# Using Physical Informed Neural Networks to solve quasinormal modes

(… and how to solve eigenvalue problems with PyTorch.)

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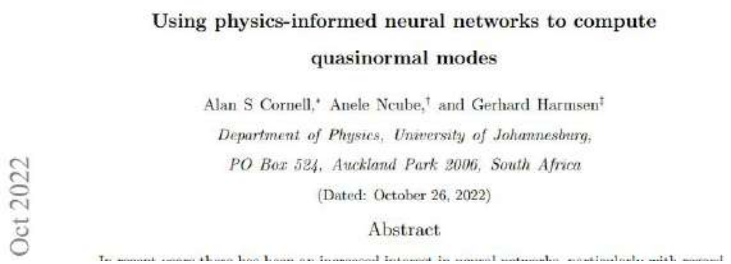
# Content


Oct 2022

**Using physics-informed neural networks to compute quasinormal modes**

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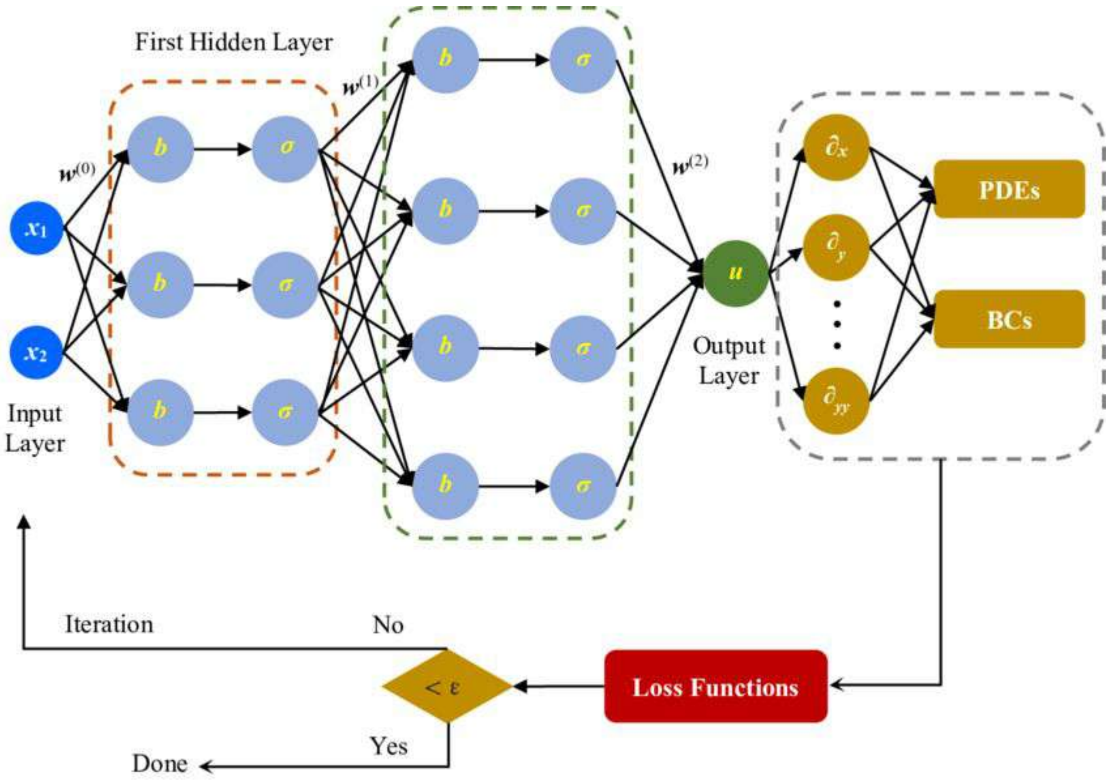
Abstract

1. A brief review of physical informed neural networks (PINNs).
2. The problem we want to solve: Some basics about quasinormal modes (QNM).
3. Example of **inverse problem**: The Posh-Teller potential.
4. Introduction to eigenvalue problems with PINNs.
5. Example of **eigenvalue problem**: Infinite potential (quantum) well.
6. Solution to the Regge-Wheeler equation so far.

# … then again, what's a PINN?



- The structure of the (general) neural network is:

$$\text{input layer:} \quad \mathcal{N}^0(\mathbf{x}) = \mathbf{x} \in \mathbb{R}^{N_0},$$

$$\text{hidden layers:} \quad \mathcal{N}^\ell(\mathbf{x}) = \sigma(\mathbf{W}^\ell \mathcal{N}^{\ell-1}(\mathbf{x}) + \mathbf{b}^\ell) \in \mathbb{R}^{N_\ell}, \quad \text{for} \quad 1 \leq \ell \leq L -$$

$$\text{output layers:} \quad \mathcal{N}^L(\mathbf{x}) = \sigma(\mathbf{W}^\ell \mathcal{N}^{L-1}(\mathbf{x}) + \mathbf{b}^L) \in \mathbb{R}^{N_L},$$

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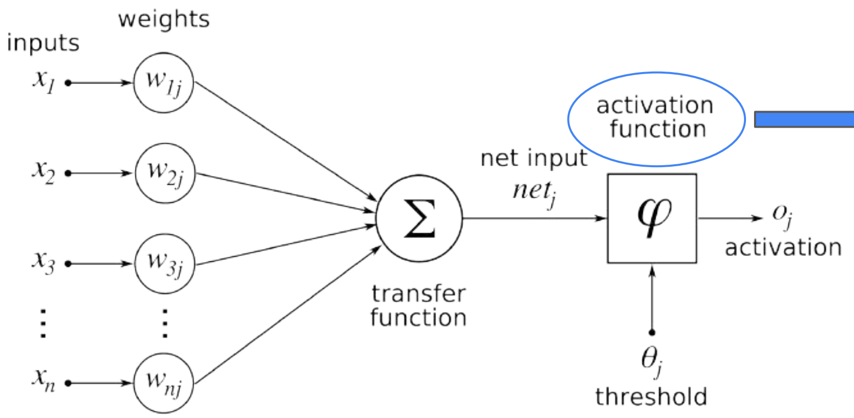
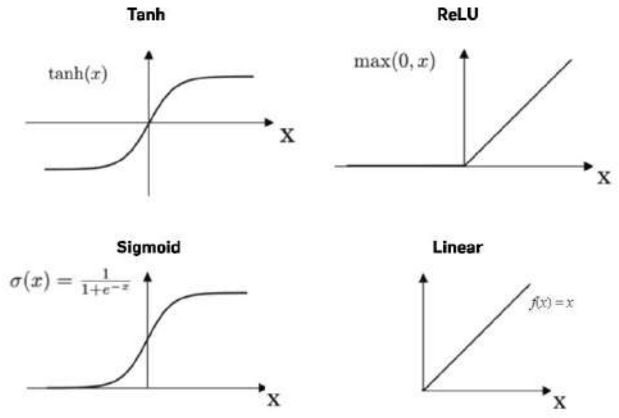


# How do machines learn?

- We first choose a **loss function** that contains what a good prediction actually is.

