Physics-Informed Neural Networks

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Outline

- Learning Goals
- Physics informed neural networks
  - What are they?
  - Why are they useful?
  - How do we implement them?
  - What are some of the challenges of using them?
- Summary

Learning Goals

- Understand what a physics-informed neural network (PINN) is
- Discuss PINN applications and where they are advantageous
- Learn how to develop a PINN
- Discuss some of the challenges in PINN research

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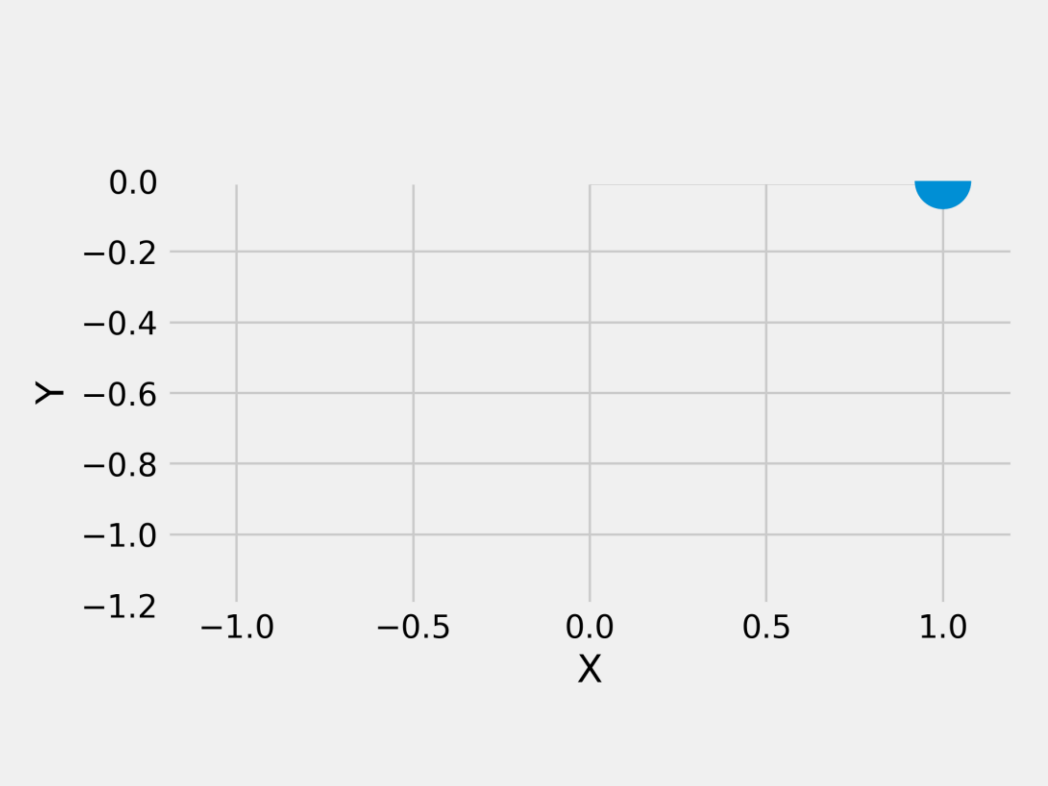
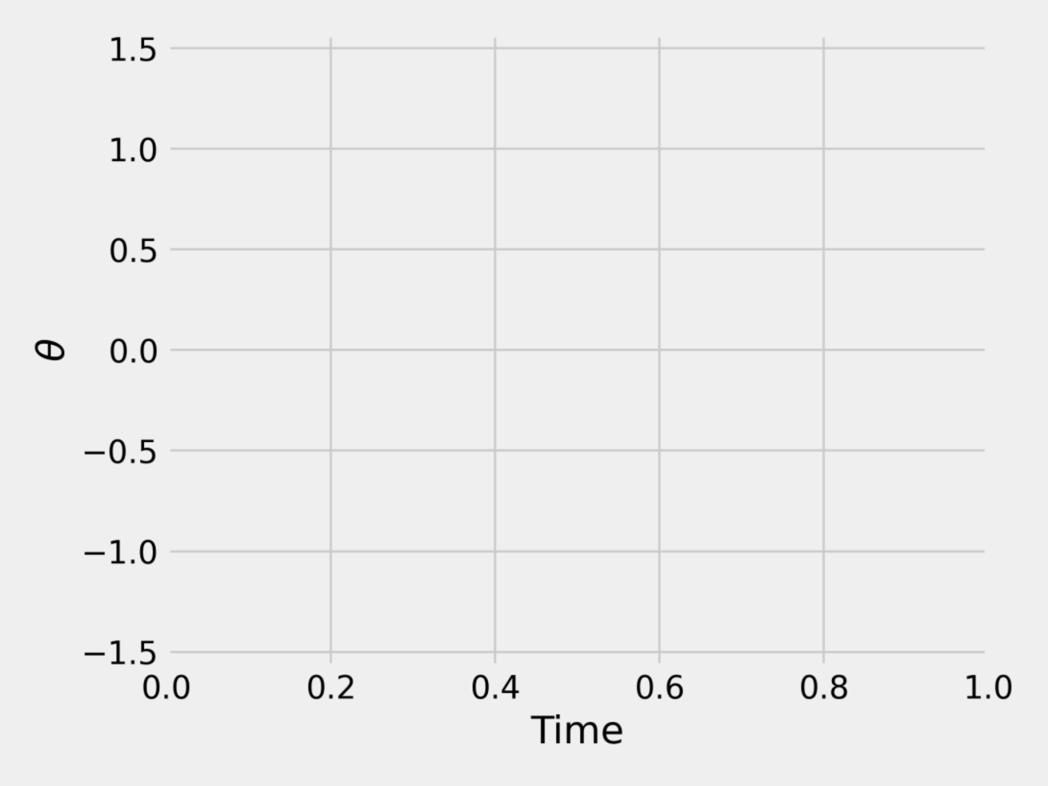
Setting the stage

