Machine Learning and Non-linear Schrödinger Equation

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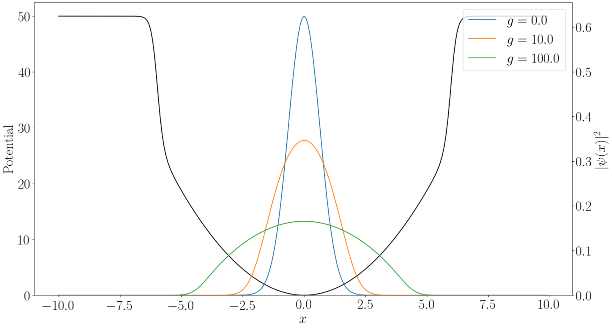
Graduation Project

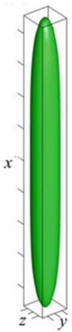
June 11, 2018

Outline

Gross-Pitaevskii Equation in Random 1D Potentials

- Bose-Einstein Condensate at zero temperature
- $\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi_x}{\mathrm{d}x^2} + V(x)\psi + g_{1\mathrm{D}}|\psi|^2\psi = \mu_{1\mathrm{D}}\psi$
- $g|\psi|^2$ term introduces non-linearty. (Interactions between bosons)
- Numerically solved in XMDS Framework.





Random Potential Generation

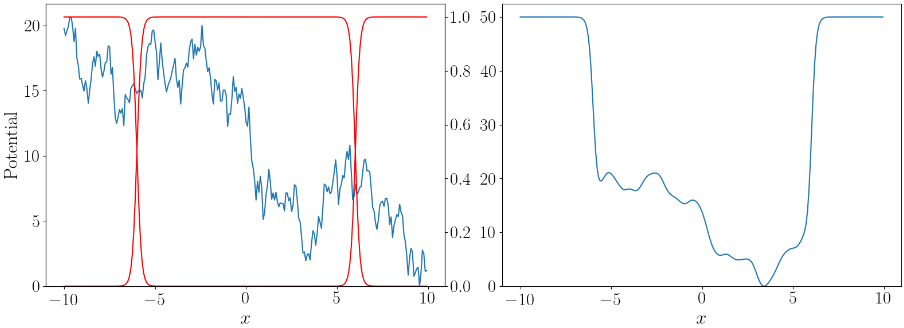
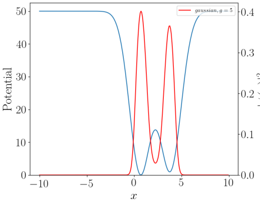
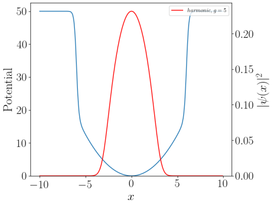


Figure 1: Envelope functions are applied to a random potential. After that, a gaussian filter is applied for smoothness. We also make sure that the minimum value of the potential is zero at re-scaling process.

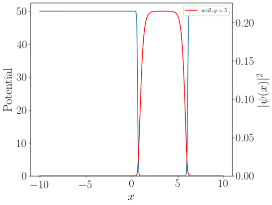
Random Potential Generation



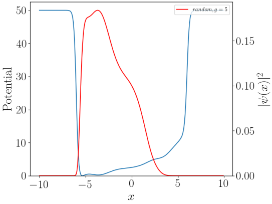
(a) DIG



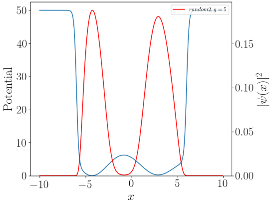
(b) Harmonic



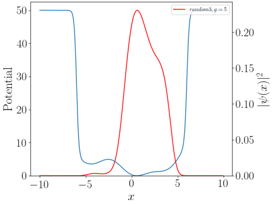
(c) Well



(d) Random Type 1



(e) Random Type 2



(f) Random Type 3

Energy Distribution

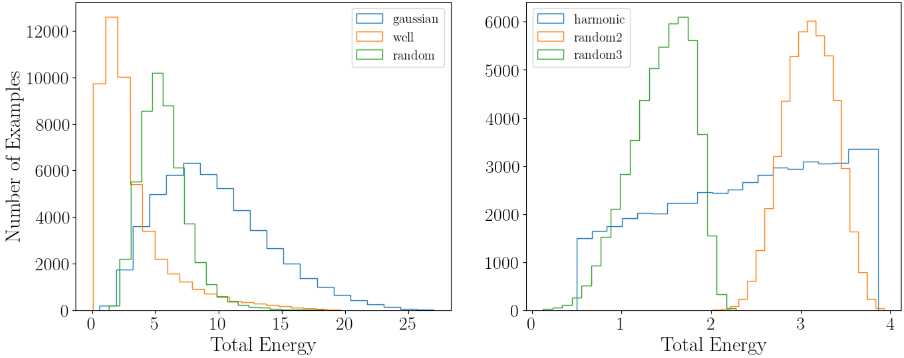
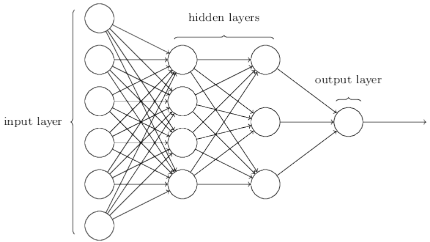