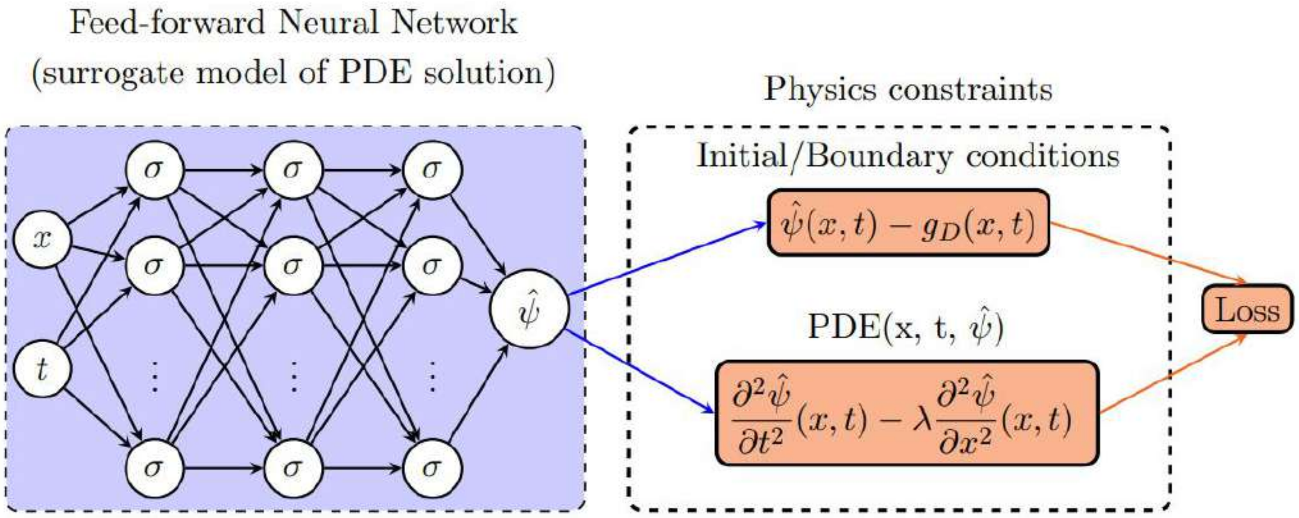
$$C(w, b) = \mathrm{MSE} = \frac{1}{N}\sum(\bar{Y} - Y)^2$$

- Then we apply **backpropagation** to update the weights and bias of **ALL** the neurons in the network. This is done from back to front using the **chain rule**:

$$\boxed{w_{jk}^{\ell} \rightarrow w_{jk}^{\ell} - \frac{\eta}{m}\sum_x \frac{\partial C_x}{\partial w_{jk}^{\ell}},}$$

$$\boxed{b_j^{\ell} \rightarrow b_j^{\ell} - \frac{\eta}{m}\sum_x \frac{\partial C_x}{\partial b_j^{\ell}},}$$

PINNs : Traditional physics model **+** data-driven neural network




The loss function contains the physical information
(Differential equation and boundary conditions).

# Encoding the physics

Dirichlet, Newman, Robin boundary conditions...

- The physical problem is defined as follows:

$$f\left(\mathbf{x}; \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d}; \frac{\partial^2 u}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_d \partial x_d}; \lambda\right) = 0 \text{ on } \Omega \quad / \quad \mathcal{B}(u, \mathbf{x}) = 0 \text{ on } \partial\Omega$$

- **Loss function:** Euclidean norm of the ODE **+** boundary conditions **+** other regularization functions

$$\mathcal{L}(\theta; \mathcal{T}) = w_f \mathcal{L}_f(\theta; \mathcal{T}_f) + w_b \mathcal{L}_b(\theta; \mathcal{T}_b) + w_r \mathcal{L}_r(\theta; \mathcal{T}_r)$$

$$\boxed{\mathcal{L}_f(\theta; \mathcal{T}_f) = \frac{1}{|\mathcal{T}_f|} \sum_{\mathbf{x} \in \mathcal{T}_f} \left\| f\left(\mathbf{x}; \frac{\partial \hat{u}}{\partial x_1}, \ldots, \frac{\partial \hat{u}}{\partial x_d}; \frac{\partial^2 \hat{u}}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 \hat{u}}{\partial x_d \partial x_d}; \hat{\lambda}\right) \right\|_2^2}$$

$$\boxed{\mathcal{L}_b(\theta; \mathcal{T}_b) = \frac{1}{|\mathcal{T}_b|} \sum_{\mathbf{x} \in \mathcal{T}_b} \|\mathcal{B}(\hat{u}, \mathbf{x})\|_2^2}$$

# Problems we could solve with PINNs:

- **Forward problems** : Well defined boundary-value ODE (or PDE) problems.
- **Inverse problems** : DEs with known data values but missing parameters.
- **“Eigenvalue” problems** : Unknown pairs eigenfunction-eigenvalue.
- **Operator learning** : Learning the behavior of the operator itself.

## Advantages

- Unsupervised solutions with only the boundary and PDE information.
- Able to generate more robust models with fewer data.
- In some cases, lower computational cost.
- Easy evaluation points of solutions

## Disadvantages

- Difficult to define some geometries.
- Problems with higher dimensions.
- Stochastic problems.
- Non-local behavior.
- Less precision.

# Black hole perturbation theory

**Quasinormal modes** (QNMs) appear in the analysis of **linear perturbations** of fixed gravitational backgrounds. These perturbations obey **linear second-order differential** equations.

$$S = \frac{1}{16\pi G}\int d^dx\sqrt{-g}\,(R-2\Lambda) + \int d^dx\sqrt{-g}\,\mathcal{L}_m$$

$$\boxed{g_{\mu\nu} = g^{BG}_{\mu\nu} + h_{\mu\nu}} \qquad \boxed{\Phi = \Phi^{BG} + \phi}$$

**Schwarzschild BH**

Spherical symmetry.

$$f(r) = 1 - \frac{2M}{r} - \frac{\Lambda}{3}r^2 \quad / \quad ds^2 = -f dt^2 + \frac{1}{f}dr^2 + r^2(d\theta^2 + \sin^2\theta d\phi)$$

$$\phi(t,r,\theta) = \sum_{lm} e^{-i\omega t}\frac{\Psi_s(r)}{r^{(d-2)/2}}Y_{lm}(\theta) \longrightarrow \frac{d^2\Psi_s}{dr_*^2} + (\omega^2 - V_s)\,\Psi_s = 0$$

$$dr_*/dr = 1/f$$

Regge-Wheeler:

$$\frac{d^2\Psi_s}{dr_*^2} + \left(\omega^2 - V_s\right)\Psi_s = 0$$

$$\boxed{V(r) = f(r)\left[\frac{\ell(\ell+1)}{r^2} + (1-s^2)\left(\frac{2M}{r^3} - \frac{(4-s^2)\Lambda}{6}\right)\right]}$$

Here ***s* = *0, 1, 2*** denotes the spin of the perturbation: scalar, electromagnetic and gravitational

**Boundary conditions**

$$\psi(x) = \begin{cases} e^{-i\omega x}, & x \to -\infty \\ e^{+i\omega x}, & x \to +\infty \end{cases}$$

The **horizon** leads to a boundary value problem which is **non-hermitian**, with associated **complex eigenvalues**.

