

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

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  - Neural Network

- 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.

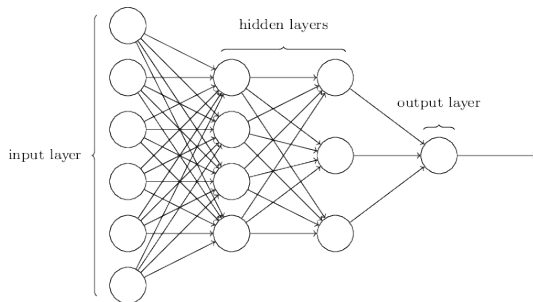


Figure 1: An example of artificial neural network (Multi-layer perceptron)

# Deep Learning and Schrödinger Equation

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

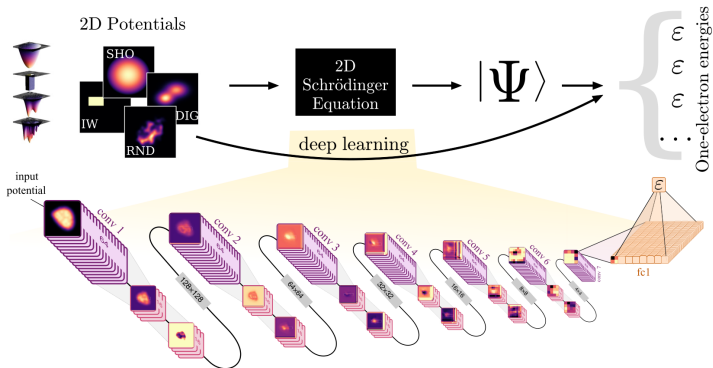


Figure 2: Deep Learning and Schrödinger Equation.

# Deep Learning and Schrödinger Equation

- The article shows that a convolutional neural network can learn the mapping between  $V(r)$  and physical features of the system.
- It also shows that partial differential equations can be solved approximately with machine learning.

# Applying ML to the non-linear Schrödinger Equation

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

- Gross-Pitaevskii Equation has non-linear term called as interaction parameter.
- Interaction Parameter determines whether interaction is repulsive or attractive.
- 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

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

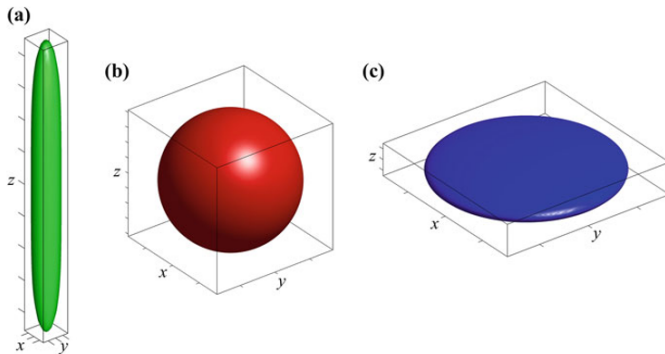


Figure 3: Bose-Einstein Condensates in different trapping potentials.



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

Table 1: My caption

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

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

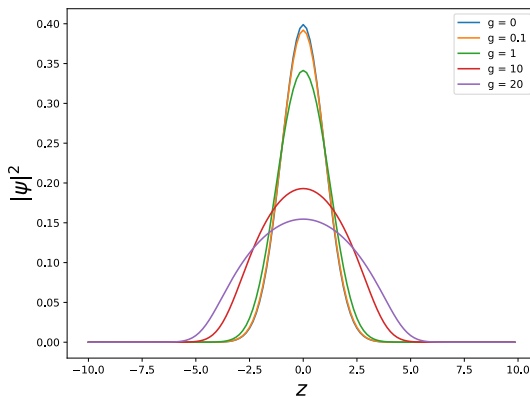


Figure 4: Density

- 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.