Figure 3: The energy distribution of the random potentials are similar but it is clear that the random potential generation method directly affects the energy spectrum. There is a shift between energy spectrum of the random2 and random3. The random's spectrum is completely different and contains both random2's and random3's.

Machine Learning with Neural Networks

• 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 $||\boldsymbol{g}(\boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x})|| < \epsilon$.



• Many different kind of applications of machine learning have already been implemented in physics.

Deep Learning and Schrödinger Equation

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

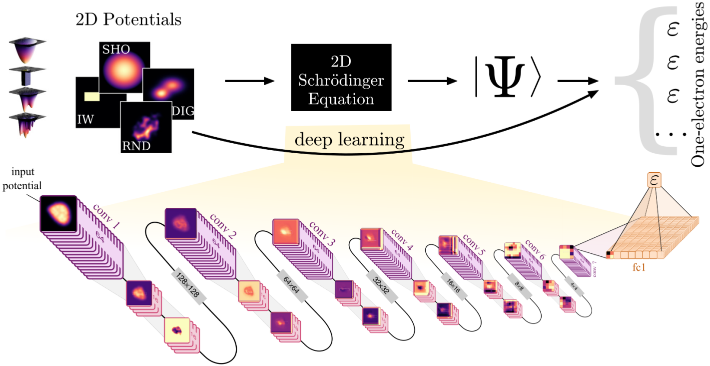


Figure 4: Deep Learning and Schrödinger Equation.

Convolutional Neural Networks

Convolution Network for Energy Prediction:

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

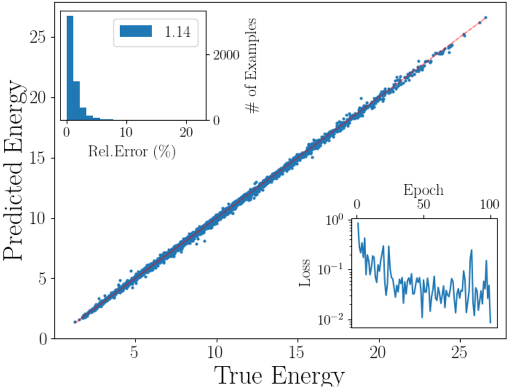
Convolution Network for Interaction Parameter:

- 5 convolution layers, 5 maxpool layers, 4 fully connected layer.
- Adaptive Learning Rate (Adam)
- ReLU activation function

Ground State Energy Predictions

Table 1: Prediction Errors

Potential Type	REM (%)
DIG	1.14
Harmonic	0.05
Infinite Well	2.13
Random #1	2.24
Random #2	0.55
Random #3	0.67

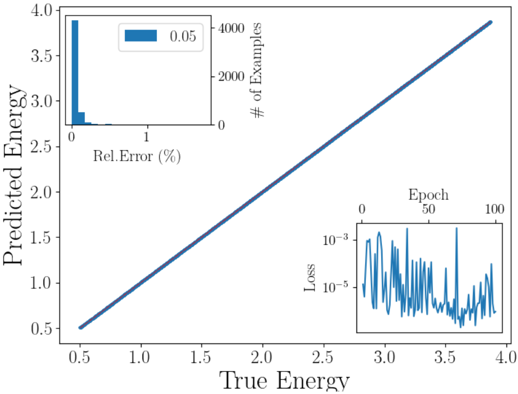


(a) Double Inverted Gaussian

Ground State Energy Predictions

Table 2: Prediction Errors

Potential Type	REM (%)
DIG	1.14
Harmonic	0.05
Infinite Well	2.13
Random #1	2.24
Random #2	0.55
Random #3	0.67

