

ISTANBUL TECHNICAL UNIVERSITY

FACULTY OF SCIENCE AND LETTERS

Graduation Project



Machine Learning and Non-linear Schrödinger Equation

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Summary

We train an artificial neural network to estimate the ground state energy of a one-dimensional Bose-Einstein condensate in harmonic trapping potential. Such a system can be described by the solution of a non-linear Schrödinger equation also called a Gross-Pitaevskii equation. We also use the method for the inverse problem of predicting the non-linearity parameter using the ground state density profile for a given harmonic trapping potential.

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1 Introduction and Motivation

Machine learning is a growing research area, not only its theoretical base but also its share in applications in different areas. One of the reason why machine learning is used increasingly today is that artificial neural networks used in machine learning can approximate any continuous function within desired accuracy. This means that if we take $\epsilon > 0$ as desired accuracy, $\mathbf{y} = \mathbf{f}(\mathbf{x})$ output of the network and $\mathbf{g}(\mathbf{x})$ real value of the function, then it is guaranteed that there exists a network that satisfies the relation $|\mathbf{g}(\mathbf{x}) - \mathbf{f}(\mathbf{x})| < \epsilon$. From this point of view, a process or calculation that can be thought of as a function can be represented by a corresponding neural network that mimics this function in desired accuracy [1]. With this in mind, neural networks have the potential to learn general functions and be exploited for their advantages. Approximate value of the quantity can be determined for different scenarios.

Many different kind of applications of machine learning have already been implemented in physics¹. For example, In [3, 4] machine learning is applied to quantum many body problems. A machine learning method called Unsupervised Learning to detect patterns in big datasets is used for discovering phase transitions [5]. There are also developed techniques in machine learning inspired from physics such as quantum tensor networks [6]. Relation between physics and machine learning also caused foundation of a new branch called Quantum Machine Learning which aims to implement a quantum software to make machine learning faster than its classical version [7].

In [8], machine learning approach is applied to a 2D Schrödinger Equation with random potentials. The authors built a convolutional deep neural network, and trained it to predict ground state energy of the system under four different two dimensional confining potentials including some random potentials. Their study showed that machine learning is a promising alternative in electronic structure calculations of quantum systems. In our study inspired from the article mentioned above, we apply machine learning method to the nonlinear Schrödinger equation to predict ground state energy of a Bose-Einstein condensate at absolute zero temperature in one dimensional harmonic trapping potentials.

¹For a detailed list, see [2]

2 Conclusion

Lorem Ipsum

References

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A APPENDIX A

A.1 Comment on Python Codes

There are two neural network codes and three utility codes. Code of FCN is `feedforwardnetwork.py`, CNN is `cnnnetwork1d.py`. `analyzer.py` is kind of a network tracer. All information about network internals and iteration information is saved and traced by class inside this module. `readdata.py` reads the data generated by XMDS and produces proper representations of the data. `sample-trainloader.py` takes the data from `readdata.py` and produces Pytorch’s tensors. `run_training.py` automatizes the training process.

Codes are not optimized and consistency of the naming convention is poor. But volume of the code is small and it is self explanatory. Code can be obtained from: goo.gl/8Fm8yt