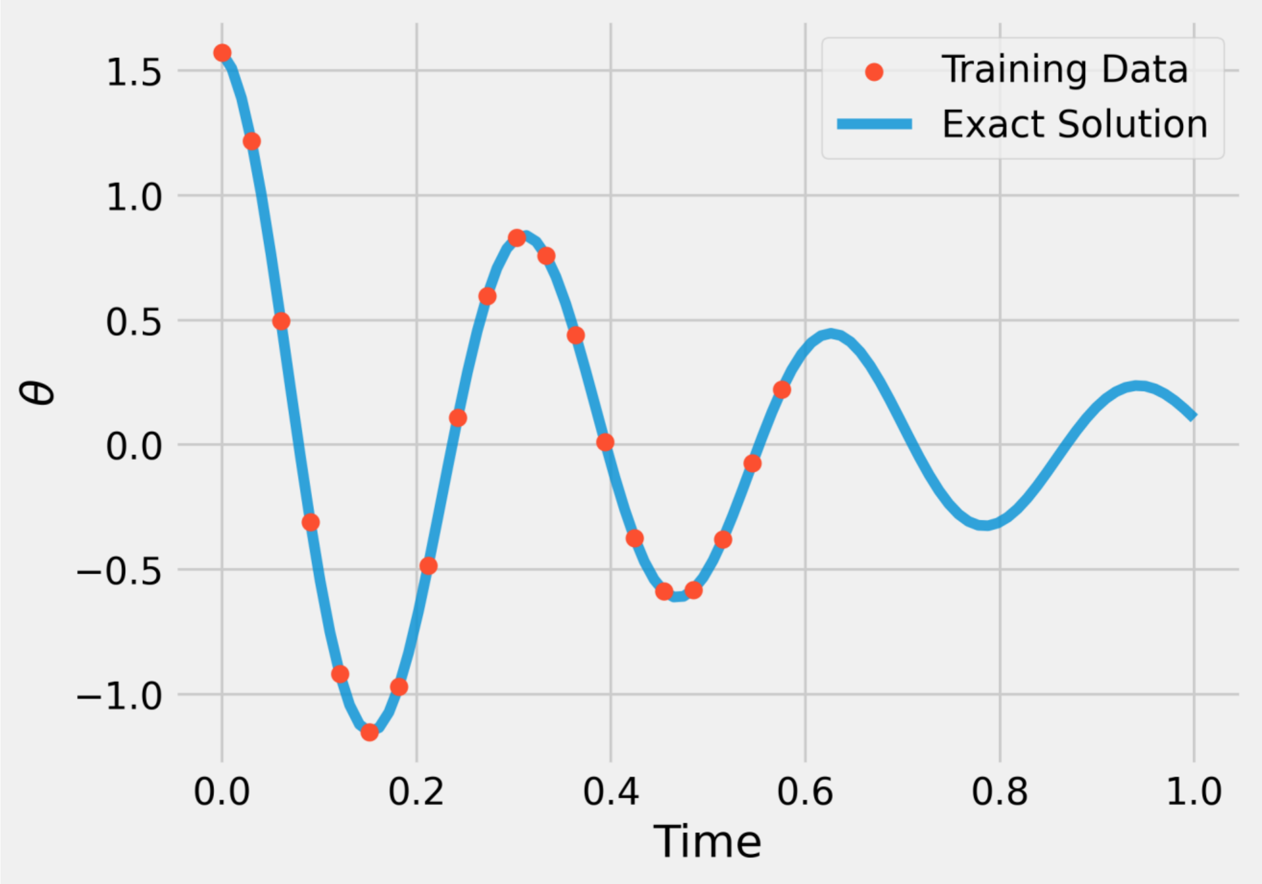
- Consider the damped pendulum





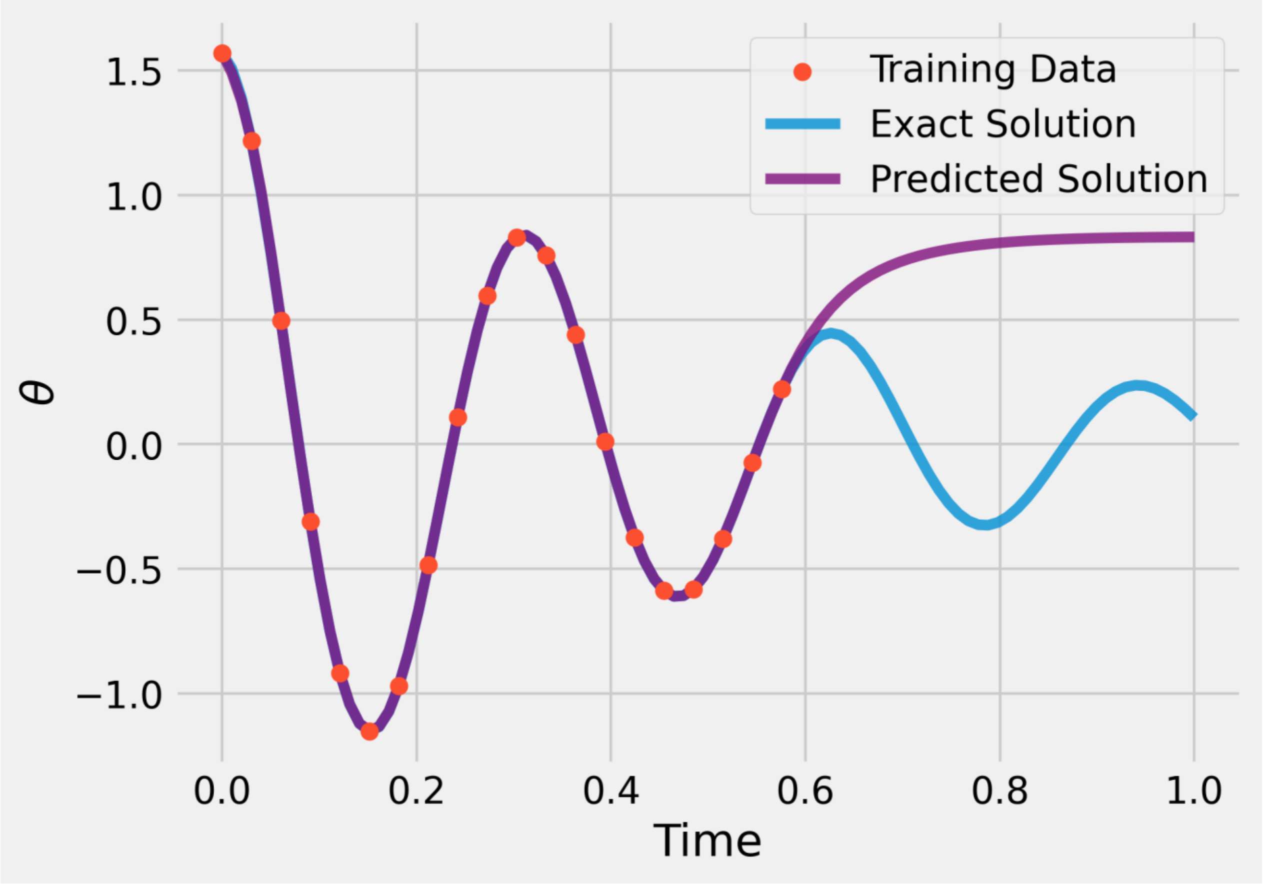
Setting the stage

$$\mathrm{MSE} = \frac{1}{N}\sum_{i}^{N}\left|\theta_{PINN}\left(t^{i}\right) - \theta_{\mathrm{data}}^{i}\right|^{2}$$



Setting the stage

$$\text{MSE} = \frac{1}{N}\sum_{i}^{N}\left|\theta_{PINN}(t^i) - \theta^i_{\text{data}}\right|^2$$



