# Physics-Informed and Data-Driven methods for Pedagogical Toy Models

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DSECOP Proposal

**Summary:**

I propose 3 modules to study physical systems using machine learning. The modules begin with the analysis of a toy problem with possible extensions to more complex systems. Numerical simulation is an important part of these modules and material about numerical techniques will also be included. Comparison of analytical, numerical and ML simulation should be done by the student to better understand the advantages and disadvantages of these techniques. These modules are interrelated and techniques mentioned in one modules can be used in other modules as well.

## Module 1: Schrödinger Equation

**Summary:**

This module can be used can be used for a Quantum Mechanics course. The module will begin with introduction to the Schrödinger Equation including a tutorial on analytical solutions for different toy systems such as Particle-In-A-Box, Quantum Harmonic Oscillator etc. The second portion of this module will consist of a brief primer on numerical techniques for solving differential equations. Finally, deep learning will be introduced with code examples and students would be expected to compare the numerical and deep learning methods with the analytical solution for a system of their choice.

**Description:**

**Physics** The Schrödinger Equation (SE) is an important part of any Quantum Mechanics course and students are expected to solve it for increasingly complex systems throughout the course. In this module, I introduce Physics-Informed Neural Networks (PINNs) and demonstrate the effectiveness of numerical techniques and deep learning for solving the SE with different potentials even in the absence of analytical solutions. This is especially important because SE becomes analytically intractable for even the smallest practical systems and formulations such as Density Functional Theory are used to simulate such systems. The time dependent Schrödinger Equation (TDSE) is (in atomic units)

$$\hat{H}\psi(\mathbf{r},t) = i\frac{\partial\psi(\mathbf{r},t)}{\partial t}$$

with time independent case (TISE)

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

where $\hat{H}$ is the Hamiltonian and $E$ is the total energy of the system.

**ML** PINNs [1, 2] are a novel class of machine learning algorithms for solution of partial differential equations. This is achieved by incorporating structured prior information derived from physical laws into the learning algorithm. PINNs are constructed by encoding the constraints posed by a given differential equation and its boundary conditions into the loss function of a NN. This constraint guides the network to approximate the solution of the differential equation.

Relevant courses: Quantum Mechanics
Computational/ML topics covered: Numerical techniques for solving PDEs, Neural Networks, Physics-Informed Neural Networks, Gaussian Processes

**Representative system:**

**Time Dependent Schrödinger Equation** Quantum Harmonic Oscillator is a representative system commonly used in QM courses. In the 1D case, the Hamiltonian is (atomic units)

$$\hat{H}_x = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\omega^2}{2}x^2$$

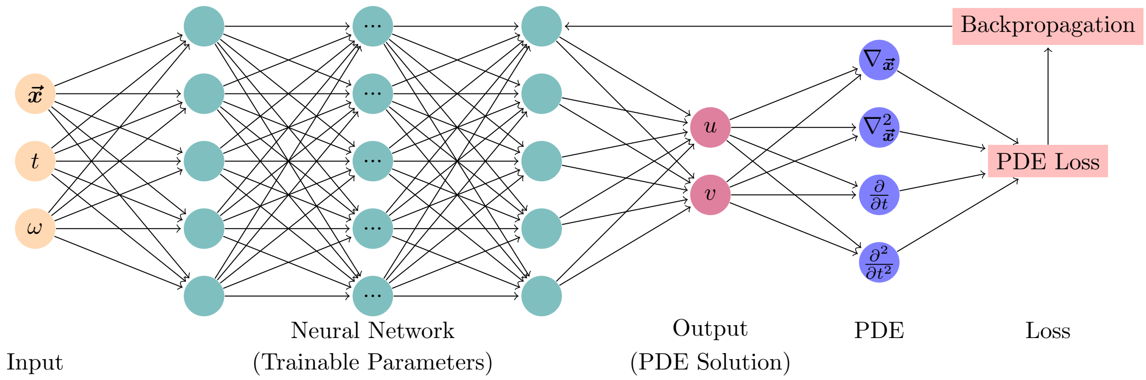


Figure 1: PINN architecture

The analytical solution $\psi(x,t) \in \mathbb{C}$ is

$$\psi_{m,n}(x,t) = \frac{1}{\sqrt{2}}\left(e^{(-iE_m t)}\phi_m(x) + e^{(-iE_n t)}\phi_n(x)\right)$$

where $\psi_{m,n}$ is the wavefunction for a QHO consisting of the superposition of eigenstates $\phi_m$ and $\phi_n$ with $E_i$ being the energy level of state $\phi_i$.