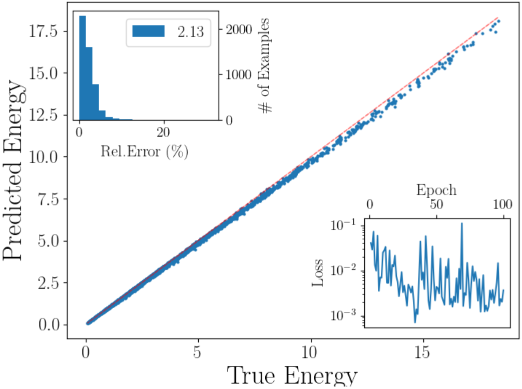


(a) Harmonic

Ground State Energy Predictions

Table 3: Prediction Errors

Potential Type	REM (%)
DIG	1.14
Harmonic	0.05
Infinite Well	2.13
Random #1	2.24
Random #2	0.55
Random #3	0.67

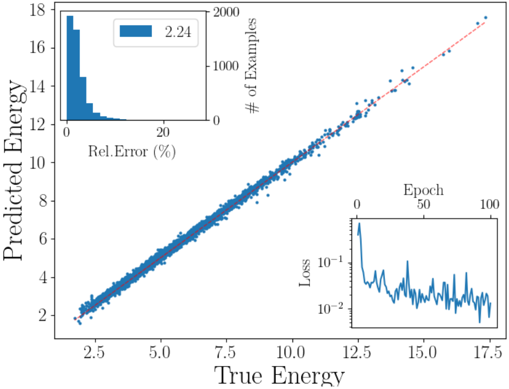


(a) Infinite Well

Ground State Energy Predictions

Table 4: Prediction Errors

Potential Type	REM (%)
DIG	1.14
Harmonic	0.05
Infinite Well	2.13
Random #1	2.24
Random #2	0.55
Random #3	0.67

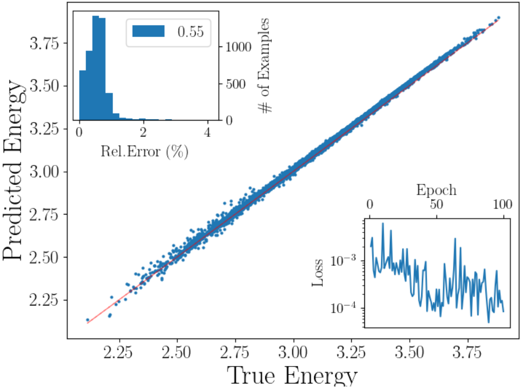


(a) Random Type 1

Ground State Energy Predictions

Table 5: Prediction Errors

Potential Type	REM (%)
DIG	1.14
Harmonic	0.05
Infinite Well	2.13
Random #1	2.24
Random #2	0.55
Random #3	0.67

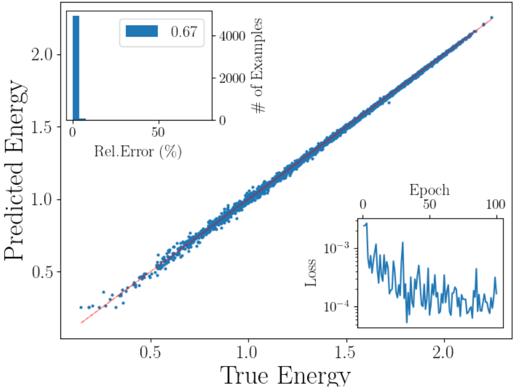


(a) Random Type 2

Ground State Energy Predictions

Table 6: Prediction Errors

Potential Type	REM (%)
DIG	1.14
Harmonic	0.05
Infinite Well	2.13
Random #1	2.24
Random #2	0.55
Random #3	0.67

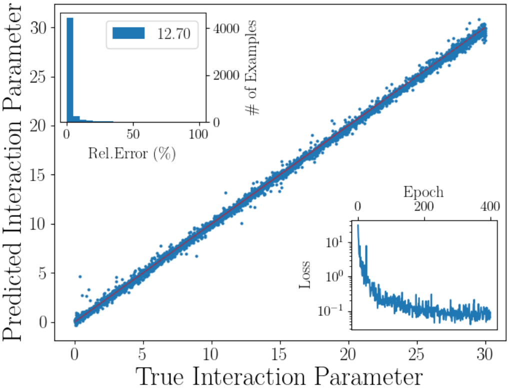


(a) Random Type 3

Inverse Problem: Interaction Parameter Prediction

Table 7: Prediction Errors

Potential Type	REM (%)
DIG	1.33
Harmonic	1.33
Infinite Well	17.29
Random #1	12.77
Random #2	10.41
Random #3	6.96