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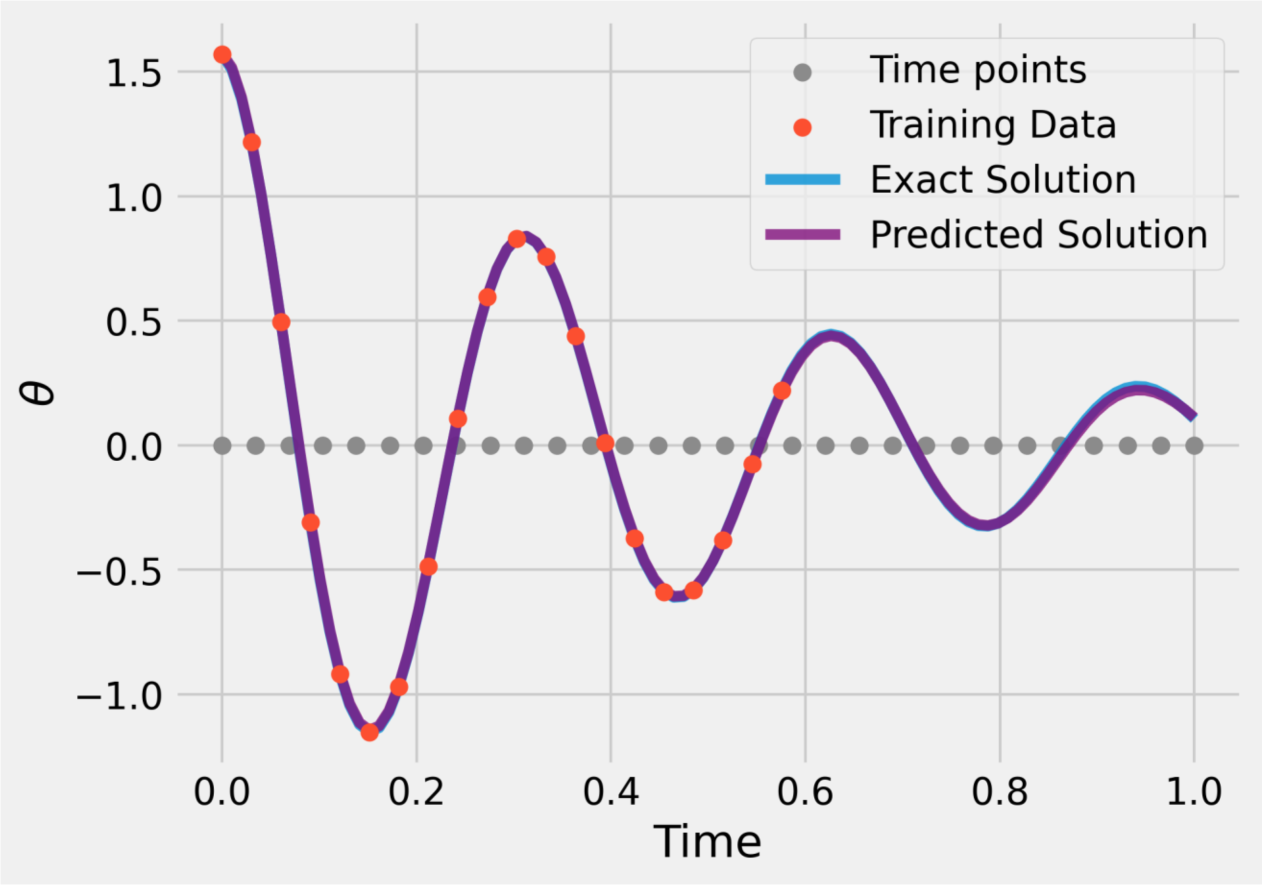
Setting the stage

- We know something about this system that can help us!

