Quantum Systems Solutions with PINNs

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Overview of the Presentation

QUANTUM SYSTEMS SOLUTIONS WITH PINNS

1. **ARCHITECTURE**
   Physics informed loss functions
2. **1D HYDROGEN ATOM**
   Schrödinger equation solution for one dimensional hydrogen atom.
3. **3D HYDROGEN ATOM**
   Schrödinger equation solution for three dimensional hydrogen atom.
4. **3D DIHYDROGEN CATION**
   Schrödinger equation solution for three dimensional dihydrogen cation molecule.

Physics-Informed Method

- Other methods to solving Schrödinger equation:
  - Hartee-Fock Method
  - Variational Monte Carlo(VMC) Method
  - Neural Networks + VMC

- Physics-informed loss differs from typical VMC function

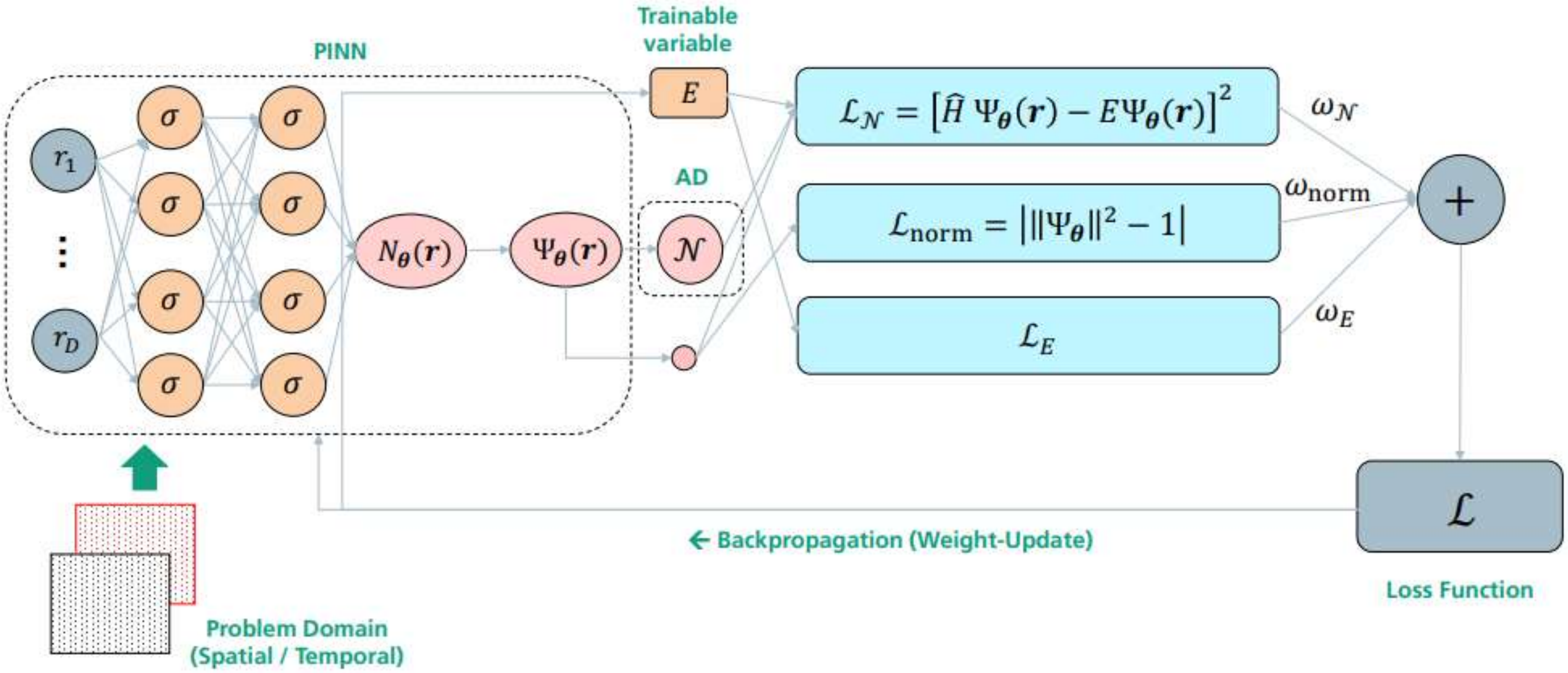
$$\mathcal{L}_{\mathcal{N}}(\boldsymbol{\theta}) = \frac{1}{N_f} \sum_{i=1}^{N_f} \left[\hat{H}\, \Psi_{\boldsymbol{\theta}}(\mathbf{r}^i) - E\, \Psi_{\boldsymbol{\theta}}(\mathbf{r}^i) \right]^2,$$