# Inverse problem with the DeepXDE library

We are first interested in a kind of potentials with exact solution.

$$\frac{d^2\psi}{dx^2} + \left\{\omega^2 - V(r)\right\}\psi = 0$$

$$-\infty < x < +\infty$$

Inverted symmetric **Poschl-Teller** potential

$$\boxed{V_{PT}(x) = \frac{1}{2\cosh^2(x)}.}$$

$$\boxed{\begin{gathered}\psi_n(x) = (\cosh(x))^{(i+1)/2}\chi_n(\sinh(x)) \\ \omega_n = \pm\frac{1}{2} - i(n + \frac{1}{2}),\end{gathered}}$$

We need a **compact domain**:

$$y = \tanh(\mathrm{x}) \quad / \quad -1 < y < +1$$

And so, we get the differential equation:

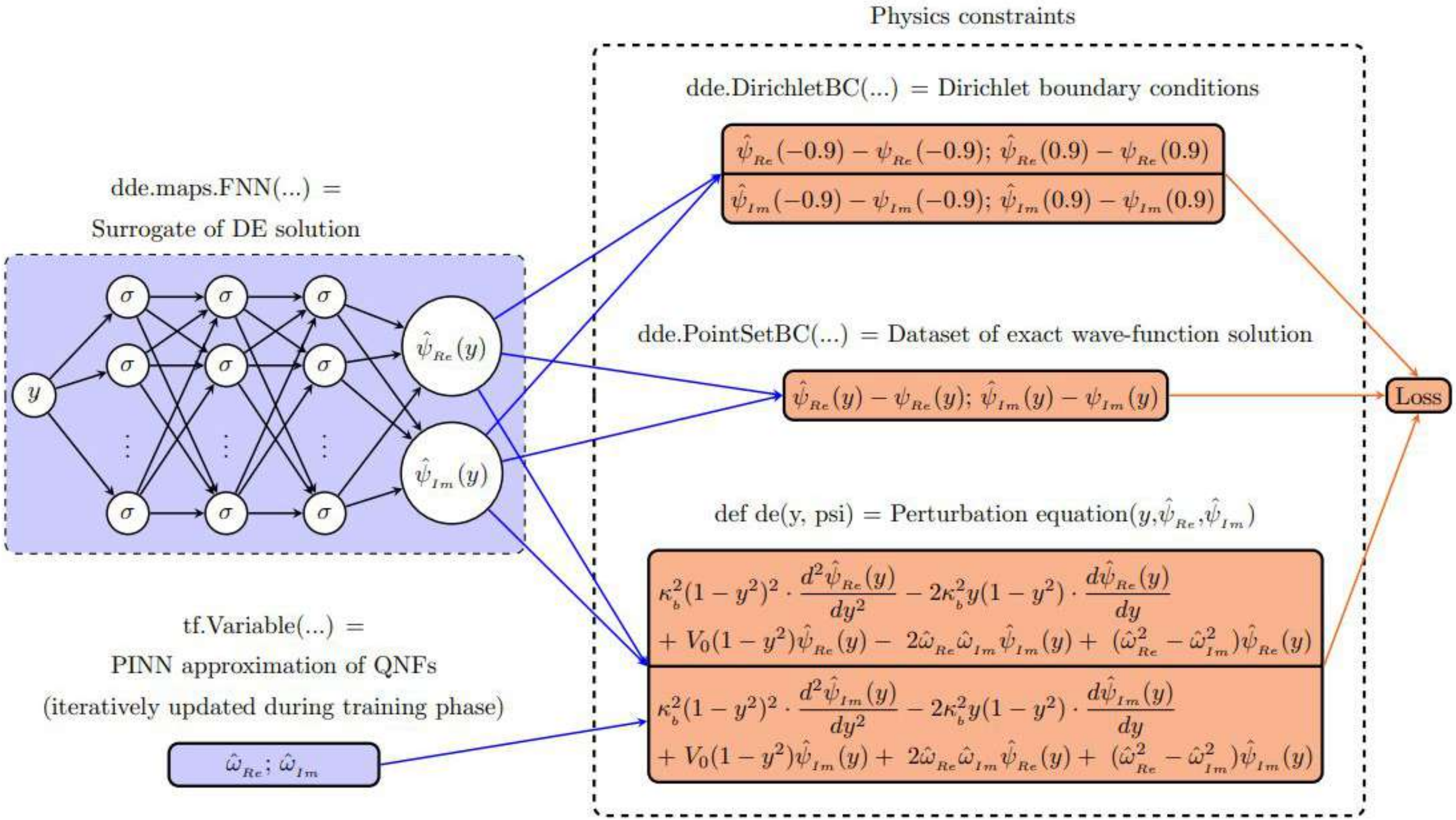
$$(1-y^2)^2\frac{d^2\psi(y)}{dy^2} - 2y(1-y^2)\frac{d\psi(y)}{dy} + \left[\omega^2 - \frac{1}{2}(1-y^2)\right]\psi(y) = 0.$$

...with solutions:

$$\psi_n = (1-y^2)^{-\frac{i+1}{4}}\chi_n\left(y\sqrt{1-y^2}\right)$$

$$\omega_n = \pm\frac{1}{2} - i(n+\frac{1}{2}),$$

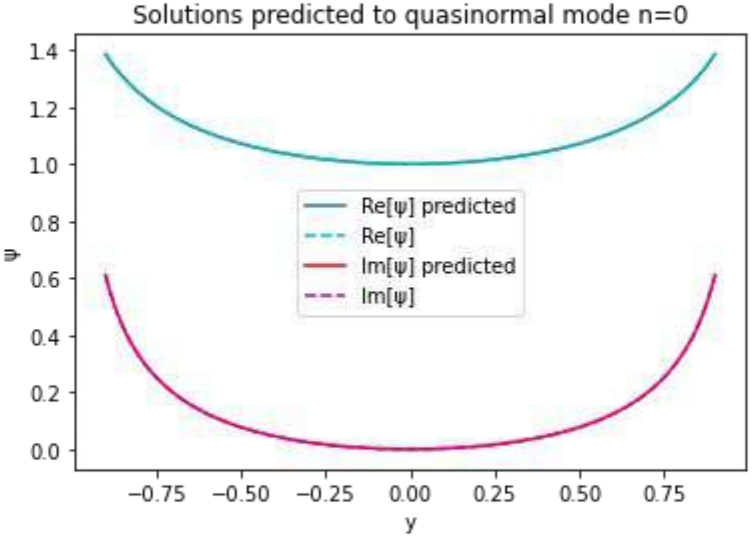
# Let's go to the code…



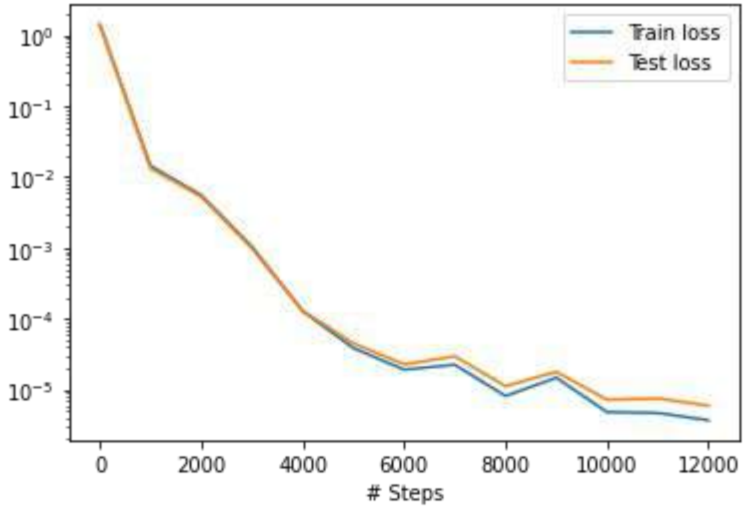
# Results

| Our PINN Aproximación | | | |
|---|---|---|---|
| $n$ | $\omega_{exact}$ | $\omega_{predict}$ | MSE |
| 0 | 0.5000 -$i$0.5000 | 0.4999 -$i$0.4997 | 0.0003- $i$0.0002 |
| 1 | 0.5000 -$i$1.5000 | 0.4985 -$i$1.4971 | 0.0029 - $i$0.0017 |
| 2 | 0.5000 -$i$2.5000 | 0.4931 -$i$2.4908 | 0.0097 - $i$0.0038 |
| 3 | 0.5000 -$i$3.5000 | 0.5014 -$i$3.4564 | 0.0205 - $i$0.0121 |

