Unsupervised Neural Networks for Quantum Eigenvalue Problems

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Abstract

Eigenvalue problems are critical to several fields of science and engineering. We present a novel unsupervised neural network for discovering eigenfunctions and eigenvalues for differential eigenvalue problems with solutions that identically satisfy the boundary conditions. A scanning mechanism is embedded allowing the method to find an arbitrary number of solutions. The network optimization is data-free and depends solely on the predictions. The unsupervised method is used to solve the quantum infinite well and quantum oscillator eigenvalue problems.

Introduction

- Neural networks solve differential equations with derivatives taken through auto-differentiation [1, 2, 3, 4, 5].
- We designed unsupervised networks for solving eigenvalue problems of the form

$$\mathcal{L}f(x) = \lambda f(x) \tag{1}$$

$\mathcal{L}$ is a differential operator, λ is the eigenvalue, and $f(x)$ is the eigenfunction.

- We solve Schrodinger's equation from quantum physics, where $\psi(x)$ is the eigenfunction, E the energy eigenvalue, and $V(x)$ the potential

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x) \tag{2}$$

Methodology

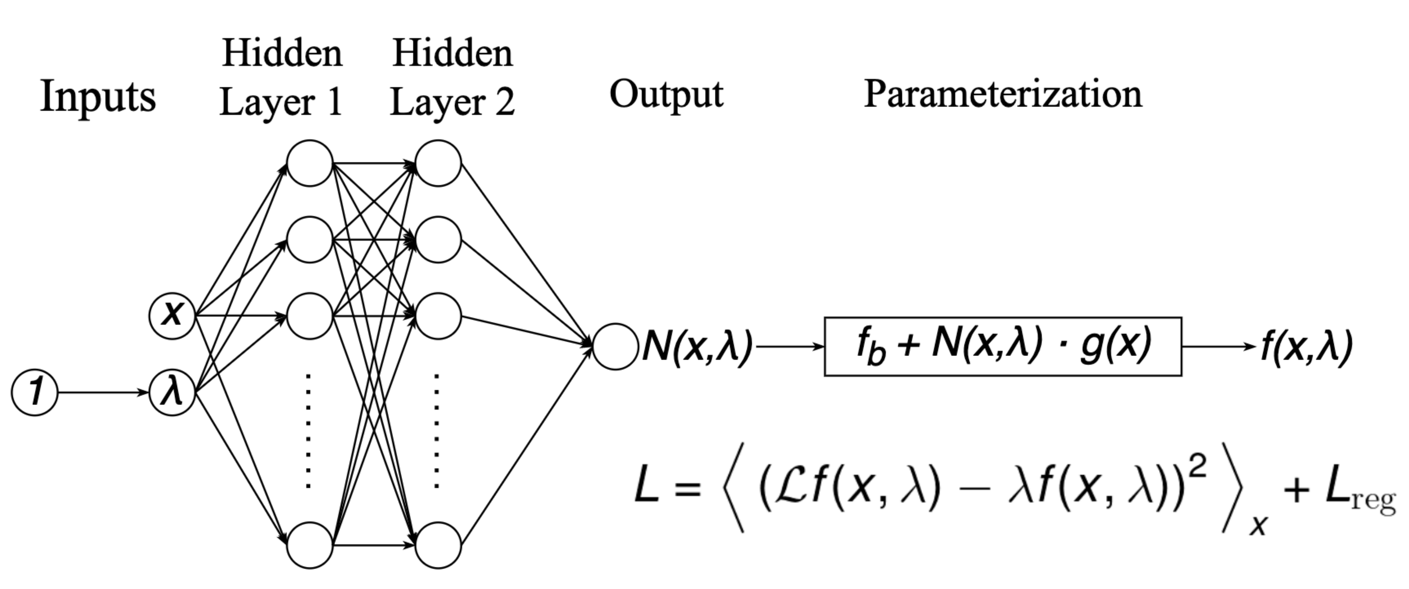

Fig. 1: Neural network architecture, parameterization of network output, and loss function

