ML for Prediction of Quantum Dynamics

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PROBLEM STATEMENT

System: Particle in a 1-D box with some unknown potential inside.

Given n position measurements of the particle for each time 0, 1, 2,...T , predict the PDF ($|\psi(x)|^2$) for time $n < t < n+1$ and $t > T$.

- Classically, a particle in a 1-D box with zero potential inside is well described i.e. $x(t)$ with 3 parameters,
- They are: Its position (x_0) and velocity (v_0) at some time (t_0). It simply bounces back and forth between the walls at constant velocity.
- In quantum mechanics, a particle in a box is at all positions with different probabilities and the probability density function evolves in time [Figure - 1].

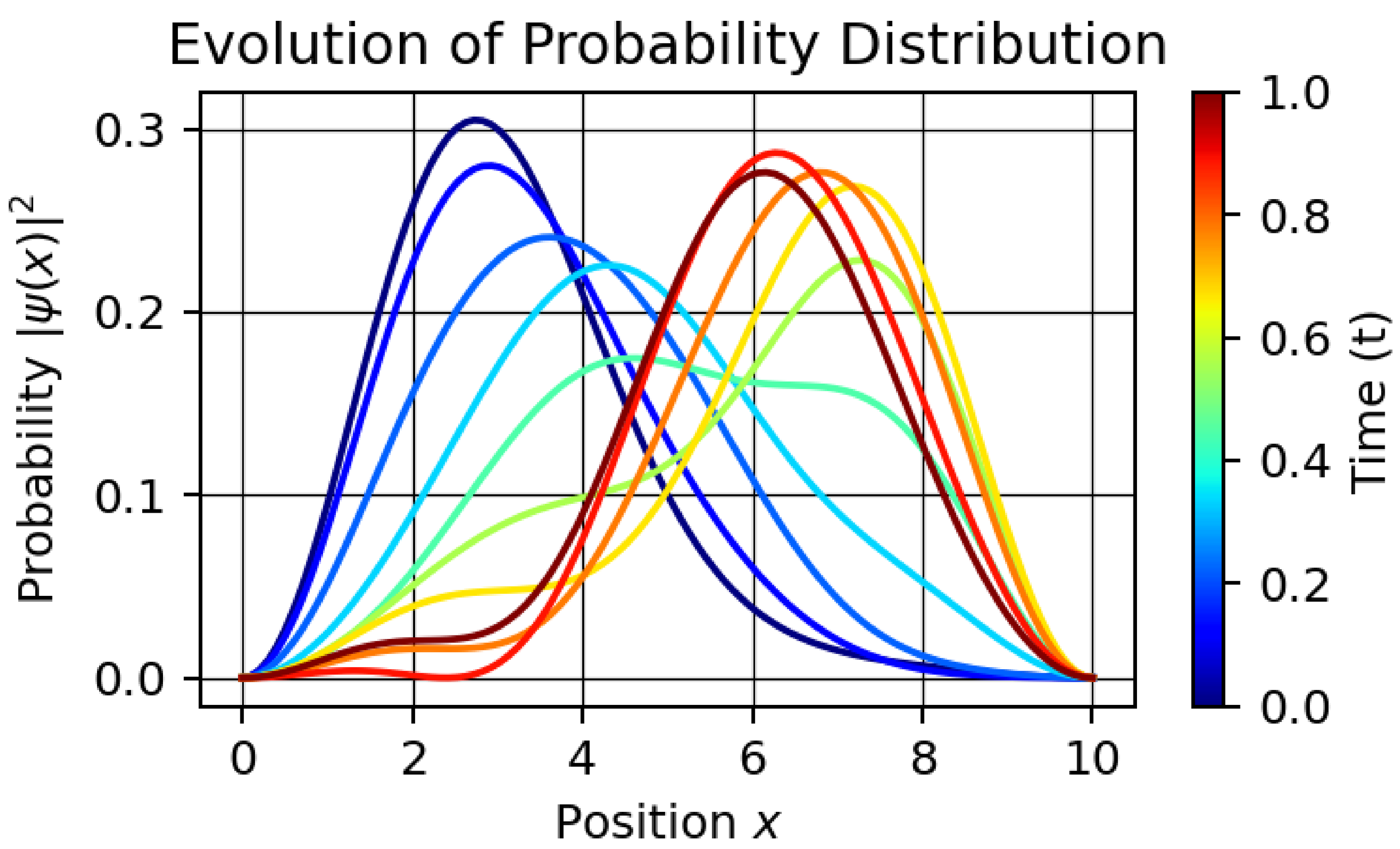

Figure 1. Sample quantum evolution of particle in a box

QUANTUM PHYSICS-INFORMED NN?

PINN [2] is a deep neural network that has been trained to solve differential equation(s) subject to a set of boundary/ initial value conditions. How to use PINN for our case?