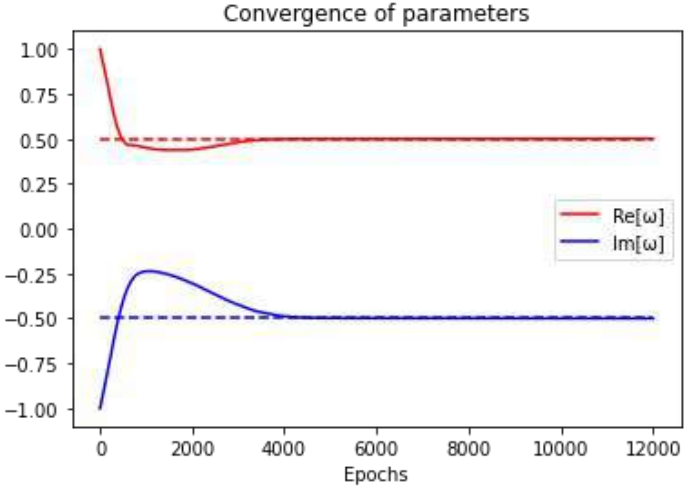
# *N = 0*



Solutions predicted to quasinormal mode n=0
Re[ψ] predicted
Re[ψ]
Im[ψ] predicted
Im[ψ]
ψ
y
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75

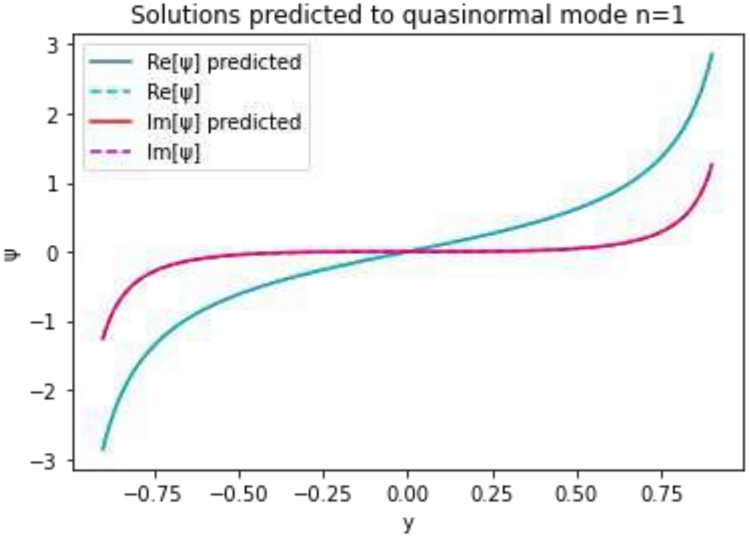



Train loss
Test loss
# Steps
0
2000
4000
6000
8000
10000
12000

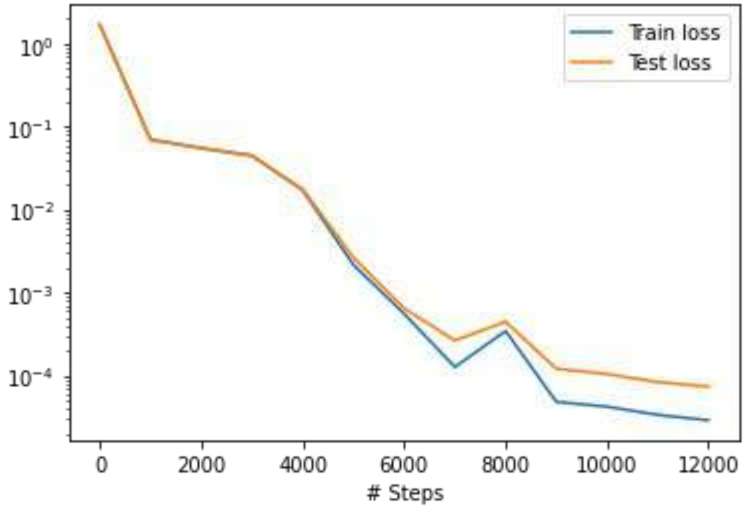



Convergence of parameters
Re[ω]
Im[ω]
Epochs
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
2000
4000
6000
8000
10000
12000

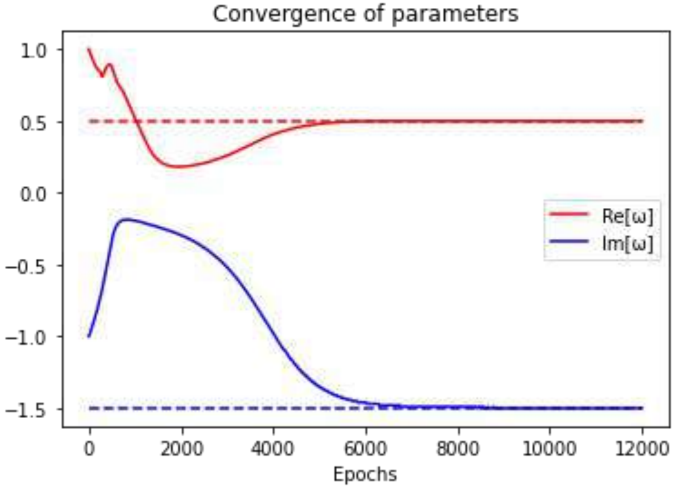
# N = 1



Solutions predicted to quasinormal mode n=1
Re[ψ] predicted
Re[ψ]
Im[ψ] predicted
Im[ψ]
ψ
y