- The network takes in inputs x and a constant 1. The constant 1 is fed into a single neuron, which learns solution eigenvalues.
- Impose homogeneous Dirichlet boundary conditions with parametrization

$$g(x) = \left(1 - e^{-(x-x_L)}\right)\left(1 - e^{-(x-x_R)}\right) \tag{3}$$

- Physics-informed loss function is given by

$$\begin{aligned} L &= L_{\text{DE}} + L_{\text{reg}} \\ &= \left\langle \left(\mathcal{L}f(x,\lambda) - \lambda f(x,\lambda)\right)^2 \right\rangle_x + L_{\text{reg}} \end{aligned} \tag{4}$$

- Data-free training since the L solely depends on network predictions.
- The regularization loss terms are given by

$$L_f = \frac{1}{f(x,\lambda)^2}, \qquad L_\lambda = \frac{1}{\lambda^2}, \qquad L_{\text{drive}} = e^{-\lambda + c}. \tag{5}$$

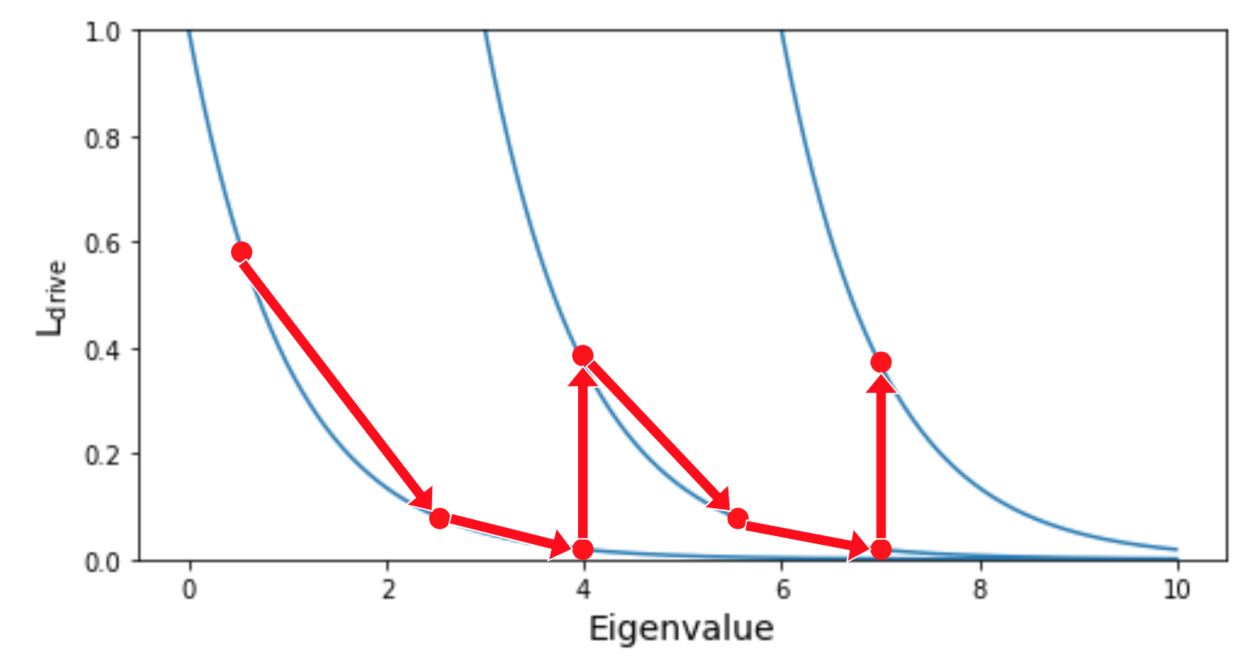

Fig. 2: The scanning mechanism pushing eigenvalue upwards. Red dot is eigenvalue, and blue curve is the shifting L_{drive}

- We used Adam optimizer for training, two hidden layers, 50 neurons each. We also used $\sin(\cdot)$ instead of more common activation functions because we found that it accelerates the convergence to a solution.