$$\frac{d^2\theta}{dt^2} + \lambda \frac{d\theta}{dt} + \omega^2\theta = 0$$

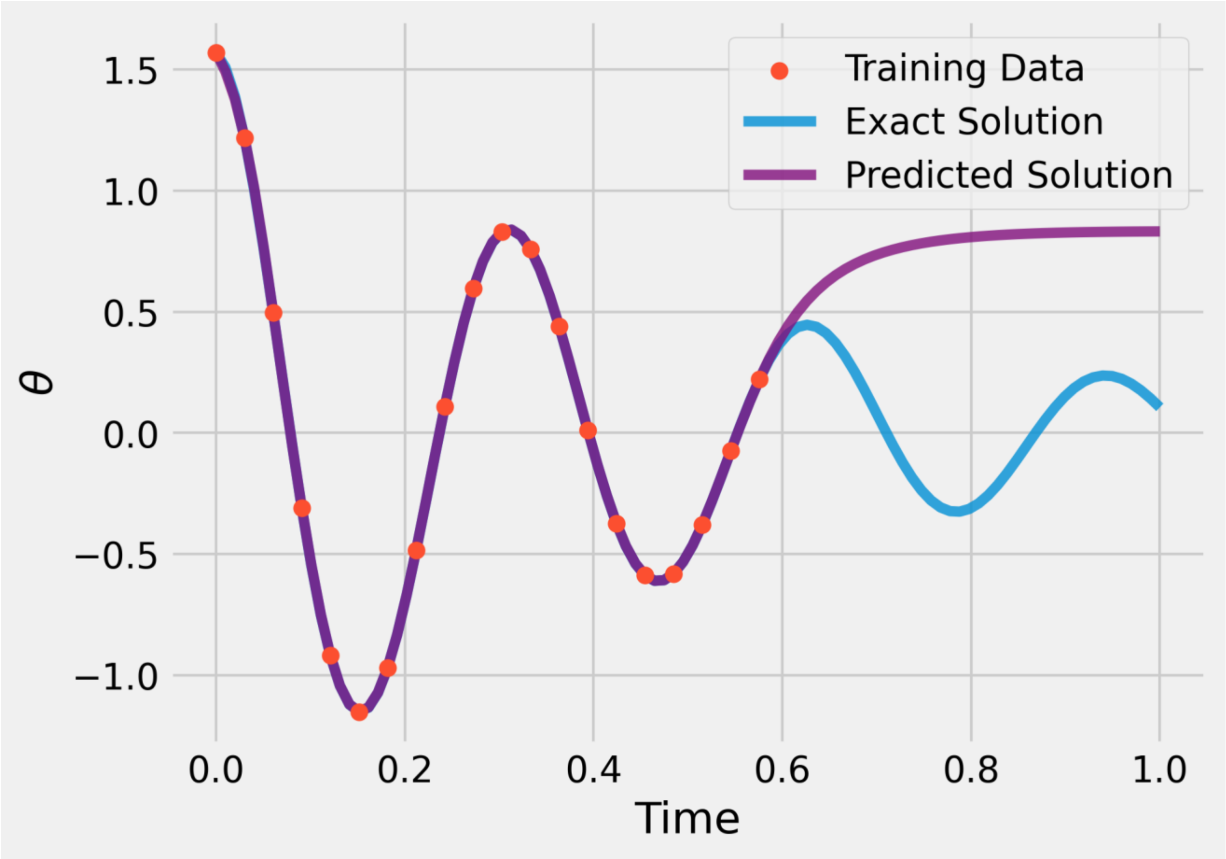
$$\frac{d\theta}{dt}(0) = 0$$

$$\theta(0) = \frac{\pi}{2}$$

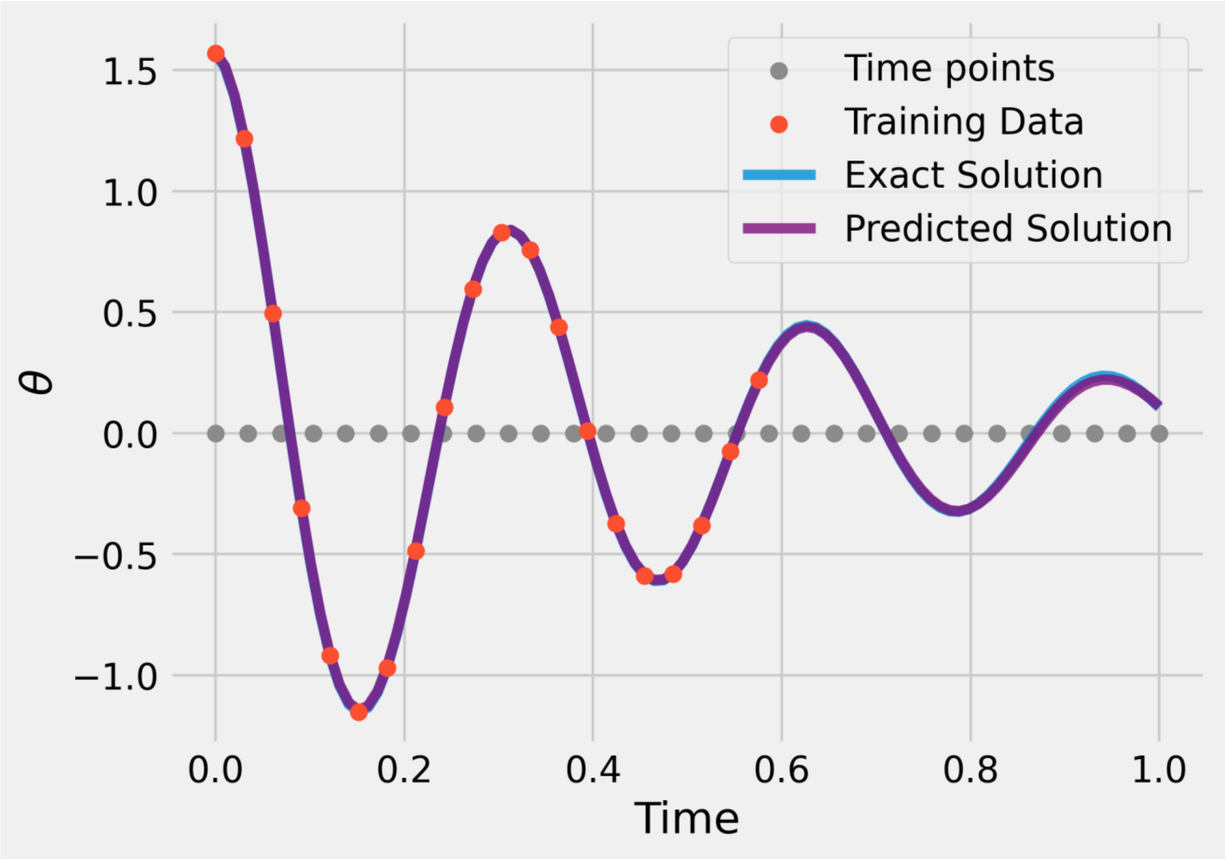


Setting the stage

Supervised Neural Network



Physics Informed Neural Network



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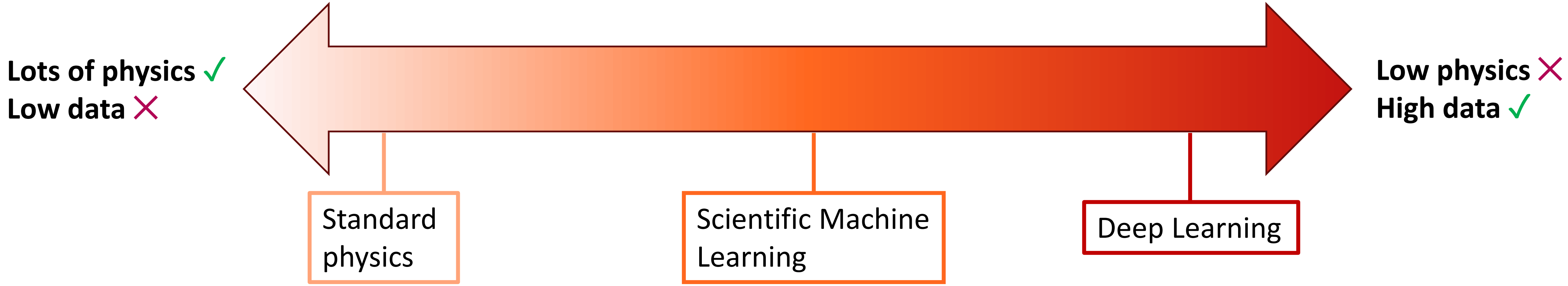
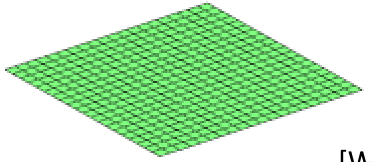
So what IS a Physics Informed Neural Network?

- **Physics Informed Neural Network (PINN):** NNs that are trained to respect the physical laws given by a differential equation
- PINNs fall under the category of ‘Scientific Machine Learning’