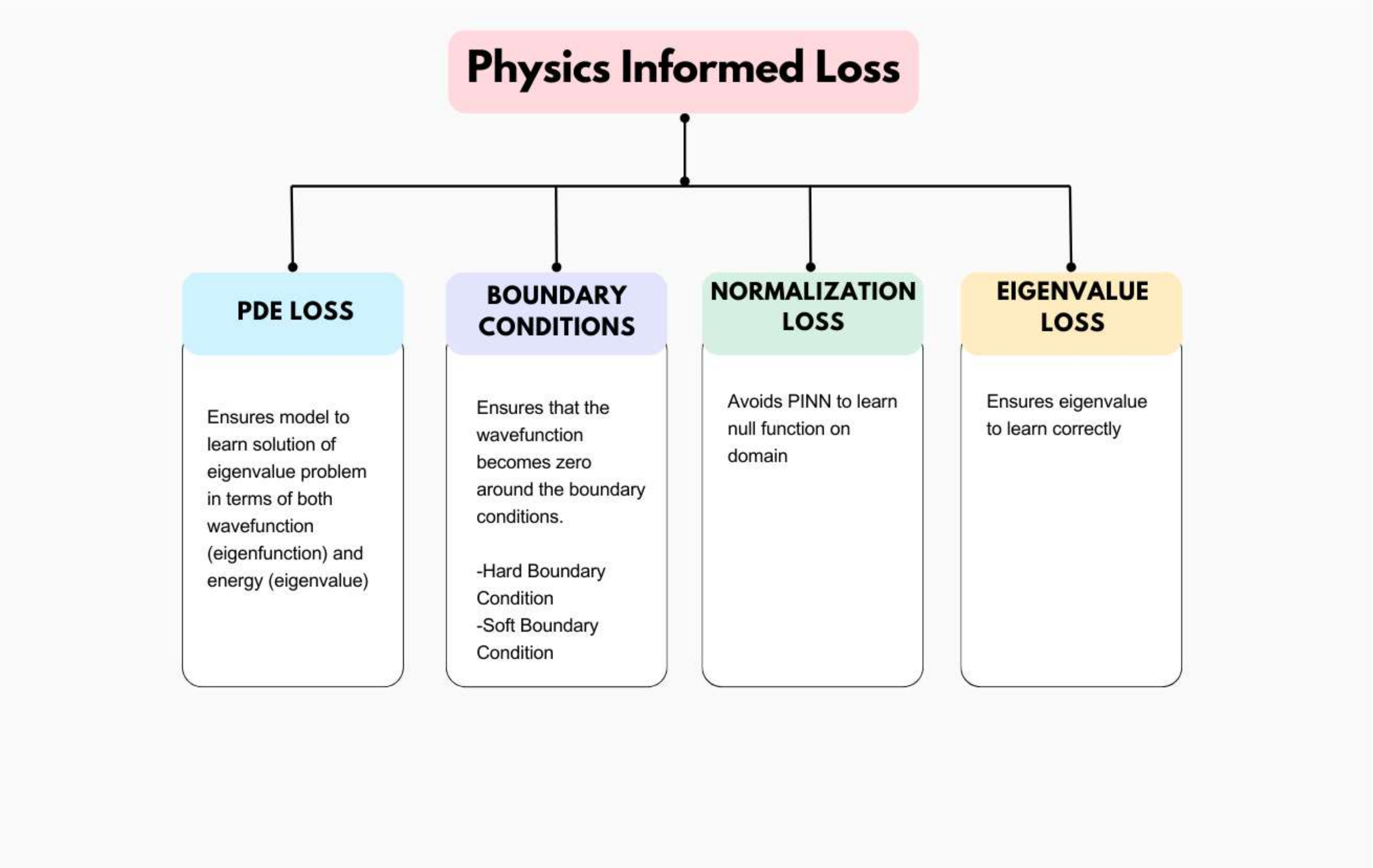
- Eigenvalue problem **differs** from PDE solution with PINNs!

Approach and Methodology

- Many-electron hamiltonian for hydrogen atom: $$\hat{H} = -\frac{1}{2}\nabla^2 - \frac{1}{|\mathbf{r}|},$$
- For hydrogen ion: $$\hat{H} = -\frac{1}{2}\nabla^2 - \frac{1}{|\mathbf{r} - \mathbf{R}_1|} - \frac{1}{|\mathbf{r} - \mathbf{R}_2|},$$
- All variables defined in atomic unites are **nondimensionalized** which is standard procedure in PINNs
- Selected domain: Ω = [0,10] for 1D and Ω = for 3D
- Wavefunction is **spin invariant**!
- Sampling points: **Quasi-random sampling**

Schematic of PINN Architecture




Physics Informed Loss
PDE LOSS
Ensures model to learn solution of eigenvalue problem in terms of both wavefunction (eigenfunction) and energy (eigenvalue)
BOUNDARY CONDITIONS
Ensures that the wavefunction becomes zero around the boundary conditions.
-Hard Boundary Condition
-Soft Boundary Condition
NORMALIZATION LOSS
Avoids PINN to learn null function on domain
EIGENVALUE LOSS
Ensures eigenvalue to learn correctly

PDE Loss

- PDE loss is according to eigenvalue problem

$$\mathcal{L}_{\mathcal{N}}(\boldsymbol{\theta}, E) = \frac{1}{N_f} \sum_{i=1}^{N_f} \left[\hat{H}\, \Psi_{\boldsymbol{\theta}}(\mathbf{r}^i) - E\, \Psi_{\boldsymbol{\theta}}(\mathbf{r}^i) \right]^2 ,$$

- are sampled inside Ω with **quasi-random sampling**

Boundary Conditions

- Domain almost certainly **contains** the electron

$$\Psi_{\boldsymbol{\theta}}(\mathbf{r}) = 0, \qquad \mathbf{r} \in \partial\Omega,$$

- Therefore, probability of finding the electron around the domain boundaries is **approximately null**
- This condition can be implemented with two ways

BOUNDARY CONDITIONS

HARD BOUNDARY CONDITIONS

- **Design the output to adhere to the provided boundary conditions.**
- **Easy to implement only for relatively simple domain**

$$\Psi_{\boldsymbol{\theta}}(\mathbf{r}) = \mathbb{I}_{\mathbf{r} \notin \partial\Omega} \cdot N_{\boldsymbol{\theta}}(\mathbf{r}),$$

- **For our model:**

$$\Psi_{\boldsymbol{\theta}}(\mathbf{r}) = \left[\prod_{i=1}^{D} \left(1 - e^{-\alpha(r_i - r_L)}\right)\left(1 - e^{-\alpha(r_R - r_i)}\right)\right] \cdot N_{\boldsymbol{\theta}}(\mathbf{r}),$$

- **Ensure that boundary points are set to zero while leaving other points unaffected.**
- **Avoids the use of an additional loss function**

SOFT BOUNDARY CONDITIONS

- **Ensure the boundary conditions with the help of loss function**
- **Easier to implement more complex domain geometries**

$$\mathcal{L}_{\mathcal{B}}(\boldsymbol{\theta}) = \frac{1}{N_g} \sum_{i=1}^{N_g} \left[\mathcal{B}[u_{\boldsymbol{\theta}}](\mathbf{x}_i^g) - g(\mathbf{x}_i^g)\right]^2, \qquad \{\mathbf{x}_i^g\}_{i=1 \ldots N_g} \in \partial\Omega.$$

- **Less stable training due to competition of losses**

Normalization Loss

- Normalization of Schrödinger equation on normal solution vs. PINNs solution
- PINN tends to learn **null function** since is a valid solution and minimizes exactly the PDE loss
- To prevent this:

$$\mathcal{L}_{\text{norm}}(\boldsymbol{\theta}) = \left| \|\Psi_{\boldsymbol{\theta}}\|^2 - 1 \right| ,$$

- **Problem:** Integration of $\|\Psi_{\boldsymbol{\theta}}\|^2 = \int_{\Omega} d^D\mathbf{r}\ |\Psi_{\boldsymbol{\theta}}(\mathbf{r})|^2$kpropagation

