

Predicting energy expectation values for one-dimensional non-linear Schrödinger Equation in random harmonic potentials using artificial neural network

Hüseyin Talha Şenyaşa
090120132

Advanced Physic Project Presentation

January 5, 2018

- 1 Machine Learning
 - Machine Learning
 - Deep Learning and Schrödinger Equation
 - Applying Machine Learning to the NLSE
- 2 Dataset Generation
 - Numerical Solution
- 3 Neural Network
 - Neural Network
- 4 Training Results
 - Ground State Energy Predictions
 - Predicting Interaction Parameter
- 5 Conclusion

- Artificial neural networks used in machine learning can approximate any continuous function within desired accuracy.
- It is guaranteed that there exists a network that satisfies the relation $|g(x) - f(x)| < \epsilon$.
- Many different kind of applications of machine learning have already been implemented in physics.

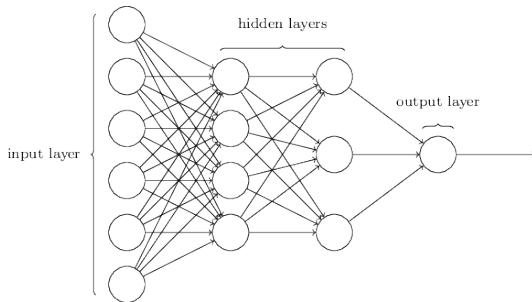


Figure 1: An example of artificial neural network (Multi-layer perceptron)

Deep Learning and Schrödinger Equation

- Application of machine learning to a 2D Schrödinger Equation with random potential.

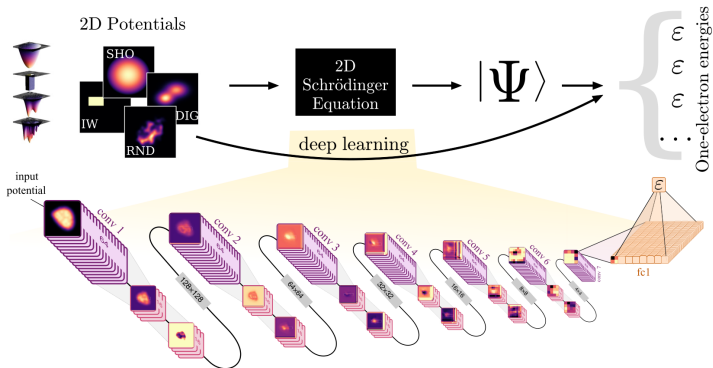


Figure 2: Deep Learning and Schrödinger Equation.

Applying ML to the non-linear Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r}, t) \Psi + g |\Psi|^2 \Psi$$

- Non-linear term results from the interactions between bosons.
- Analytic solutions are known for only few cases.
- Generally solved by numerically or by approximation.

Applying ML to the non-linear Schrödinger Equation

- GPE can also be studied in 1D

$$\mu' \psi_z = \frac{-\hbar^2}{2m} \frac{d^2 \psi_z}{dz^2} + \frac{1}{2} m \omega_z^2 (z - z_0)^2 \psi_z + g' |\psi_z|^2 \psi_z$$

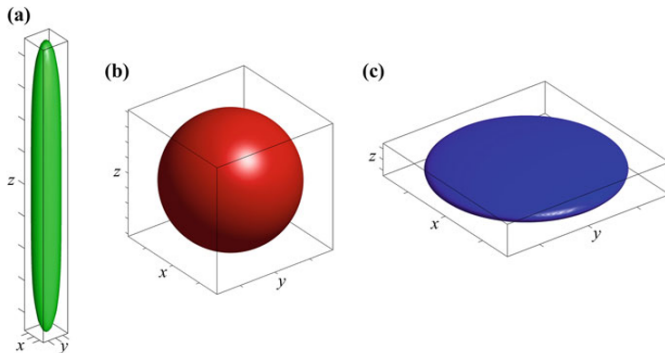


Figure 3: Bose-Einstein Condensates in different trapping potentials.

