac.at