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.

Contents

1 Introduction and Motivation

Machine learning.
General usage area.
ML in physics and Phyiscs in ML.
ML&SE article.
Ours difference.

2 Gross Pitaevskii Equation

General information about GPE
Why and how nonlinearty is introduced.
Physical and mathematical interpretation of interaction parameter. (phy: attractive, repulsive math:dominance of the terms)
Stationary form.
Potential, kinetic and interaction energy expressions.
Reduction of dimension.
Analytic solution and approximation.

2.1 Numeric Solution and Dataset Generation

Potential types (with analytic forms etc.)
Scaling, $\alpha\beta$ case etc
Brief info about imaginary time evolution. (detailed in APPENDIX)
XMDS framerwork and other programs.
Potential generation.
Random potential generations with different method. (Reason)
Boundaries. (Table)
Convergence (detailed in APPENDIX).
Dataset generation. (Total number of examples etc)

2.1.1 Scaling

$$V(z) = \widetilde{V}(z)\gamma E_0$$

$$z = \beta L \widetilde{z}$$

$$\mu = \widetilde{\mu}\gamma E_0$$

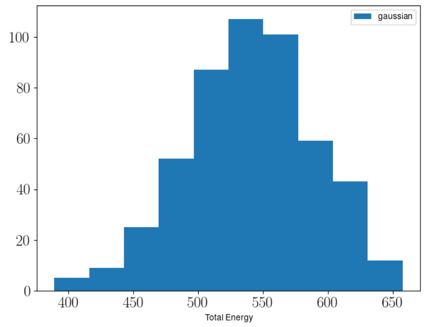
$$\frac{\hbar^2}{2m\gamma E_0}\frac{1}{\beta^2 L^2} = \alpha$$

$$\psi = \widetilde{\psi}\sqrt{\frac{N}{\beta L}}$$

$$-\alpha\frac{d^2\widetilde{\psi}}{d\widetilde{z}^2} + \widetilde{V}(z)\widetilde{\psi} + \widetilde{g}|\widetilde{\psi}|^2\widetilde{\psi} = \widetilde{\mu}\widetilde{\psi} \tag{1}$$

2.2 Dataset Features

2.2.1 Energy distribution



(a) g = 0

Figure 1: Total energy distributions of the generated solution for different interaction parameter values.

3 Machine Learning

3.1 Network architecture

Architecture of the network.
A general figure like in the ML&SE article that describes the work done.
Another figure about internals of the network such as number of layers, how interaction parameter is introduced to the network etc.
Hyperparameters.

3.2 Training

Detailed info about dataset (energy distribution etc).
Indicate that if there is any method to increase the number of examples in low and high energy values.

3.3 Results

4 Inverse Problem

5 Conclusion and Discussion

Conclusion.

Discussion.

Effects of random potential generation method.

Are there problems in low and high energies compared to the mean?

Inverse problem.

A APPENDIX A