Normalization Loss

- **Solution:** Specific Architecture or **Monte Carlo Methods**
- Importance of **quasi-random sampling**

$$\|\Psi_{\boldsymbol{\theta}}\|^2 = \int_{\Omega} d^D\mathbf{r}\; |\Psi_{\boldsymbol{\theta}}(\mathbf{r})|^2 \approx \sum_{i=1}^{N_f} \frac{V(\Omega)}{N_f} \left|\Psi_{\boldsymbol{\theta}}(\mathbf{r}^i)\right|^2 := \|\Psi_{\boldsymbol{\theta}}\|^2_{N_f},$$

$$\mathcal{L}_{\text{norm}}(\boldsymbol{\theta}) = \left|\|\Psi_{\boldsymbol{\theta}}\|^2_{N_f} - 1\right| = \left|V(\Omega) \sum_{i=1}^{N_f} \frac{1}{N_f} \left|\Psi_{\boldsymbol{\theta}}(\mathbf{r}^i)\right|^2 - 1\right|$$

- An accurate estimation of the integral is computed at each step
- Normalization loss → Soft Constraint → **Unnormalized** Final Wavefunction
- To prevent that <u>normalization with traditional computational heavy integration</u>!

Eigenvalue Loss

- Presence of this loss → **Unpredictable behavior** of the eigenvalue
- Known true ground-state energy → simple direct problem
- Full eigenvalue problem → find true ground-state energy with PINN in a **unsupervised** way

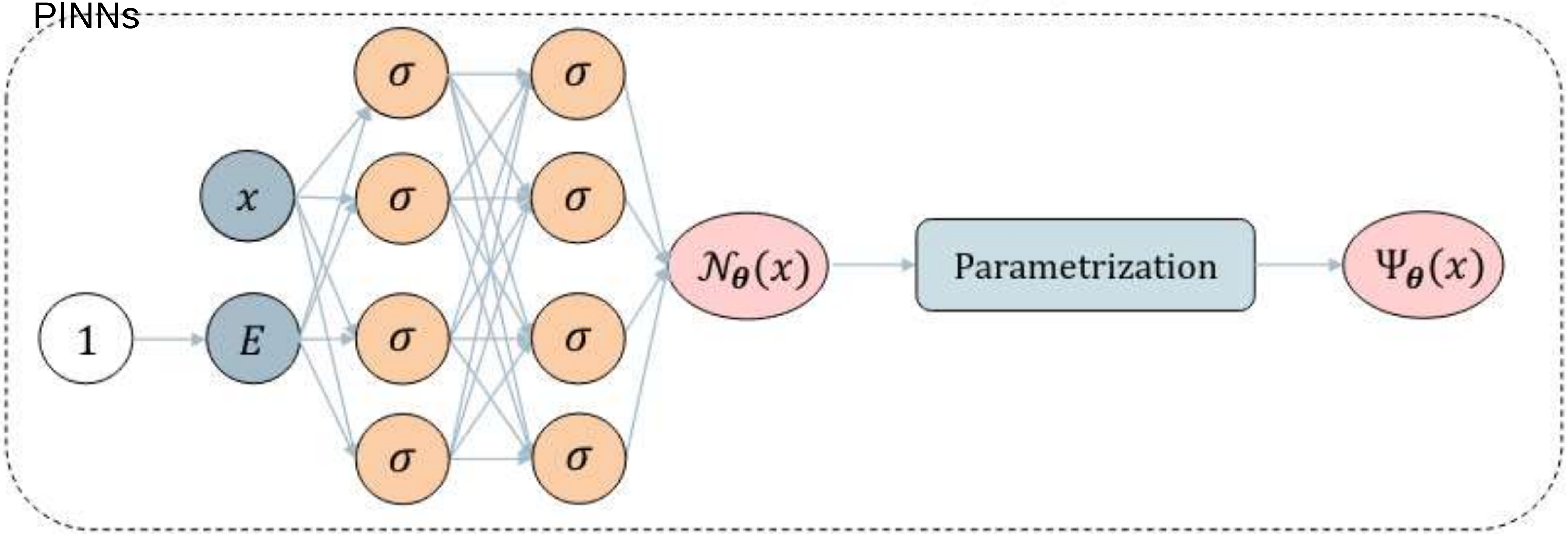
$$\mathcal{L}_{E1}(E) = E,$$ → Not a traditional loss, it is not **null** when true eigenvalue is found

$$\mathcal{L}_{E2}(E) = (E - E_{\text{ref}})^2$$ → Allows to **restrict** the eigenvalue range

Reference energy must be closer to the true ground state energy than any other valid eigenvalue

Particle in a Box

Schematic of proposed PINNs



Particle in a Box

Physics Informed Loss Functions

Schördinger Equation Loss:

$$\mathcal{L}_{Schrodinger} = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + E\psi$$

Eigvenvalue Drive Loss:

$$\mathcal{L}_{Eigen} = e^{-E+c}$$

Non-trivial Wavefunction Loss:

$$\mathcal{L}_{Psinontriv} = \left(\frac{1}{\psi(x, E)}\right)^2$$

Non-trivial Energy Loss:

$$\mathcal{L}_{Enontriv} = \left(\frac{1}{E}\right)^2$$

Analytical Solution

Time independent Schrödinger equation of infinite square well is:

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

Where:

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq 1 \\ \infty & \text{otherwise} \end{cases}$$

