CEMRACS 2023 mini-project proposal

2 pages maximum (references included)

Title: Scientific machine learning and tensor methods for electronic structure computations in quantum chemistry

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1. **Context**

   Computing the electronic structure of molecules with a very large number of electrons is a very challenging problem. Indeed, this amounts to solving the electronic Schrödinger problem, which is an eigenvalue problem defined on a space of dimension three times the number of electrons. Standard numerical methods are doomed to fail because of the so-called curse of dimensionality.

2. **Description and objectives**

   The aim of this project is to use scientific machine learning so as to compute the ground state wavefunctions of electrons within a molecule for large systems. More precisely, we wish to solve the electronic Schrödinger equation by means of neural networks. This has already been undertaken by several groups including the FermiNet group for instance. However, the fact that the wavefunction of a system of electrons is antisymmetric, due to the fermionic nature of the electrons, makes these approaches difficult to carry out. Here we wish to use an alternative formulation of the electronic Schrödinger equation, using the so-called second quantization formalism, which enables to avoid these problems linked to antisymmetry. The idea is then to use a Physically Informed Neural Network so as to minimize the Rayleigh quotient associated to the eigenvalue problem and compare this approach together with the state-of-the-art method for solving the Schrödinger problem in this second quantization formulation, which relies on the use of Tensor Trains (this is the so-called DMRG method in quantum chemistry).

3. **Proposed methodology**

   We already have a home-made code in Julia implementing the DMRG method (based on Tensor Trains) for the resolution of the electronic Schrödinger equation in the second quantization formalism for various molecules. This code will be used by the students so as to make DMRG computations which will serve as a reference.
   For the PINN formulation, we wish to investigate in a first step simple feed-forward neural networks so as to minimize the Rayleigh quotient associated to the eigenvalue problem. We will investigate the influence of various parameters defining the architecture of the neural network (including depth, number of neurons per layer, activation function...) on the quality of the approximation we obtain.

4. **Software requirements**

   For the PINN method, the students will have to use either PyTorch or TensorFlow, depending on their preference. The home-made code in Julia will be freely shared with the students.

5. **References**

[1] CANCES, Eric, DEFRANCESCHI, Mireille, KUTZELNIGG, Werner, *et al.* Computational quantum chemistry: a primer. *Handbook of numerical analysis*, 2003, vol. 10, p. 3-270.

[2] LOU, Qin, MENG, Xuhui, et KARNIADAKIS, George Em. Physics-informed neural networks for solving forward and inverse flow problems via the Boltzmann-BGK formulation. *Journal of Computational Physics*, 2021, vol. 447, p. 110676.

[3] MARTI, Konrad Heinrich et REIHER, Markus. The density matrix renormalization group algorithm in quantum chemistry. *Zeitschrift für Physikalische Chemie*, 2010, vol. 224, no 3-4, p. 583-599.