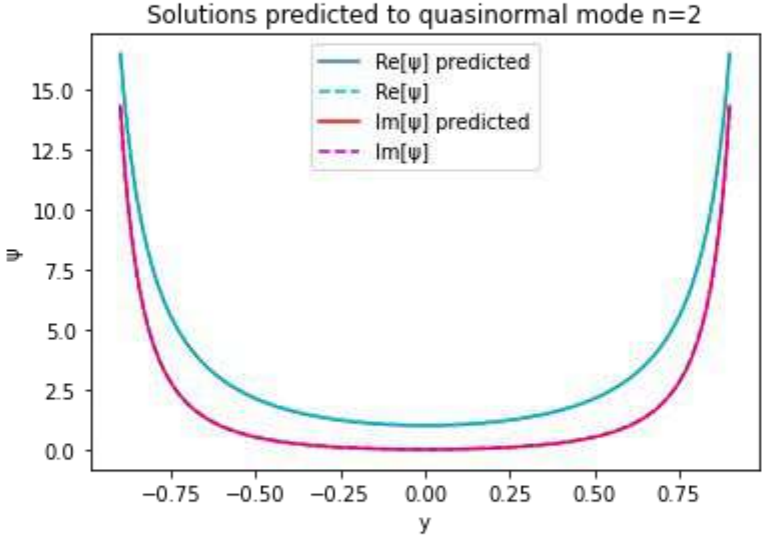



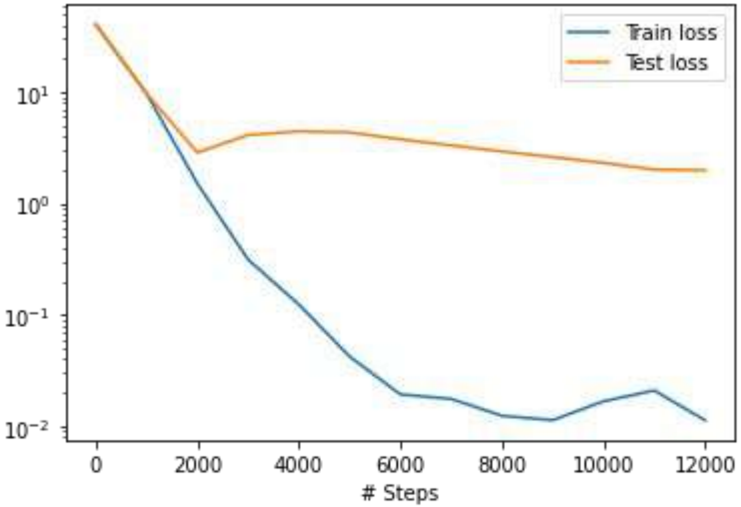
Train loss
Test loss
# Steps

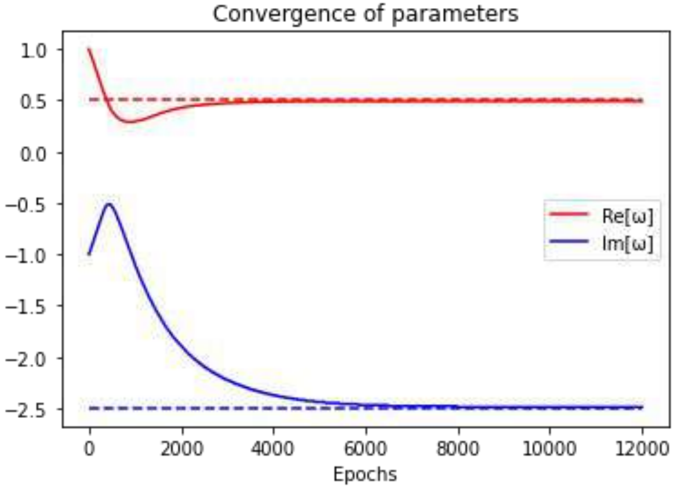



Convergence of parameters
Re[ω]
Im[ω]
Epochs

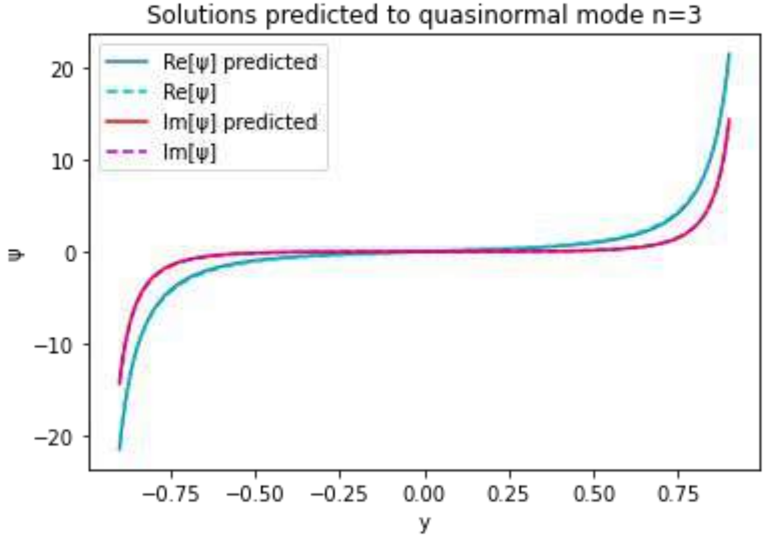
***N* = 2**


Solutions predicted to quasinormal mode n=2
Re[ψ] predicted
Re[ψ]
Im[ψ] predicted
Im[ψ]
ψ
y

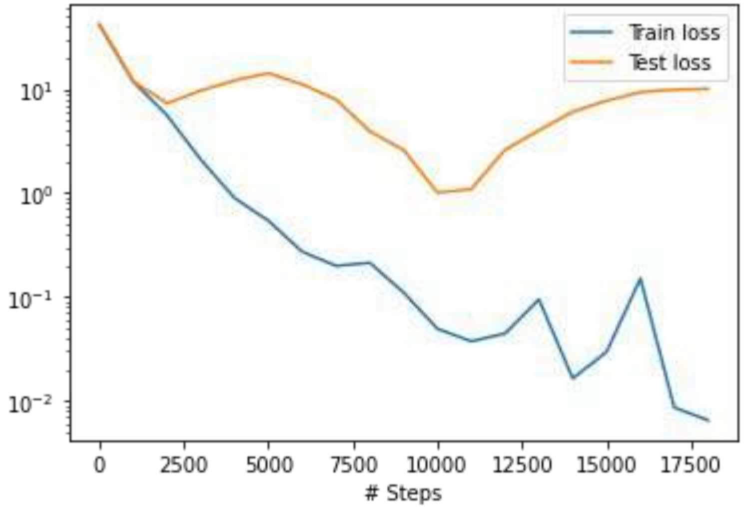

Train loss
Test loss
# Steps


Convergence of parameters
Re[ω]
Im[ω]
Epochs

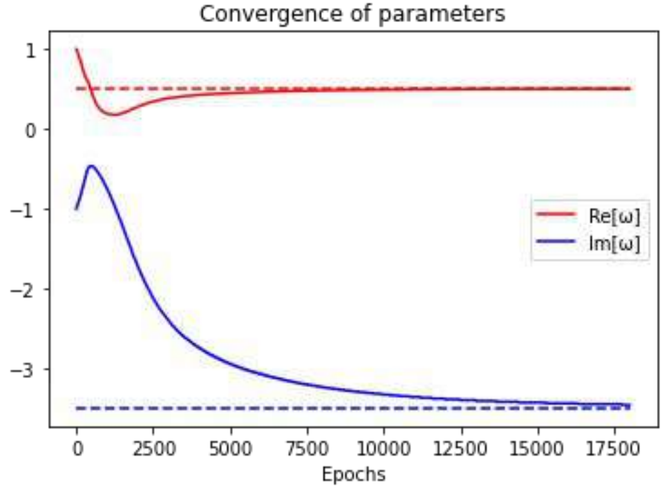
# *N = 3*



Solutions predicted to quasinormal mode n=3
Re[ψ] predicted
Re[ψ]
Im[ψ] predicted
Im[ψ]
ψ
y