$\hbar$ and m can be set to 1 without losing any generality

Solution of this eigenvalue problem:

$$\psi_n(x) = \begin{cases} \sqrt{2}\sin(n\pi x) & \text{if } 0 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

$$E_n = \frac{n^2\pi^2}{2}$$

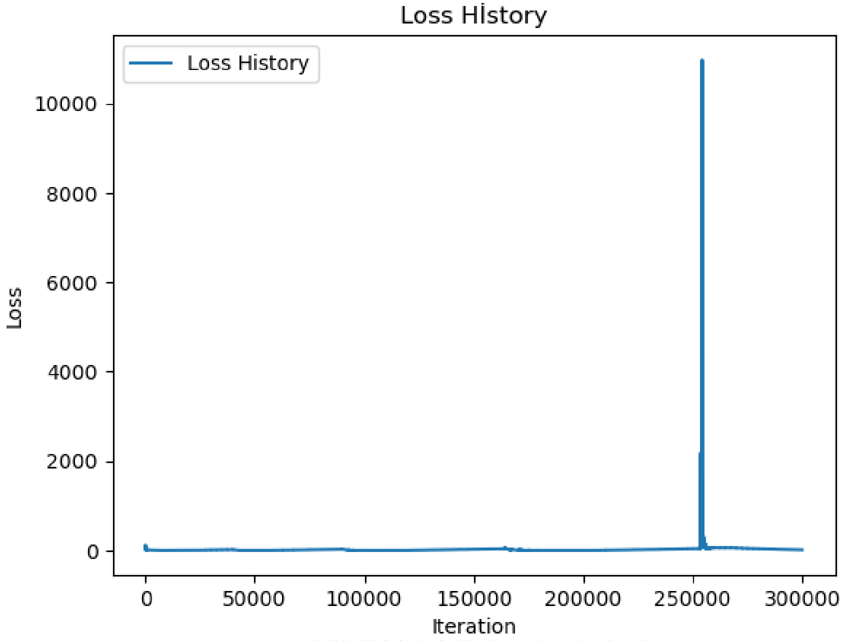
Where n represents the energy states.

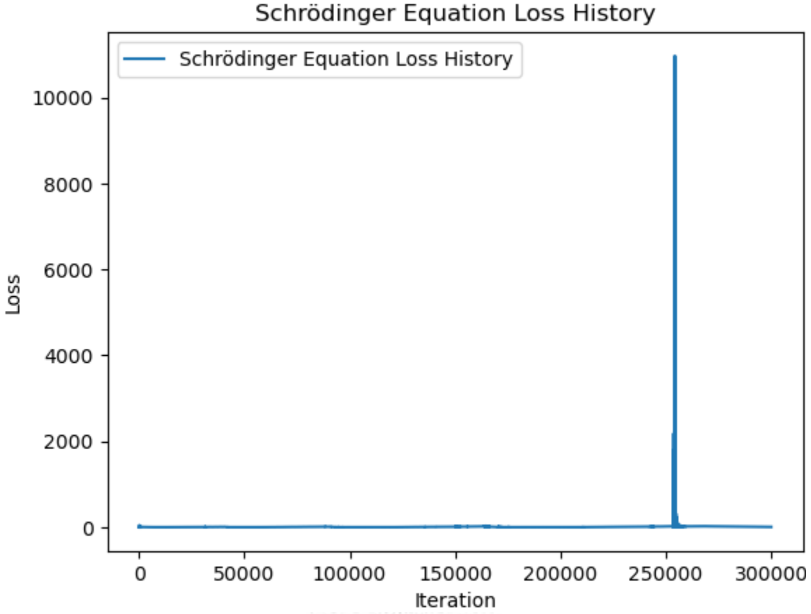
Analytical Solution

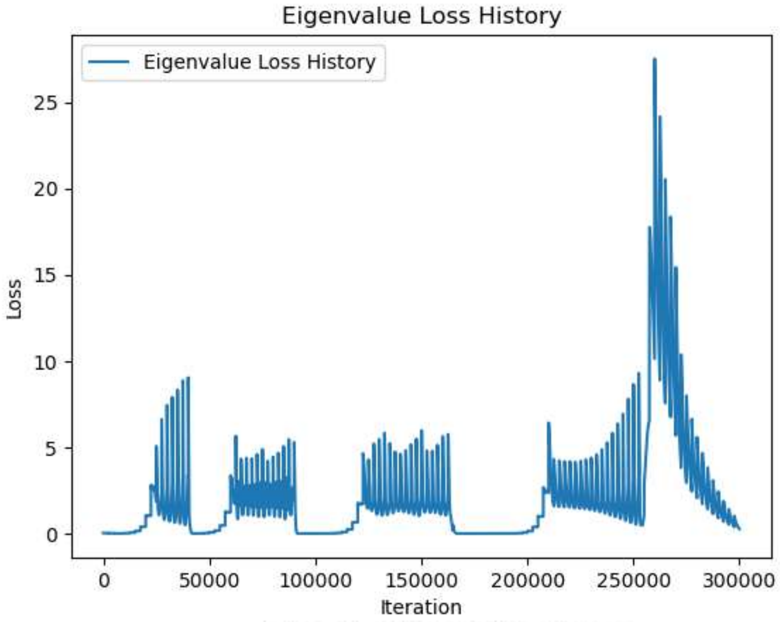
Therefore, we expect to obtain minimum loss at these energy levels, and associiated wavefunction

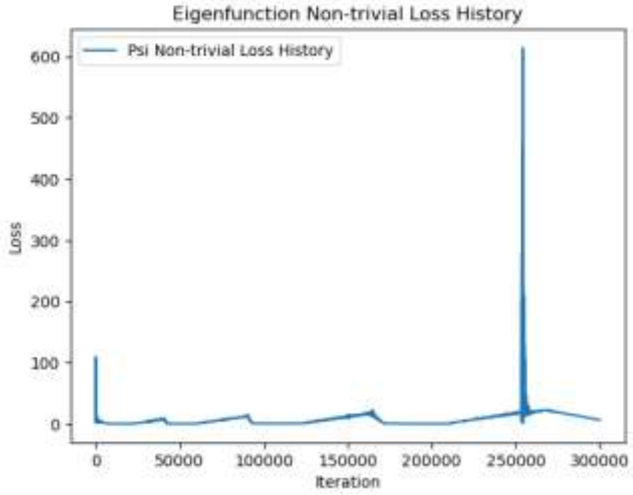
$$\psi_1 = \sqrt{2}\sin(\pi x) \quad \text{and} \quad E_1 = \frac{\pi^2}{2} = 4.934$$
$$\psi_2 = \sqrt{2}\sin(2\pi x) \quad \text{and} \quad E_2 = \frac{4\pi^2}{2} = 19.739$$
$$\psi_3 = \sqrt{2}\sin(3\pi x) \quad \text{and} \quad E_3 = \frac{9\pi^2}{2} = 44.413$$
$$\psi_4 = \sqrt{2}\sin(4\pi x) \quad \text{and} \quad E_4 = \frac{16\pi^2}{2} = 78.956$$
$$\psi_5 = \sqrt{2}\sin(5\pi x) \quad \text{and} \quad E_5 = \frac{25\pi^2}{2} = 123.37$$