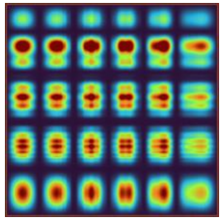
So what IS a Physics Informed Neural Network?

Wave equation: $\frac{\partial^2 u}{\partial t^2} = c^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)$

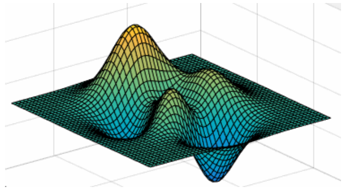


[Wikipedia.org]

Schrödinger equation: $i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi$



Heat equation: $\frac{\partial u}{\partial t} = c^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)$

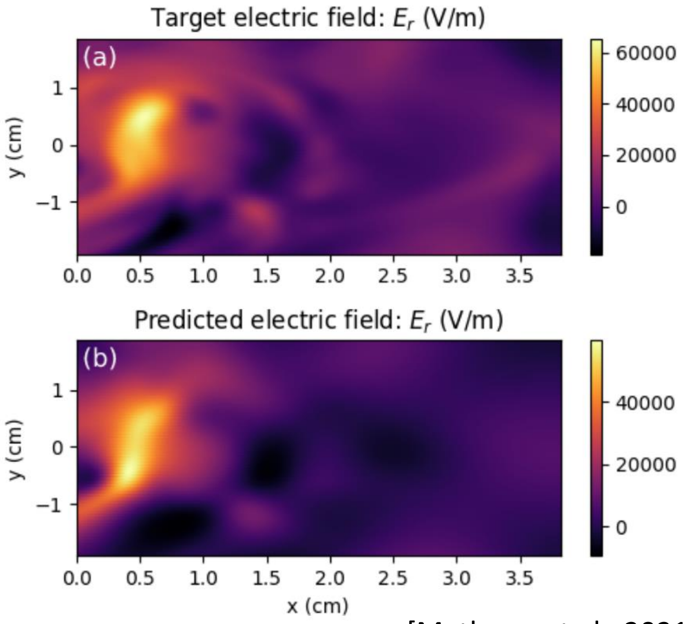


[mathworks.com]

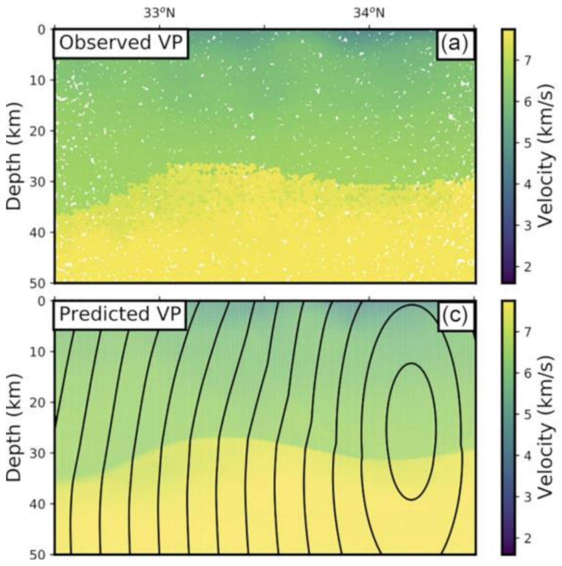
- Differential equations (DEs) means we have derivatives (or gradients)
- Deep learning frameworks are great at computing gradients!