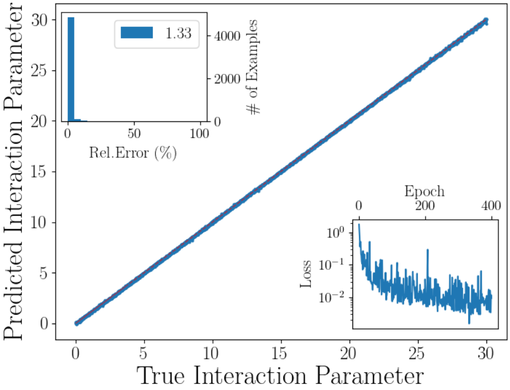


(a) Double Inverted Gaussian

Inverse Problem: Interaction Parameter Prediction

Table 8: Prediction Errors

Potential Type	REM (%)
DIG	1.33
Harmonic	1.33
Infinite Well	17.29
Random #1	12.77
Random #2	10.41
Random #3	6.96

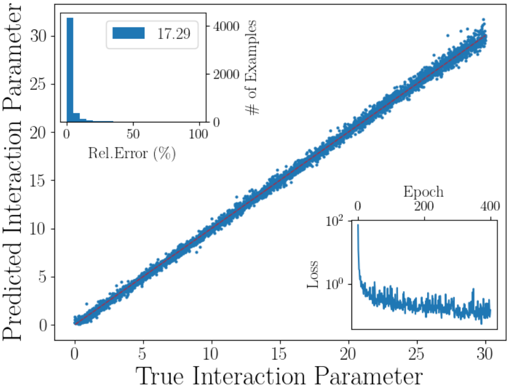


(a) Harmonic

Inverse Problem: Interaction Parameter Prediction

Table 9: Prediction Errors

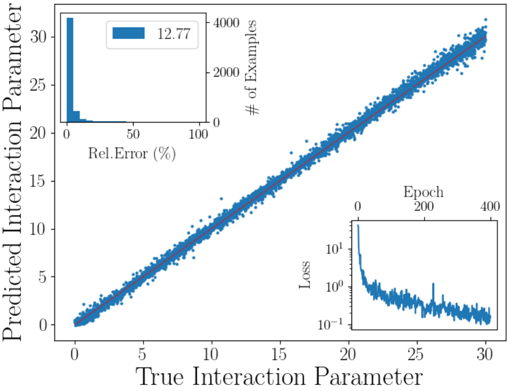
Potential Type	REM (%)
DIG	1.33
Harmonic	1.33
Infinite Well	17.29
Random #1	12.77
Random #2	10.41
Random #3	6.96



(a) Infinite Well

Table 10: Prediction Errors

Potential Type	REM (%)
DIG	1.33
Harmonic	1.33
Infinite Well	17.29
Random #1	12.77
Random #2	10.41
Random #3	6.96

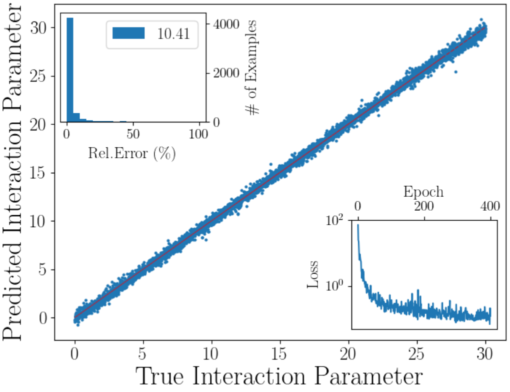


(a) Random Type 1

Inverse Problem: Interaction Parameter Prediction

Table 11: Prediction Errors

Potential Type	REM (%)
DIG	1.33
Harmonic	1.33
Infinite Well	17.29
Random #1	12.77
Random #2	10.41
Random #3	6.96

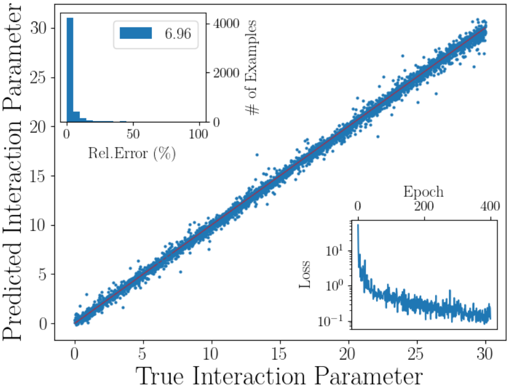


(a) Random Type 2

Inverse Problem: Interaction Parameter Prediction

Table 12: Prediction Errors

Potential Type	REM (%)
DIG	1.33
Harmonic	1.33
Infinite Well	17.29
Random #1	12.77
Random #2	10.41
Random #3	6.96



(a) Random Type 3

Conclusion and Future Plan

1. Conclusion
    1. Machine learning techniques can also be applied to non-linear Schrödinger Equation
    2. Random potential generation techniques affects the results due to corresponding energy spectrum and distribution.
2. Future Work
    1. Generating uniformly distributed dataset by using variational and approximation methods.
    2. Working in 2D.