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

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Outline

Machine Learning

• 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.

Machine Learning

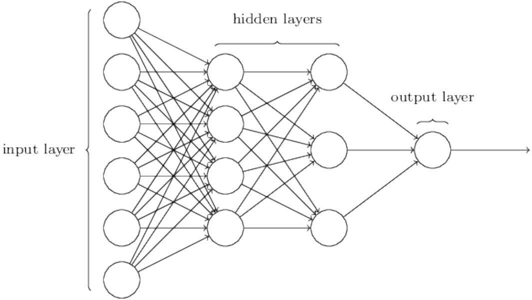


Figure 1: An example of artificial neural network (Multi-layer perceptron)

Deep Learning and Schrödinger Equation

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

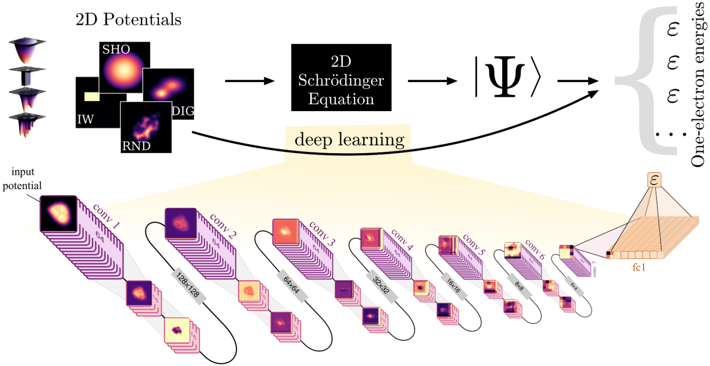


Figure 2: Deep Learning and Schrödinger Equation.

Applying ML to the non-linear Schrödinger Equation

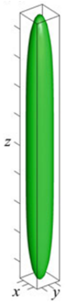
$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\Psi + V(\boldsymbol{r},t)\Psi + g|\Psi|^2\ \Psi$$

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

Numerical Solution

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

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



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.

Numerical Solution

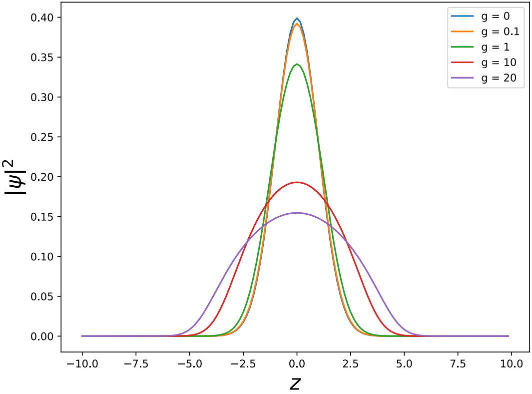


Figure 3: Density

Neural Network

- 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.

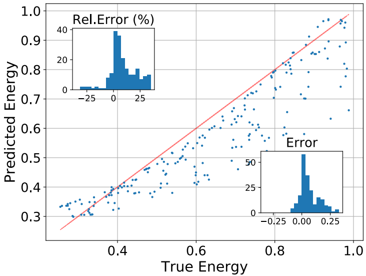
Fully Connected Network:

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

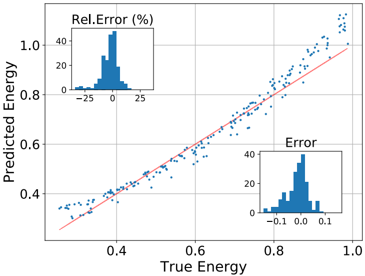
Convolution Network:

- 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 4: Hyperparameters

Ground State Energy Predictions

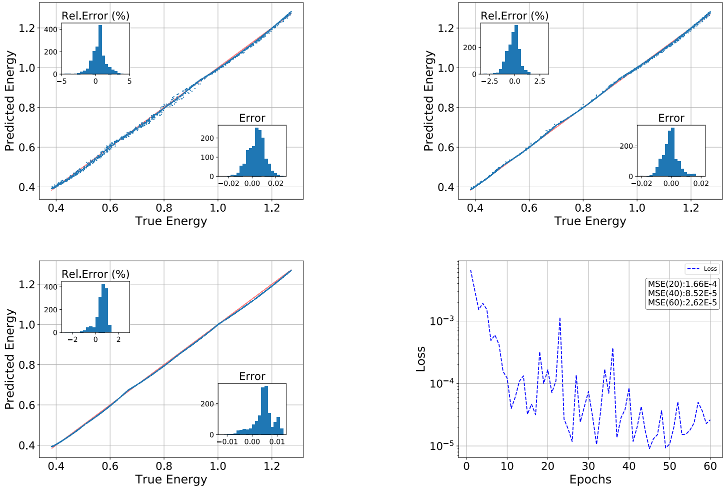


Figure 5: FCN[128, 30, 30, 10, 1] results for $g = 1$

Ground State Energy Predictions

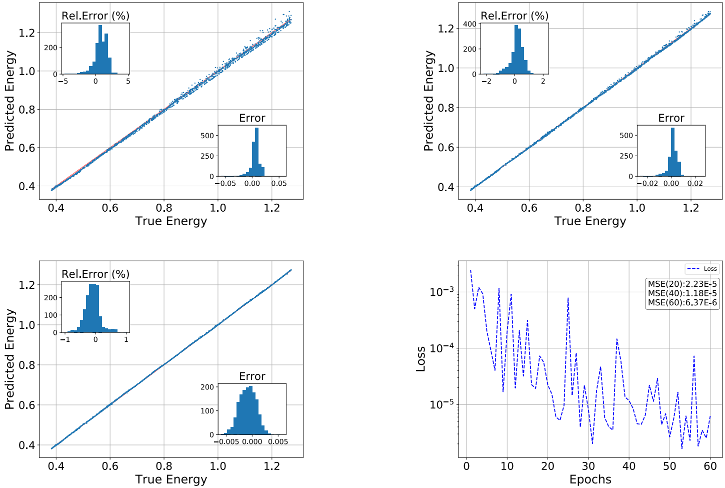


Figure 6: CNN results for $g = 1$

Ground State Energy Predictions

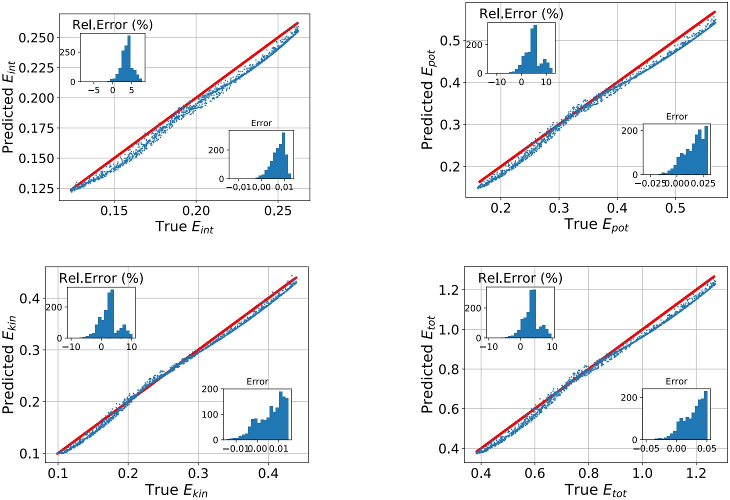


Figure 7: FCN[128, 30, 30, 10, 4], Separate energy predictions for $g = 1$.

Inverse Problem: Predicting interaction parameter

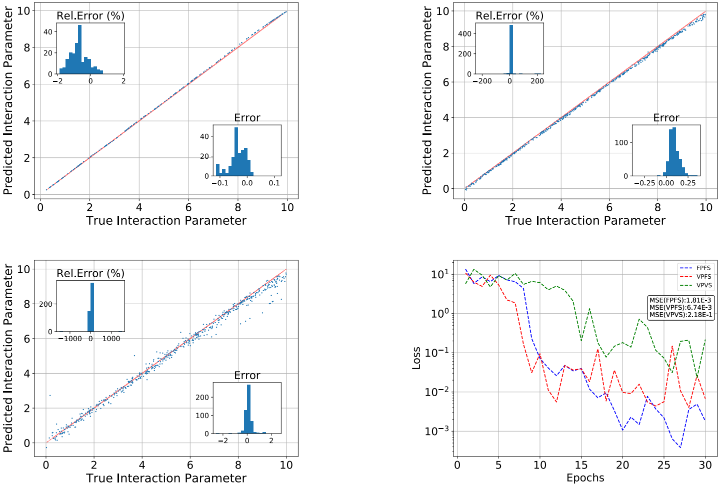


Figure 8: Prediction of interaction parameter

Conclusion and Future Plan

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

• Working with different potential types including random while the interaction parameter is also random.

• Applying this study to the 2D GPE.