Experiments

We test our method on two cases of the Schrodinger equation Eq. (2).

Infinite square well: The potential function is given by

$$V(x) = \begin{cases} 0 & 0 \le x \le \ell \\ \infty & \text{otherwise} \end{cases}. \tag{6}$$

- The analytical solutions to this problem are

$$\psi_n(x) = \begin{cases} \sqrt{2}\sin(n\pi x) & 0 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}, \qquad E_n = \frac{n^2\pi^2}{2}, \tag{7}$$

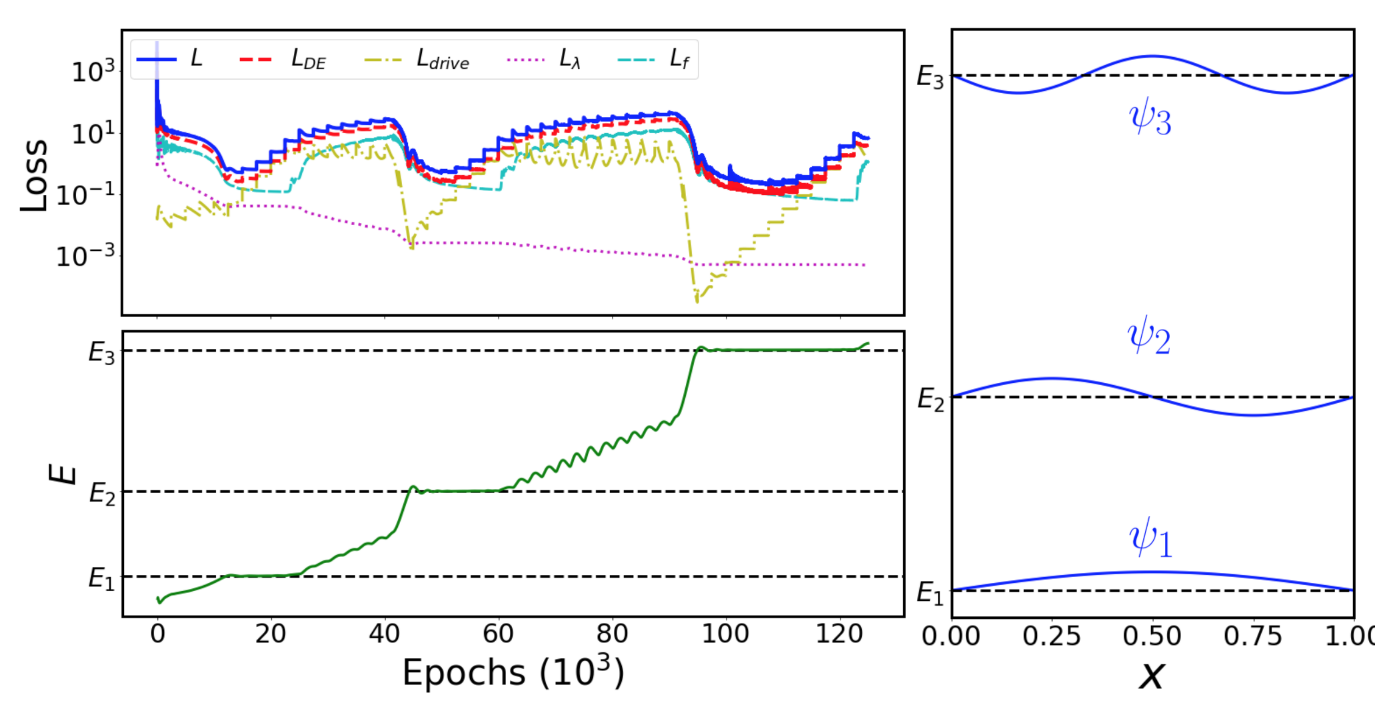

Fig. 3: Found solutions for the infinite square well. Errors are of the order 10^{-3} and 10^{-4} for ψ and E.