- GPE is solved with random harmonic trapping potential including shift while interaction parameter is kept fixed.

Table 1: Values and Ranges of Parameters

Interaction Parameter	g :	$\{0, 0.1, 1, 10, 20\}$
Shift	z_0 :	$[-5, 5]$
Angular Frequency	ω_z :	$[0.5, 2]$

- Solved by using imaginary time propagation and re-normalization in XMDS Framework.

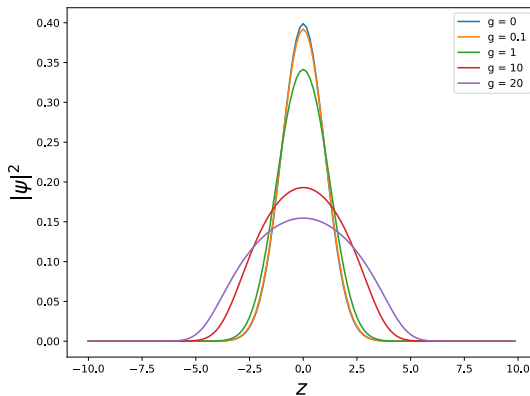


Figure 4: Density

- Implemented in Pytorch Framework.
- Two different neural network: Fully Connected, Convolutional.
- Trained to predict ground state energy of a Bose-Einstein Condensate.
- FCN is also trained to predict interaction, kinetic, potential, and total energy of the system.

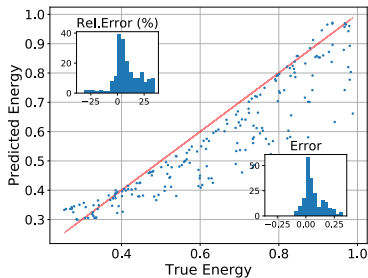
Fully Connected Network

- 1 input layer, 3 hidden layers, 1 output layer.
- Adaptive Learning Rate (Adam)
- ReLU activation function

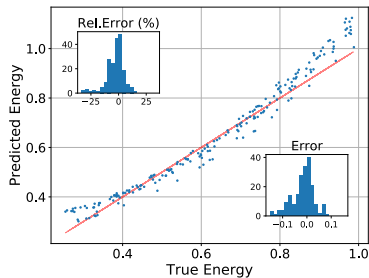
Convolutional Neural Network

- 2 convolution layers, 2 maxpool layers, 3 fully connected layer.
- Adaptive Learning Rate (Adam)
- ReLU activation function

Choosing Hyperparameters



(a) FCN[128, 40, 40, 1], $\eta = 0.003$



(b) FCN[128, 40, 40, 1], $\eta = 0.001$

Figure 5: Hyperparameters

Ground State Energy Predictions

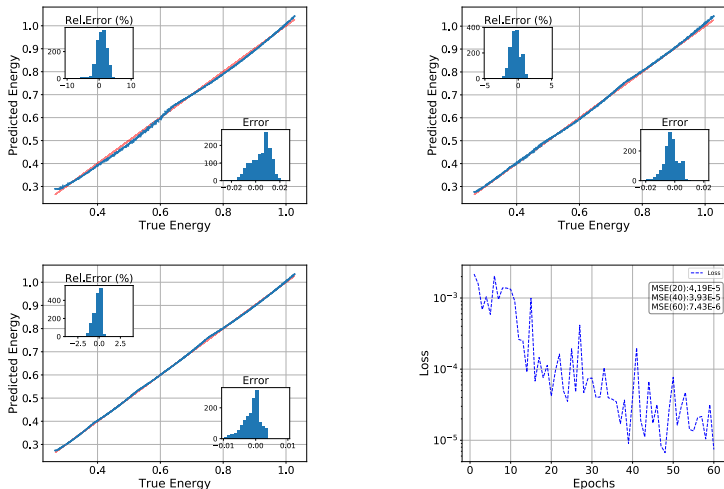


Figure 6: FCN[128, 30, 30, 10, 1] results for $g = 0.1$.