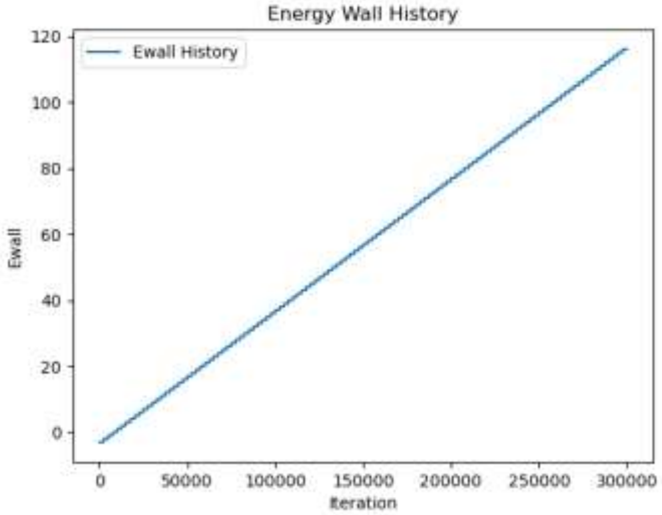
Results

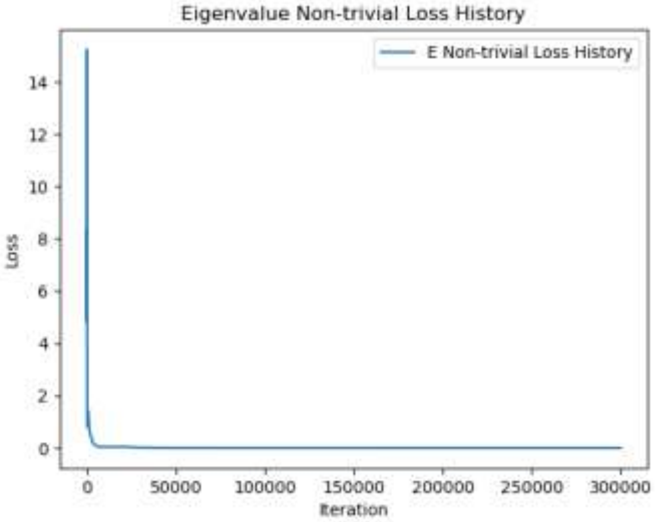

Loss Hİstory
Loss History
Loss
Iteration


Schrödinger Equation Loss History
Schrödinger Equation Loss History
Loss
Iteration

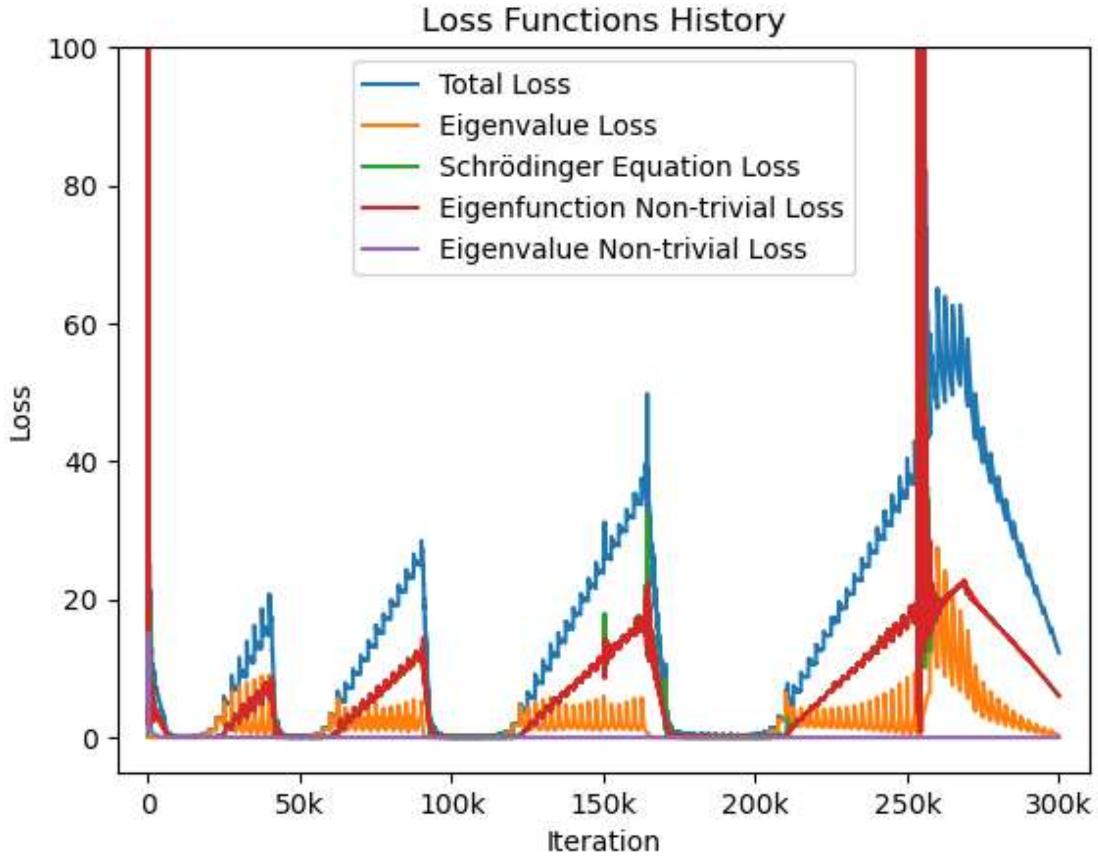

Eigenvalue Loss History
Eigenvalue Loss History
Loss
Iteration


Eigenfunction Non-trivial Loss History
Psi Non-trivial Loss History
Loss
Iteration