Quantum harmonic oscillator: The potential is given by

$$V(x) = \frac{1}{2}kx^2, \tag{8}$$

- The exact solutions for the eigenfunctions and energies are given in terms of Hermite polynomials H_n

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\frac{e^{-\frac{x^2}{2}}}{\pi^{1/4}}H_n(x), \qquad E_n = n + \frac{1}{2}. \tag{9}$$

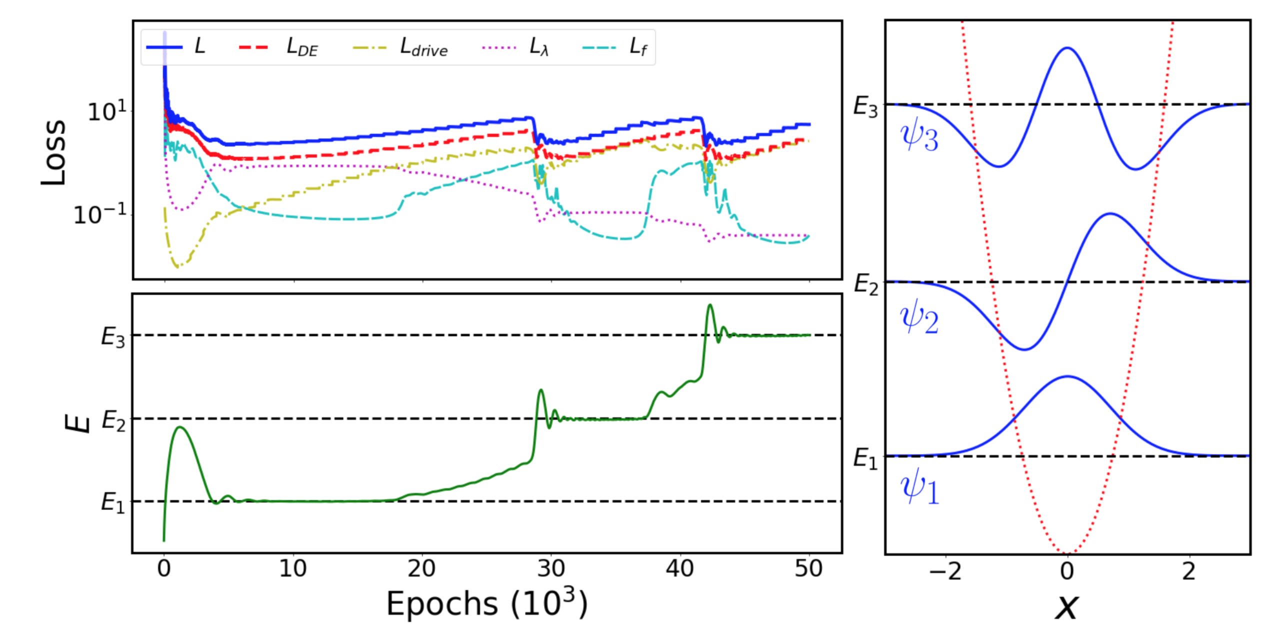

Fig. 4: Found solutions for the harmonic oscillator. Errors are of the order 10^{-2} and 10^{-2} for ψ and E.

Conclusion

- A general neural network method for discovering eigenvalues and eigenfunctions of boundary conditioned problems.
- The boundary conditions are identically satisfied through a parametrization.
- Different boundary conditions can be identically satisfied through a different parametrization.
- An embedded scanning mechanism allows the network to find different eigenvalues and eigenfunctions pairs.
- The network optimization solely depends on the predictions consisting an unsupervised data-free learning method.
- A physics-informed loss function. Dips in loss and plateaus in eigenvalue predictions indicate a solution, giving physical meaning to loss function.

References

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