Train loss
Test loss
# Steps

Convergence of parameters
Re[ω]
Im[ω]
Epochs

# Eigenvalue problem

An Eigenvalue problem is defined as:

- Given a linear operator, the eigenvalue problem asks to find a scalar value λ and a non-zero vector v such that applying the operator to v results in a scalar multiple of v:

In the context of **quantum mechanics**

$$\hat{H}\psi(x) = E\psi(x)$$

Wave functions **orthogonal to each other** and **normalizable.**

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

# Methods for solving eigenvalue problems

Change the loss **function!!**

$$\mathcal{F}_3(\mathbf{u},(x,\theta_u)) = \sum_{i=1}^{M}\left(\alpha\|\mathcal{T}u_i\|_2^2 + \mu\|\mathcal{T}u_i\|_\infty + \delta\|u_i - u_0\|_{1,\partial\Omega} + \beta\left|\|u_i\|_2^2 - c\right| + \gamma_i\|R(u_i)\|_2^2\right) + \rho\|\theta_u\|_2^2 + \nu\sum_{i<j}\langle u_i, u_j\rangle,$$

with $\boxed{\mathcal{T}u := \mathcal{L}u + \lambda u}$

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$$\mathrm{Error}(\boldsymbol{p},\boldsymbol{\lambda}) = \frac{\sum_i[H\Psi_t(\boldsymbol{r}_i,\boldsymbol{p},\boldsymbol{\lambda}) - \epsilon\Psi_t(\boldsymbol{r}_i,\boldsymbol{p},\boldsymbol{\lambda})]^2}{\int|\Psi_t|^2 d\boldsymbol{r}}$$

$$\epsilon = \frac{\int\Psi_t^{\star}H\Psi_t\, d\boldsymbol{r}}{\int|\Psi_t|^2\, d\boldsymbol{r}}$$

**Use special parametrization**

$$\begin{aligned}|\Psi_t\rangle &= (1 - |\Psi_0\rangle\langle\Psi_0|)(1 - |\Psi_1\rangle\langle\Psi_1|)\ldots(1 - |\Psi_k\rangle\langle\Psi_k|)|\tilde{\Psi}_t\rangle\\ &= (1 - |\Psi_0\rangle\langle\Psi_0| - |\Psi_1\rangle\langle\Psi_1|\ldots - |\Psi_k\rangle\langle\Psi_k|)|\tilde{\Psi}_t\rangle.\end{aligned}$$

# But…

$$\phi(\omega, x) \propto e^{+i\omega x} \qquad (x \to +\infty)$$
$$\phi(\omega, x) \propto e^{-i\omega x} \qquad (x \to -\infty)$$

$$\boxed{\phi(\omega, x) \propto e^{+i\omega |x|} \qquad (x \to \pm\infty)\,.}$$

… we need another method.

# Loss function

**Unsupervised Neural Networks for Quantum Eigenvalue Problems**


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$$\mathcal{L}(\theta;\mathcal{T}) = w_f\mathcal{L}_f(\theta;\mathcal{T}_f) + w_b\mathcal{L}_b(\theta;\mathcal{T}_b) + w_r\mathcal{L}_r(\theta;\mathcal{T}_r)$$

$$\boxed{L_{\text{reg}} = \nu_f L_f + \nu_\lambda L_\lambda + \nu_{\text{drive}} L_{\text{drive}}}$$

Where:

$$L_f = \frac{1}{f(x,\lambda)^2},$$

Non-trivial **eigenfunction**

$$L_\lambda = \frac{1}{\lambda^2},$$

Non-trivial **eigenvalue**

$$L_{\text{drive}} = e^{-\lambda + c}.$$

Explores **different eigenvalues**

# Example: Infinite potential well

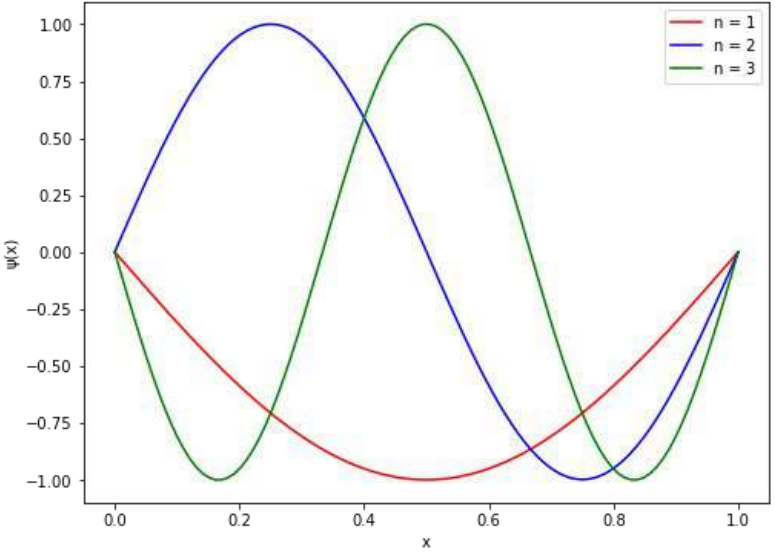
$$V(x) = \begin{cases} 0 & 0 \le x \le \ell \\ \infty & \text{otherwise} \end{cases}$$