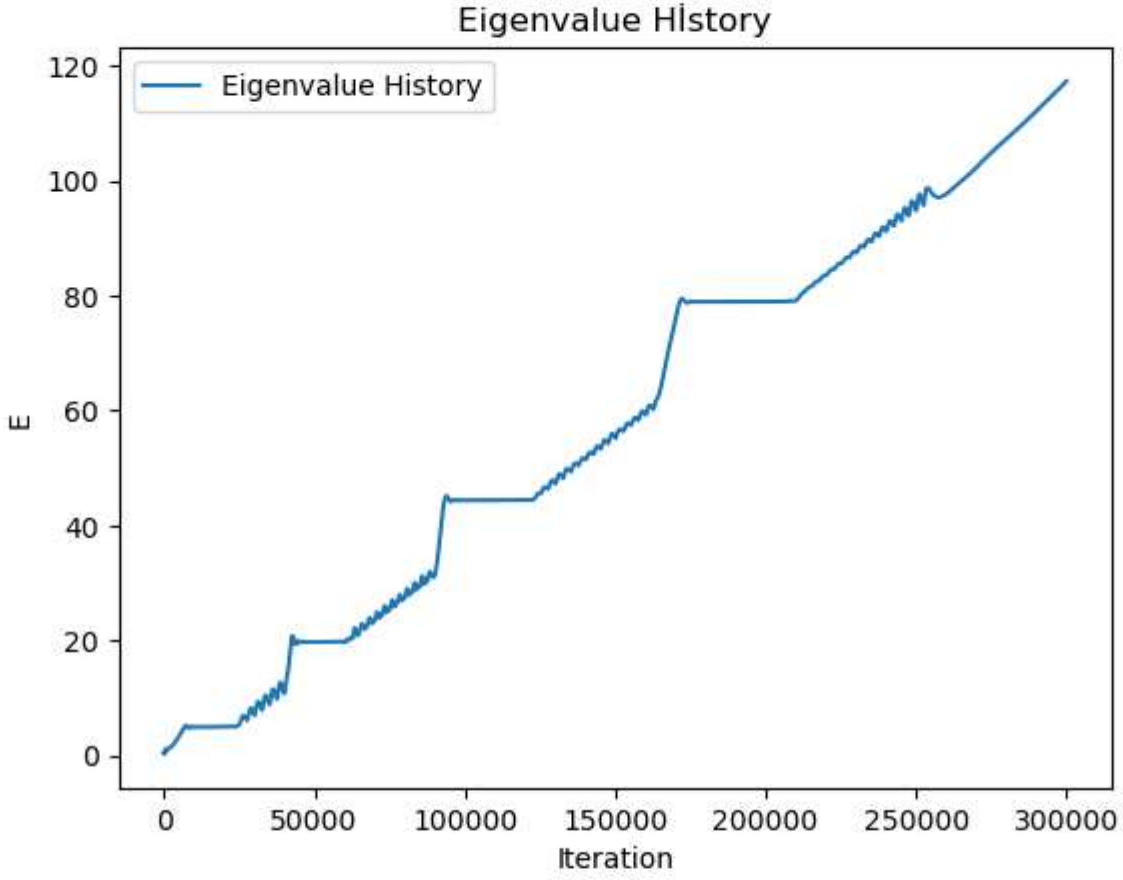

Energy Wall History
Ewall History
Ewall
Iteration


Eigenvalue Non-trivial Loss History
E Non-trivial Loss History
Loss
Iteration

Results

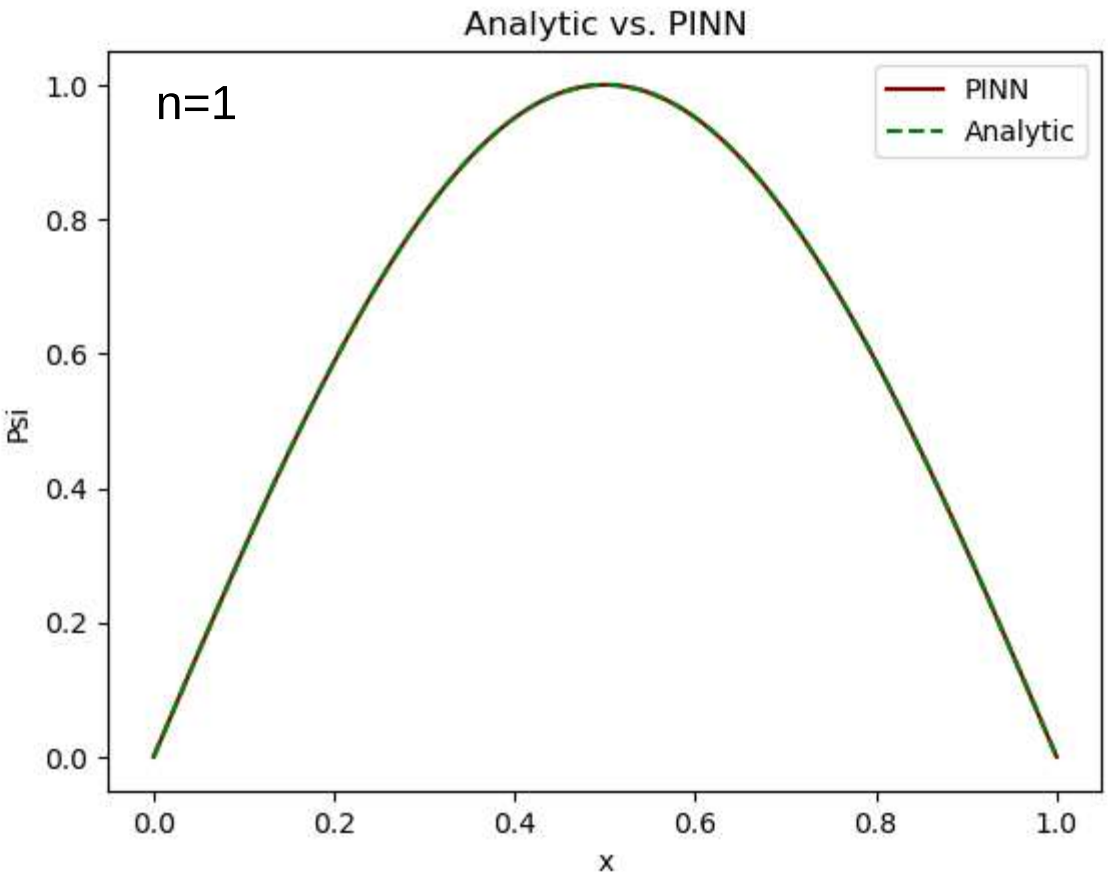


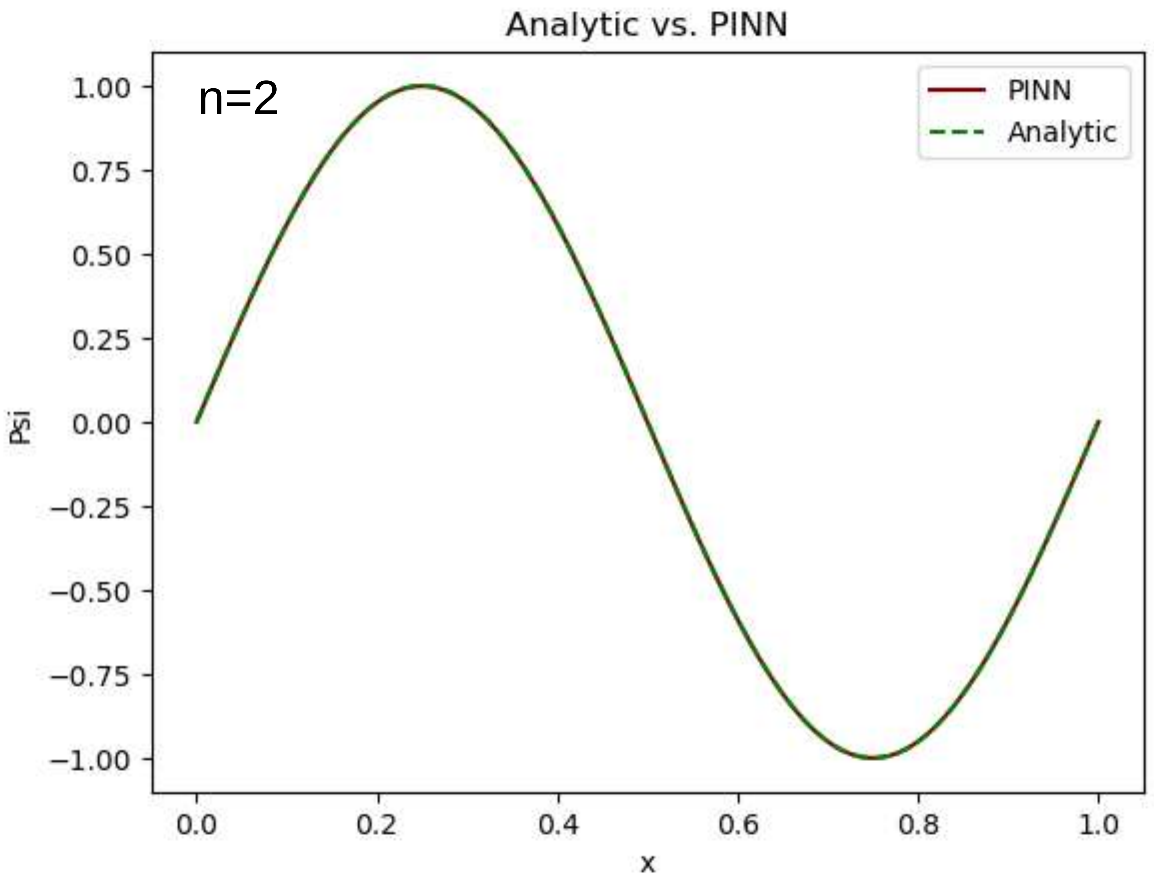
Loss Functions History
Total Loss
Eigenvalue Loss