$$\phi_0(x) = \sqrt[4]{\frac{\omega}{\pi}}\exp\left(-\frac{\omega x^2}{2}\right)$$

$$\phi_n(x) = \phi_0(x)\frac{1}{\sqrt{2^n n!}}Her_n(\sqrt{\omega}x)\exp\left(-iE_n t\right)$$

where $Her_n(y)$ is the $n$th Hermite polynomial, and phase $\exp\left(-iE_n t\right)$ where $E_n = (n+\frac{1}{2})\omega$

**Sample questions:**

1. Derive the analytical solution for QHO.
2. (a) Write a simple numerical solver (eg Runge-Kutta) to simulate the time evolution of this QHO system.
   (b) Implement a simple neural network as a surrogate model for this system. How would you represent a complex valued wavefunction in a neural network? (started code for neural network will be provided)
   (c) Now add the Physics-Informed regularization term to the simple neural network implemented in part (b).
   (d) Compare the results from approaches (a),(b) and (c) with the analytical solution.
3. TISE is an eigenvalue problem. How would you incorporate further constraints into PINNs to get solutions for specific eigenstates?
4. What are the advantages and disadvantages of ML models like PINNs over traditional numerical solvers?

**Sample simulation:**

This figure shows results inferred with a PINN for the 1D TD QHO system:

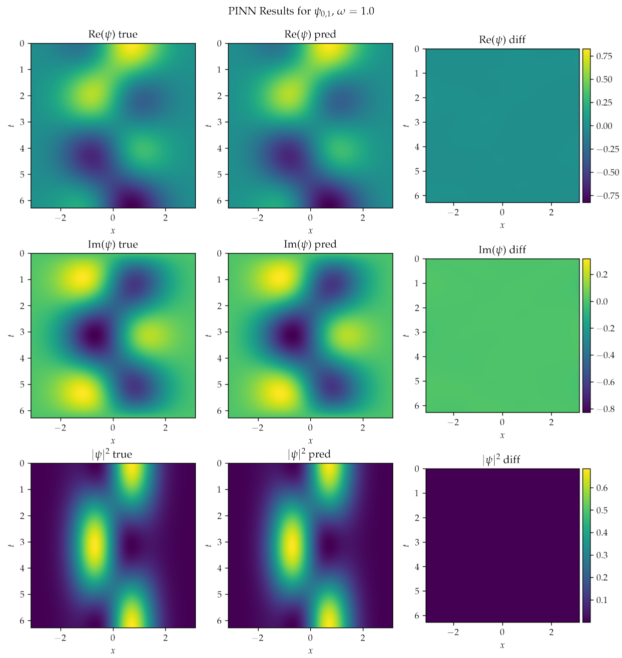


Figure 2: Real and predicted simulation for 1D QHO

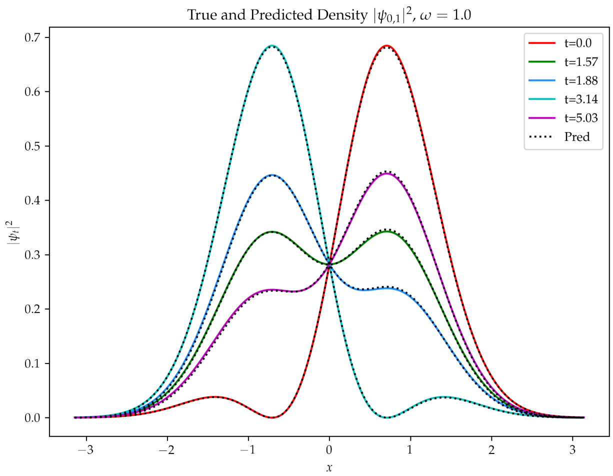


Figure 3: Density results for 1D QHO

**Extensions:**

- Content about Bayesian statistics can be incorporated by using a Gaussian Process based surrogate model for the Schrödinger equation. Example: https://karan.sh/GPNN_schrodingers_equation/
- Because of the relevance of differential equations to different physical systems, this module can be extended to multiple courses like Classical Mechanics and Electrostatics/dynamics.