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

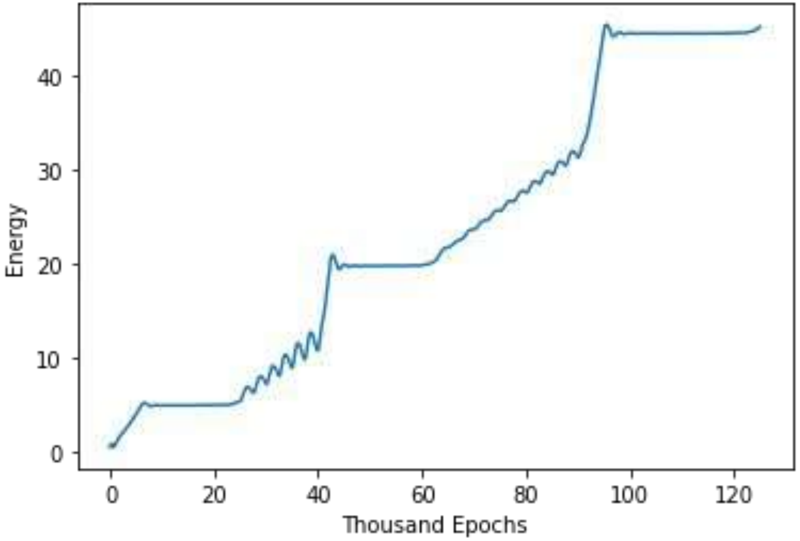
**Analytic Solutions:**

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

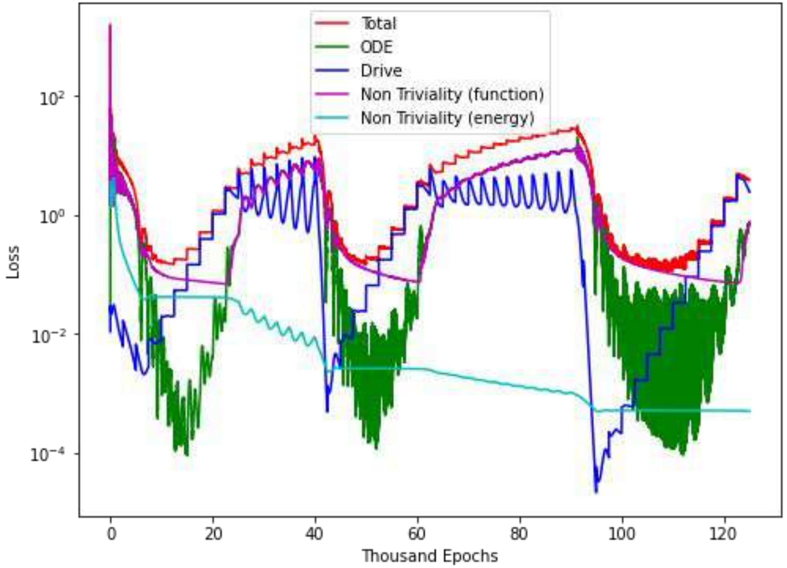
$$E_n = \frac{n^2\pi^2}{2},$$



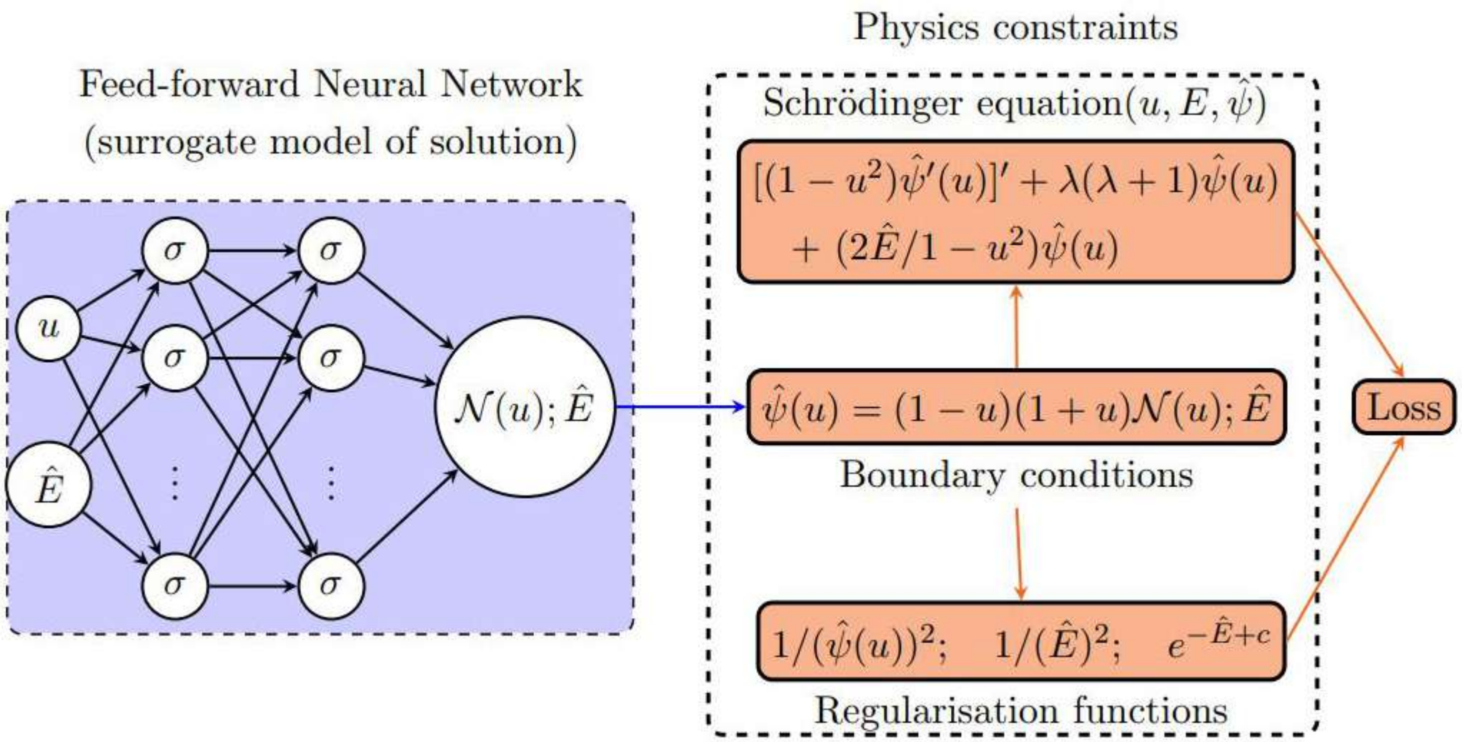
# Eigenvalues




# Cost function



# Let's go to the code…



# Asymptotically Flat Schwarzschild BH

Here:

$$\boxed{f(r) = 1 - \frac{2M}{r}} \quad \Rightarrow \quad x(r) = r + 2M \ln\left(\frac{r}{2M} - 1\right)$$

Instead, we will use the coordinates:

$$\xi = 1 - \frac{2M}{r} \quad / \quad 0 \leq \xi < 1$$

Which lead to:

$$\boxed{\frac{d^2\psi}{d\xi^2} + \frac{1-3\xi}{\xi(1-\xi)}\frac{d\psi}{d\xi} + \left[\frac{4M^2\omega^2}{\xi^2(1-\xi)^4} - \frac{\ell(\ell+1)}{\xi(1-\xi)^2} - \frac{1-s^2}{\xi(1-\xi)}\right]\psi = 0\,.}$$

And we will use the **ansatz:**

$$\psi(\xi) = \xi^{-2iM\omega}(1-\xi)^{-2iM\omega}e^{\frac{2iM\omega}{1-\xi}}\chi(\xi)$$

So the real problem becomes:

$$\chi'' = \lambda_0(\xi)\chi' + s_0(\xi)\chi \; ,$$

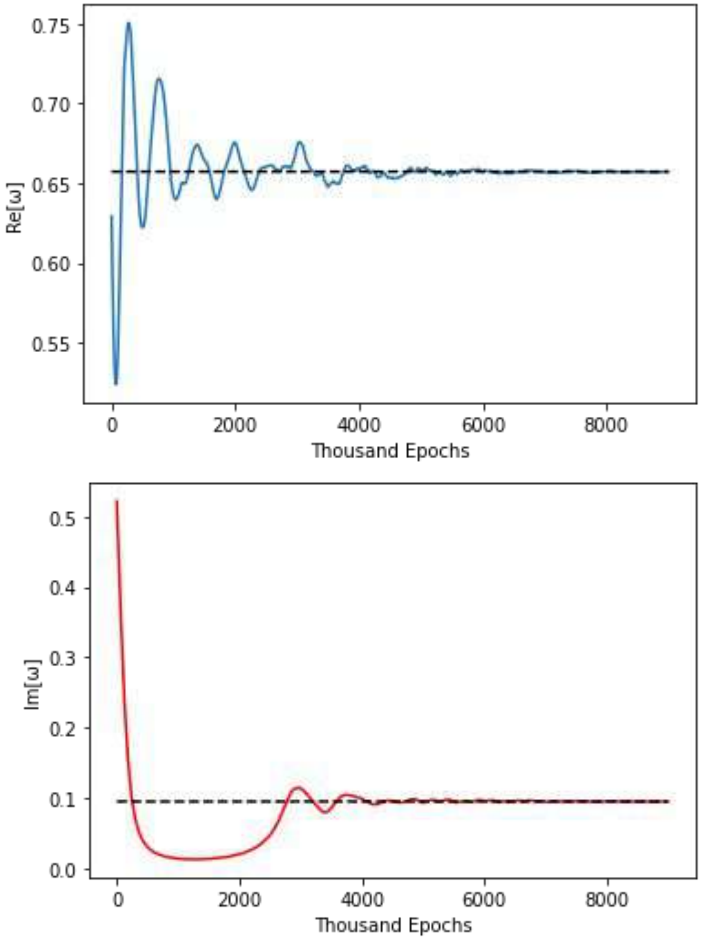
$$\lambda_0(\xi) = \frac{4Mi\omega(2\xi^2 - 4\xi + 1) - (1-3\xi)(1-\xi)}{\xi(1-\xi)^2} \; ,$$