Schrödinger Equation Loss
Eigenfunction Non-trivial Loss
Eigenvalue Non-trivial Loss
Loss
Iteration
100
80
60
40
20
0
0
50k
100k
150k
200k
250k
300k



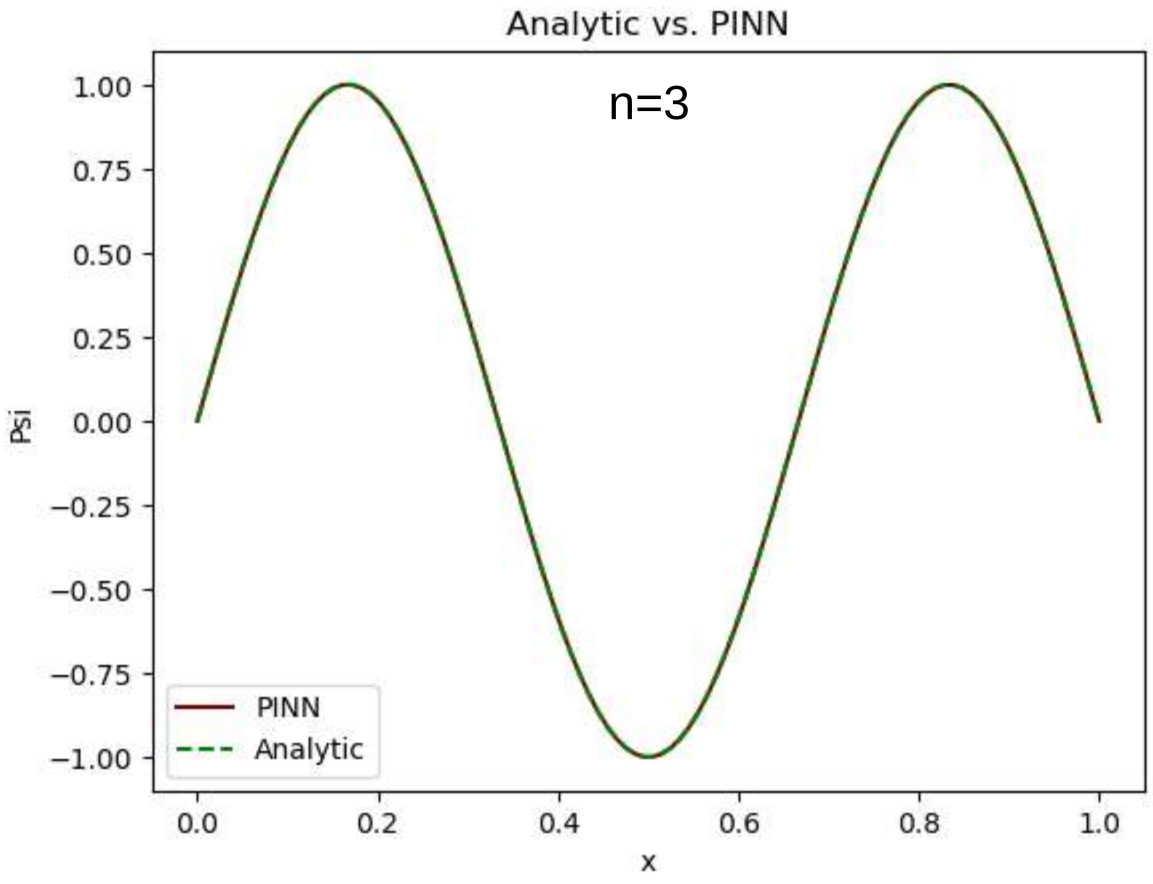
Eigenvalue HIstory
Eigenvalue History
E
Iteration
120
100
80
60
40
20
0
0
50000
100000
150000
200000
250000
300000

