Numerical solution of regular Schrödinger problems in high dimension using two-layer neural networks

The objective of this presentation is to analyse fundamental neural numerical schemes utilising two-layer neural networks for the resolution of some Schrödinger problems, specifically the inversion of the Poisson operator an the eigenproblem for the Schrödinger operator, in the high-dimensional regime.

By employing Barron's representation of the solution with a probability measure defined on the set of parameter values, the energy is minimised through a gradient curve dynamic on the 2-Wasserstein space of the set of parameter values defining the neural network. This approach is inspired by the work of Bach and Chizat.
It is demonstrated that if the gradient curve converges, then the represented function is the solution of the elliptic equation under consideration.

The method is then adapted to solve Schrödinger eigenvalue problems with smooth potentials, introducing a constrained gradient flow.
The efficiency of the method is demonstrated through the presentation of numerical experiments in both cases.

If time allows it, I will present the conceptual framework underlying the development of FermiNet and PauliNet. These are neural network-based methods whose objective is to solve the Schrödinger eigenvalue problem with Coulombic interaction and an antisymmetry constraint imposed on the wavefunction.

Links :

- https://hal.science/hal-04089961
- https://arxiv.org/abs/2409.01640
- https://sciencespo.hal.science/CHL/hal-04817039v1

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