Machine Learning Schrödinger Equation

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The main objective of this work is, using the framework given by the Machine Learning methods, to solve the Schrödinger equation that governs the wavefunction of a system for different potentials in order to obtain the ground state of the system.
The problem is solved using variational methods with an Artificial Neural Network (ANN). An ANN with simple architecture is created and used as an ansatz of the ground state wavefunction. By training the ANN and minimizing its energy we will obtain an upper bond of the ground state energy of the system.
Different methods have been used in order to compute the energy integrals and compare their results. We have focused in Monte Carlo (MC) methods for integrating due to its benefits in terms of computational cost when moving from 1D to 3D and Markov Chain Monte Carlo (MCMC) methods to distribute points according to a probability distribution from which direct sampling is difficult.

References

[1] J. W. T. Keeble and A. Rios, Phys. Lett. B, 809 (2020)
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[3] K. P. Murphy, MIT Press, (2022) pp. 441-490

Figures

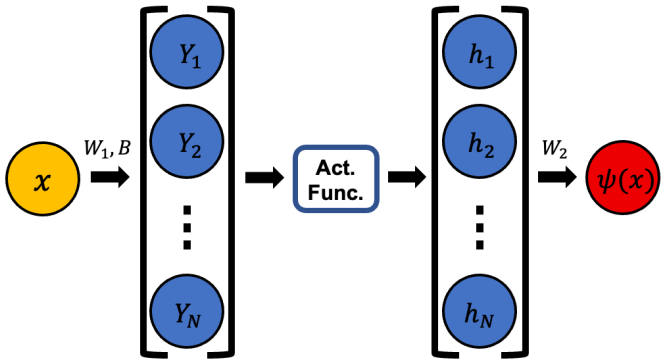

Figure 1: Architecture of the Artificial Neural Network. W_1, W_2 and B are the matrices that connect the input (in yellow), the hidden layer (in blue) and the output (in red).