Ground State Energy Predictions

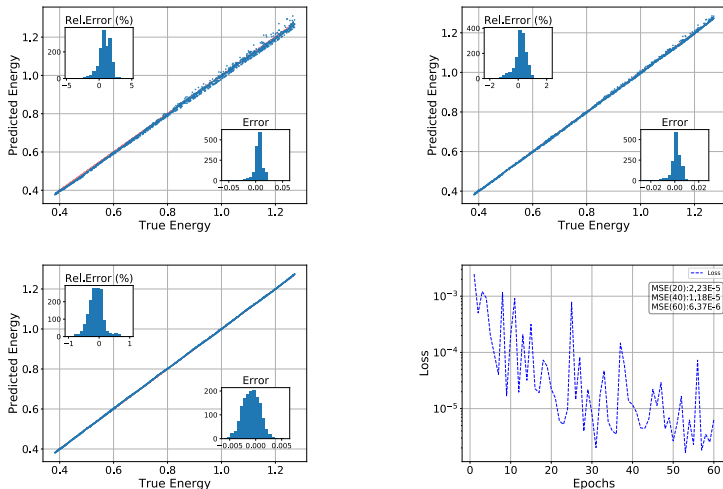


Figure 7: CNN results for $g = 1$

Ground State Energy Predictions

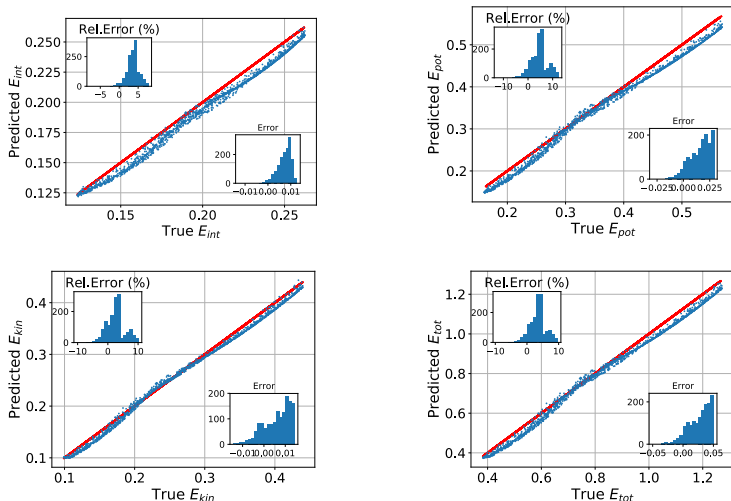


Figure 8: FCN[128, 30, 30, 10, 4], Separate energy predictions for $g = 1$.

Inverse Problem: Predicting interaction parameter

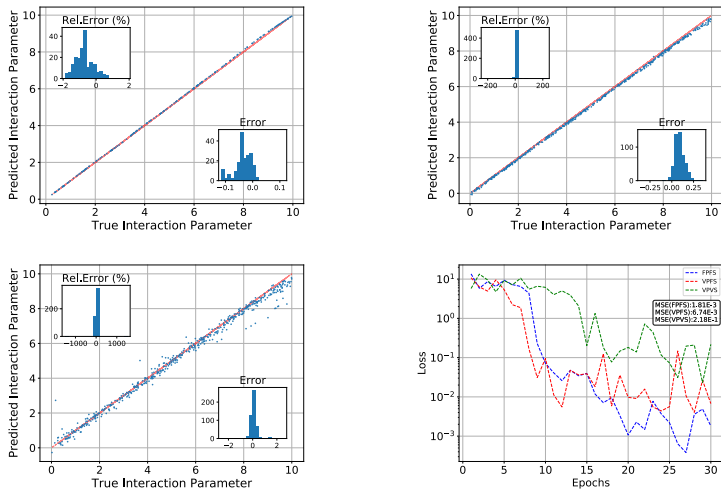


Figure 9: Prediction of interaction parameter

Conclusion

- Machine learning methods can also be applied to non-linear Schrödinger equation.