As potential $V(x)$ is unknown, one can't use the Schrodinger Equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

Use a different equation; Continuity equation of probability. (It doesn't work)

$$\frac{\partial|\psi(x)|^2}{\partial t} + \frac{\partial J}{\partial x} = 0 \quad \text{where,} \quad J = \frac{i\hbar}{2m}\left[\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right] \tag{2}$$

We tried to predict dynamics for V=0 using the Schrodinger equation, but even that didn't work.

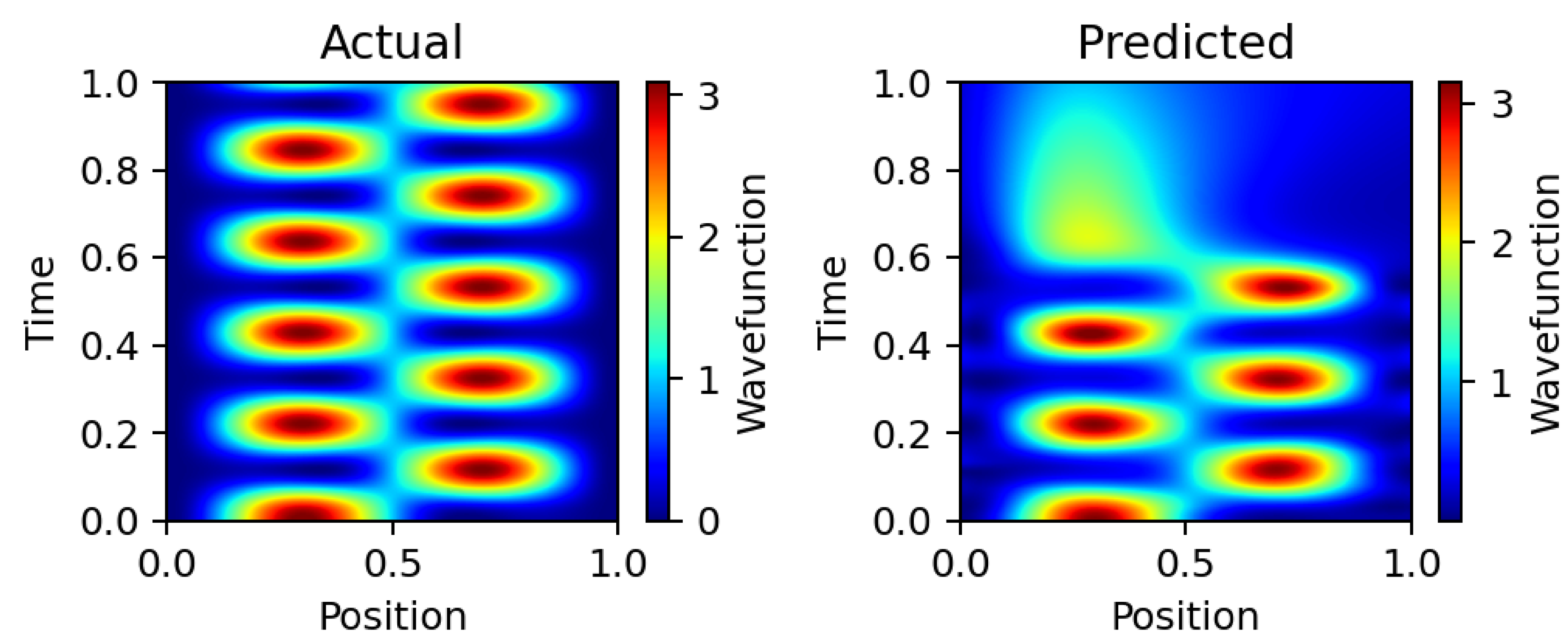

Figure 2. Failure of Q-PINN. It has been trained on data from T=0 to 0.6 (which it learns) but can't predict future.

We suspect it is not easy to train PINN to solve second order differential equations. Even if it did work for V=0, how to solve for unknown V ?

Quantum > Classical ; Regression > Neural Network

is much more difficult than — is sometimes better than

BACK TO REGRESSION

Scrap everything and start from the basics. Analytically solve S.E. for V=0. The most general solution is

$$\psi(x,t) = \sum_{n=1}^{N} a_n \psi_n^\circ(x) e^{-i(E_n^\circ t + \phi_n)}$$

$$\text{where,} \quad E_n^\circ = \frac{1}{2m}\left(\frac{n\pi\hbar}{L}\right)^2 \quad \text{and} \quad \psi_n^\circ(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi x}{L}\right)$$

Now one can use gradient descent to find the parameters (a_n and ϕ_n i.e $O(2N)$). Simple gradient decent algorithms didn't work. We finally used a **combination of LBFGS and Adam**. LBFGS is good at finding the descent path efficiently but can't jump out of local minima. Adam optimiser hot starts the gradient descent process and jumps out of it.