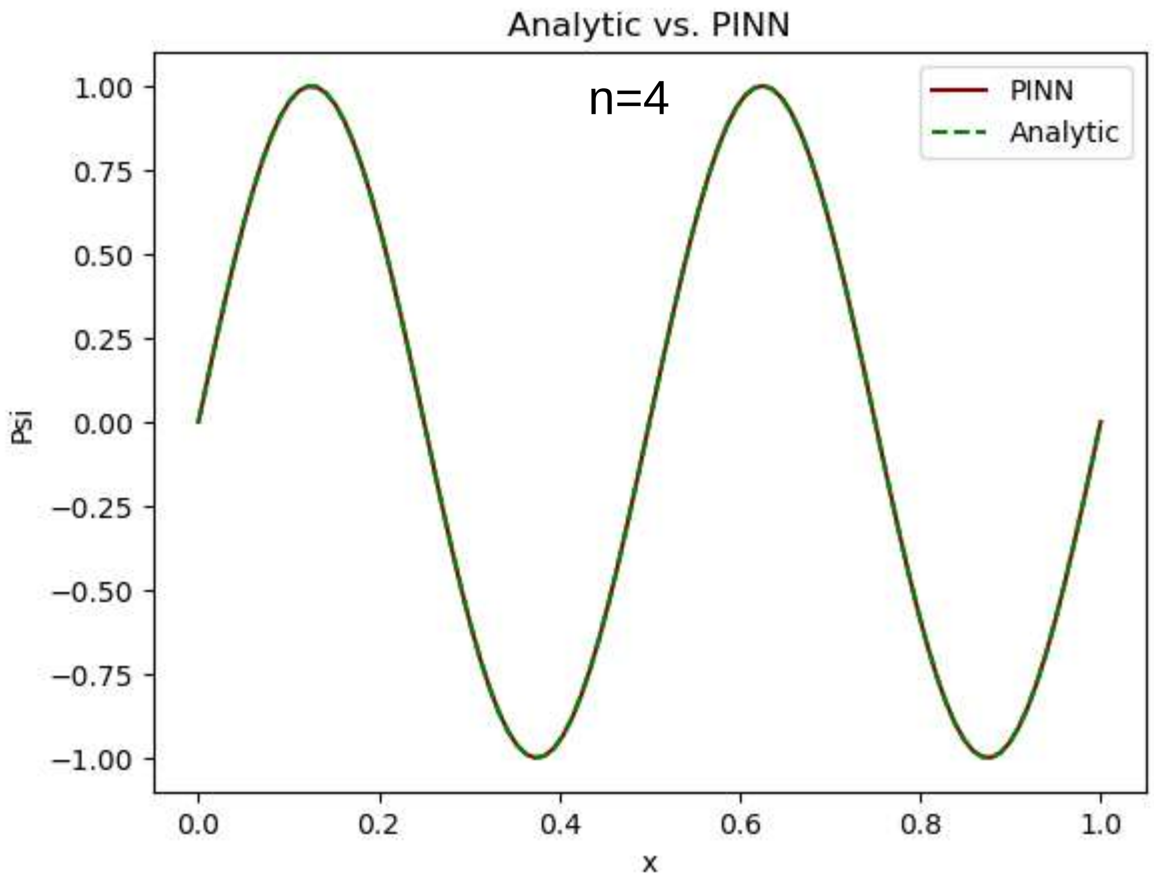
Results


Analytic vs. PINN
n=1
PINN
Analytic
Psi
x
1.0
0.8
0.6
0.4
0.2
0.0
0.0 0.2 0.4 0.6 0.8 1.0


Analytic vs. PINN
n=2
PINN
Analytic
Psi
x
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0.0 0.2 0.4 0.6 0.8 1.0

Results


Analytic vs. PINN
n=3
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Psi
0.0
0.2
0.4
0.6
0.8
1.0
x
PINN
Analytic


Analytic vs. PINN
n=4
PINN
Analytic
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Psi
0.0
0.2
0.4
0.6
0.8
1.0
x

New Physics Informed Loss Functions

- Some of the loss functions in the previous application do not arise directly from physics information.
- Therefore, I am implementing different loss functions that arise from physics knowledge for both infinite and finite square well problems

- However, I haven't been able to finalize the new models due to health problems.

- ## Orthogonality Loss:
  - Orthogonality of different wave functions with different eigenvalues is fundamental property of hermitian operator
  - Energy and wave function of different energy levels can be found with orthogonality loss instead scanning the energy values.

$$L_{\text{orth}} = \psi_{\text{eigen}} \cdot \psi,$$

```
def orthogonal_loss(self,psi,num_psi):

    psisum=0
    for oldpsi in self.old_psi:
        psisum+=oldpsi

    loss=torch.sqrt(torch.dot(psisum,psi[:,0]).pow(2))

    return loss
```

- ## Normalization Loss:

$$\mathcal{L}_{\text{norm}}(\boldsymbol{\theta}) = \left| \|\Psi_{\boldsymbol{\theta}}\|^2_{N_f} - 1 \right| = \left| V(\Omega) \sum_{i=1}^{N_f} \frac{1}{N_f} \left|\Psi_{\boldsymbol{\theta}}(\mathbf{r}^i)\right|^2 - 1 \right|$$

```
def normalization_loss(self, u):

    norm_loss =torch.sqrt((-torch.dot(u[:,0],u[:,0])+100).pow(2)).cuda()

    return norm_loss
```

- ## Symmetry:
  - Implementing correct symmetry of particular wave function may enhance the training significantly
  - Even and odd symmetry can be embedding through neural networks

References

- https://thesis.unipd.it/retrieve/6db1e530-776d-40ff-b264-bdd2ba871188/Zinesi_Paolo.pdf
- https://arxiv.org/pdf/2010.05075.pdf
- https://arxiv.org/pdf/2203.00451.pdf