$$s_0(\xi) = \frac{16M^2\omega^2(\xi - 2) - 8Mi\omega(1-\xi) + \ell(\ell+1) + (1-s^2)(1-\xi)}{\xi(1-\xi)^2}$$

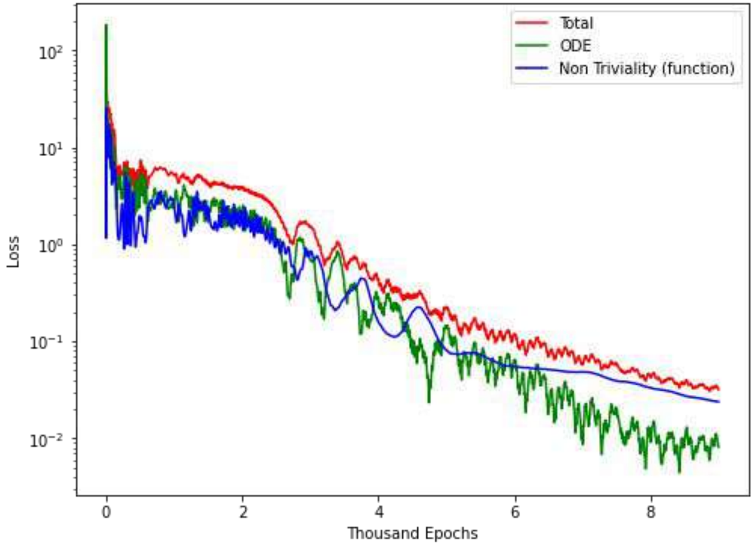
# Results

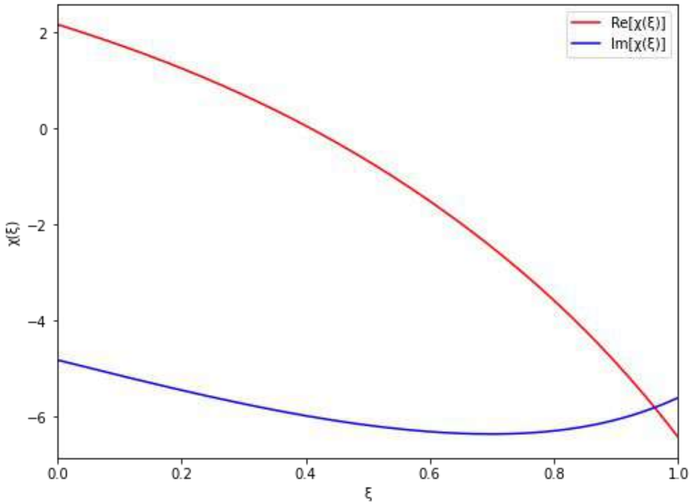
| $s$ | $l$ | $\omega$ solver | $\omega$ 6th order WKB |
|---|---|---|---|
| 0 | 0 | 0.0004 -$i$0.3456 | 0.1105 -$i$0.1008 |
| 0 | 1 | 0.2933 -$i$0.0977 | 0.2929 -$i$0.0978 |
| 0 | 2 | 0.4839 -$i$0.0966 | 0.4836 -$i$0.0968 |
| 1 | 1 | 0.2487 -$i$0.0922 | 0.2482 -$i$0.0926 |
| 1 | 2 | 0.4581 -$i$0.0949 | 0.4576 -$i$0.0950 |
| 1 | 3 | 0.6571 -$i$0.0953 | 0.6569 -$i$0.0956 |
| 2 | 2 | 0.3741 -$i$0.0889 | 0.3736 -$i$0.0890 |
| 2 | 3 | 0.6001 -$i$0.0929 | 0.5994 -$i$0.0927 |
| 2 | 4 | 0.8097 -$i$0.0942 | 0.8092 -$i$0.0942 |

## Frequencies

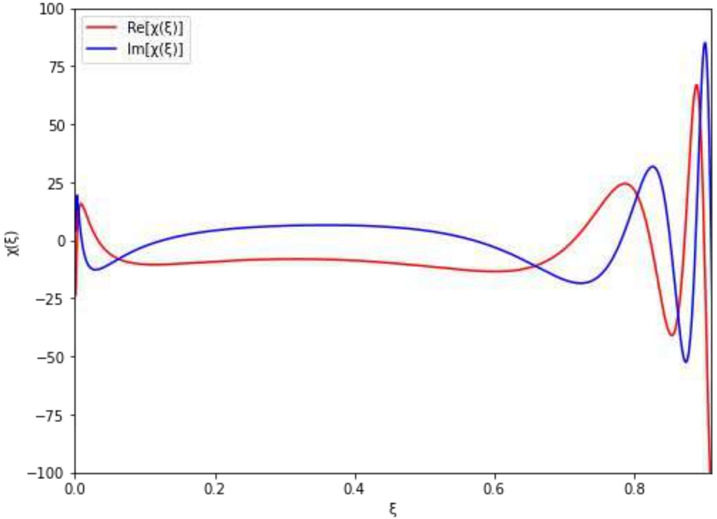



## Loss function

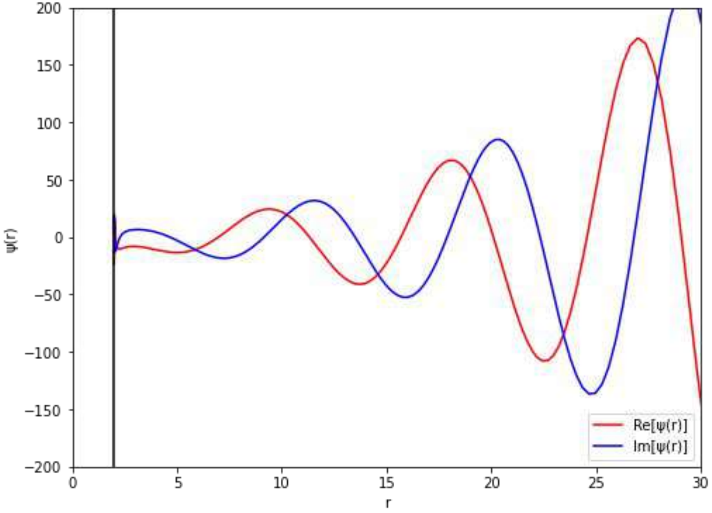





Parametrization




**<u>The physical radial coordinate</u>**




***s = 1, l = 3***

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