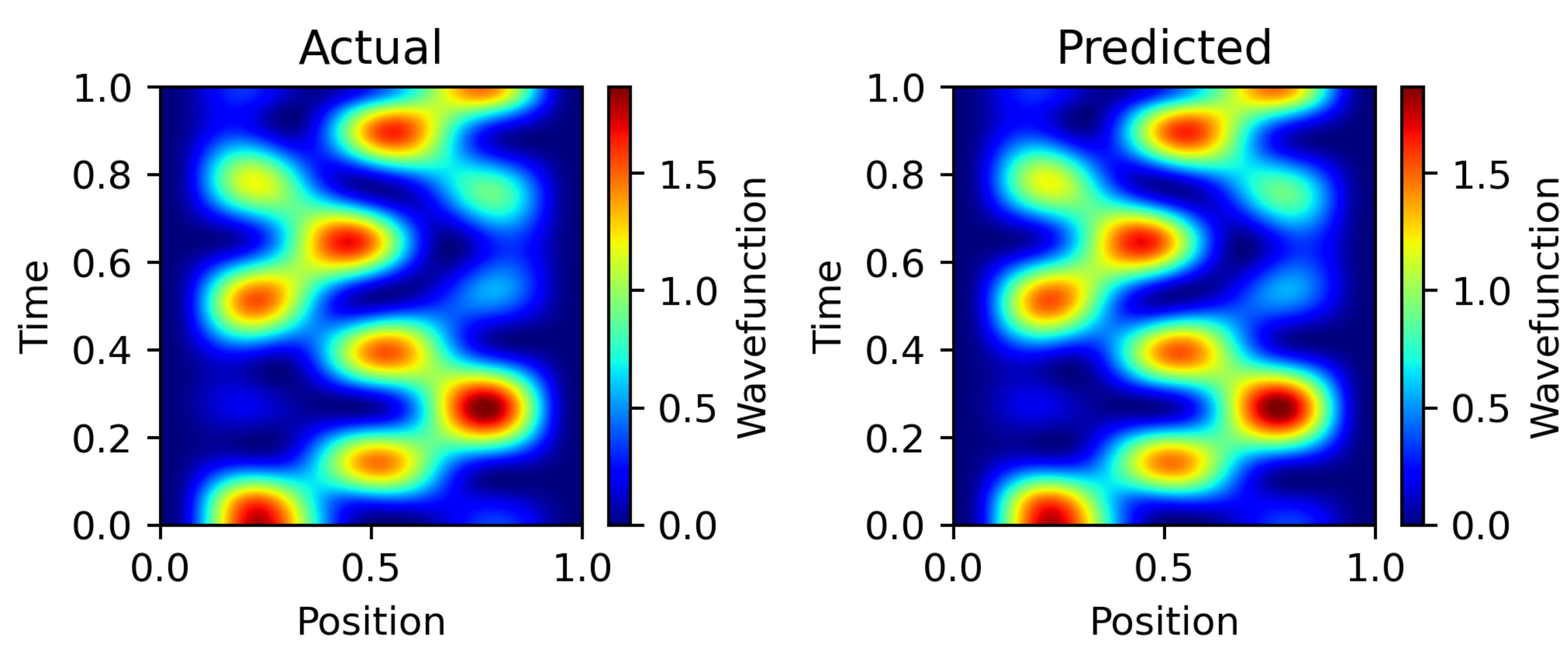

Figure 3. Success of Regression method for V = 0 case.

Non-zero V: There must be a set of Eigenstate-energy solution to the Schrodinger equation. Expand the Eigenstate in the basis of V=0 solution, making it a regression problem again.

$$\Psi_n(x,t) = \sum_{n=1}^{N} a_n \psi_n(x) e^{-i(E_n t + \phi_n)} \quad , \quad \psi_n(x) = \sum_{m=1}^{N} b_{nm}\psi_m^\circ(x) e^{i\theta_{nm}}$$

The parameters here are a_n, b_{nm}, E_n, ϕ_n and θ_{nm} i.e $O(2N^2+2N)$. It is a complex non-convex optimization problem, mostly due to unknown parameters in the exponential (Energies). **LBFGS+Adam didn't work**.

FUTURE WORK

- Resolve Q-PINN for for V = 0 cases, and extend to non-zero potentials motivated by work on HNN. [1]
- Improve upon regression for V $\neq$ 0.
- In case all of this works, explore extension to time-dependent potentials.

REFERENCES

[1] Sam Greydanus, Misko Dzamba, and Jason Yosinski. Hamiltonian neural networks, 2019.

[2] George Em Karniadakis, Ioannis G. Kevrekidis, Lu Lu, Paris Perdikaris, Sifan Wang, and Liu Yang. Physics-informed machine learning. *Nature Reviews Physics*, 3(6):422–440, May 2021.