Applications

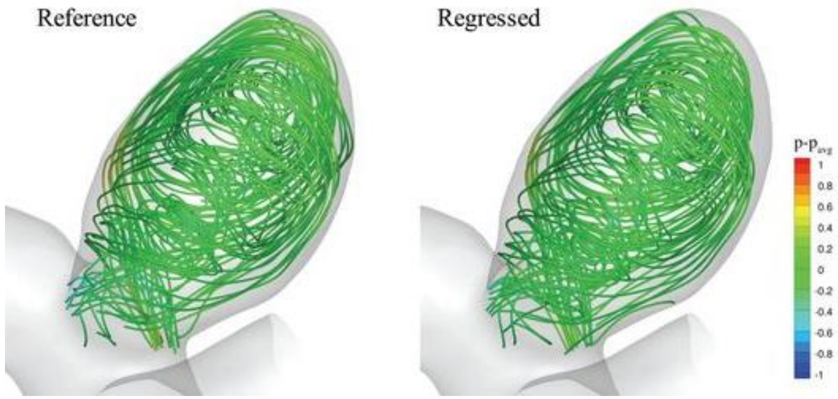
- PINNs can be useful in similar scenarios as finite element analysis
  - Plasma dynamics
  - Hemodynamics
  - Geoscience
  - …and more!
- Unlike FEA, PINNs are mesh-free
- Can be extended to equation discovery
- Work well in regimes with some noisy data and some physics



[Mathews et al., 2021]



[Smith et al., 2022]



[Raissi et al., 2020]

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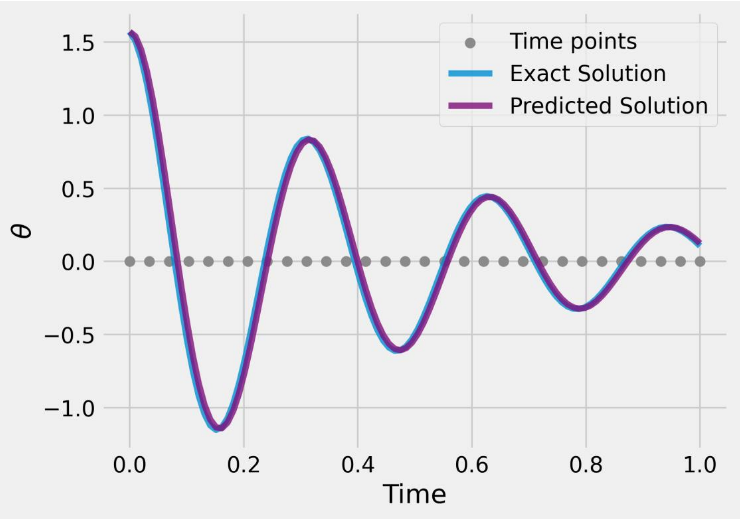
Two main tasks

Solutions of DEs

- Given a governing equation, what is the solution?



Discovery of DEs

- Given some noisy data, what is the governing equation?

$$\frac{d^2\theta}{dt^2} + \lambda\frac{d\theta}{dt} + \omega^2\theta = 0$$

What are these values?!

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DE solution

Given the following:

$$\frac{d^2\theta}{dt^2} + \lambda \frac{d\theta}{dt} + \omega^2\theta = 0$$

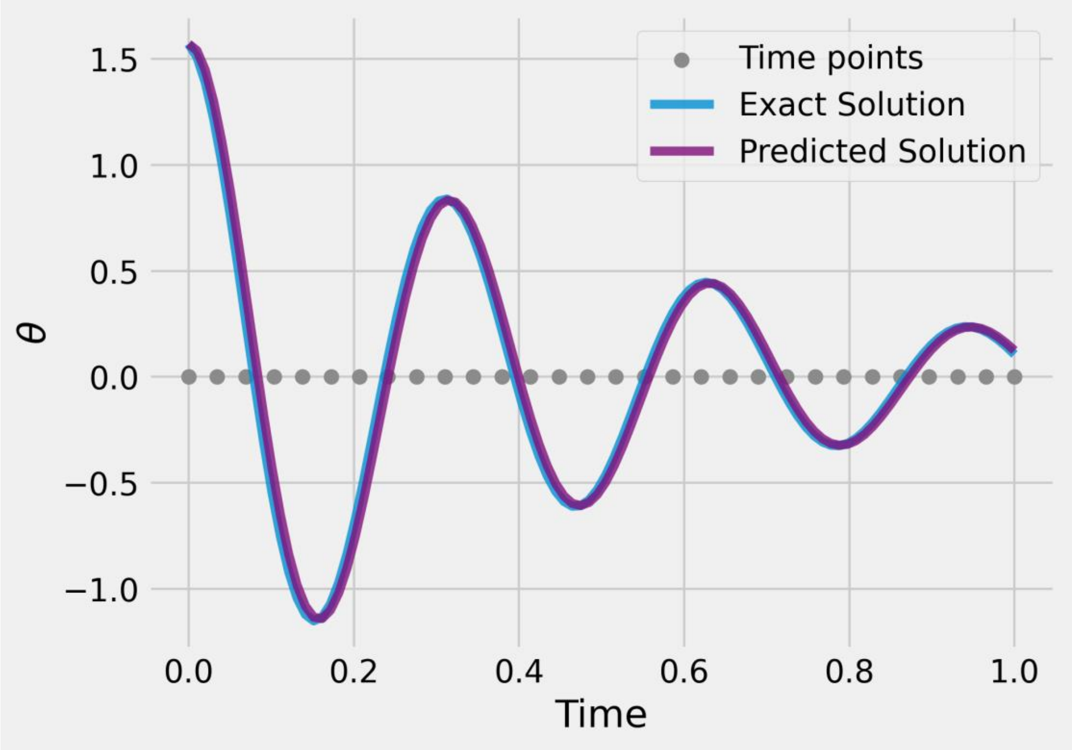
DE

$$\frac{d\theta}{dt}(0) = 0$$

$$\theta(0) = \frac{\pi}{2}$$

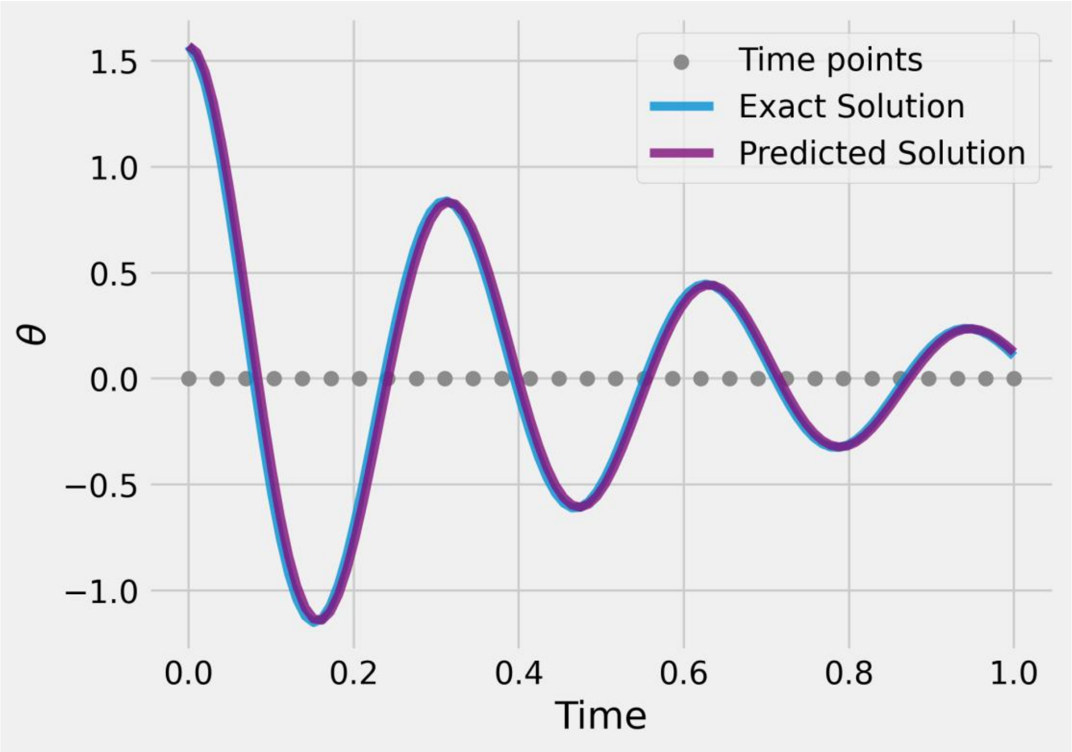
Boundary conditions

…what is $\theta(t)$?



DE solution

- We will need to choose some points to evaluate our DE at
  - A.k.a. 'collocation points'
- Define t_{col} to evaluate the DE, and t_{BC} to evaluate the boundary conditions
  - **Note:** We can have collocation points in other dimensions as well! For example: spatial dimensions
- **Question:** What are some ways we could choose collocation points?



DE solution

- We can incorporate the constraints into our loss function
- We end up wanting to minimize the following terms:
  - $\frac{d^2\theta_{PINN}}{dt^2}(t_{\mathrm{col}}) + \lambda \frac{d\theta_{PINN}}{dt}(t_{\mathrm{col}}) + \omega^2\theta_{PINN}(t_{\mathrm{col}})$ **(Physics term)**
  - $\frac{d\theta_{PINN}}{dt}(t_{\mathrm{BC}}) - \frac{d\theta_{\mathrm{BC}}}{dt}$ **(BC 1 term)**
  - $\theta_{PINN}(t_{\mathrm{BC}}) - \theta_{\mathrm{BC}}$ **(BC 2 term)**
  - **Note:** If we have some data, we could also include a data term
- **Question:** How could we go about balancing these loss terms?

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DE solution

- Assuming we use MSE, and incorporating the specific boundary values, we get:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i}^{N}\left|\frac{d^2\theta_{PINN}}{dt^2}(t_{\mathrm{col}}^{i}) + \lambda\frac{d\theta_{PINN}}{dt}(t_{\mathrm{col}}^{i}) + \omega^2\theta_{PINN}(t_{\mathrm{col}}^{i})\right|^2 + \left|\frac{d\theta_{PINN}}{dt}(0)\right|^2 + \left|\theta_{PINN}(0) - \frac{\pi}{2}\right|^2$$

Question: Is this supervised or unsupervised training?

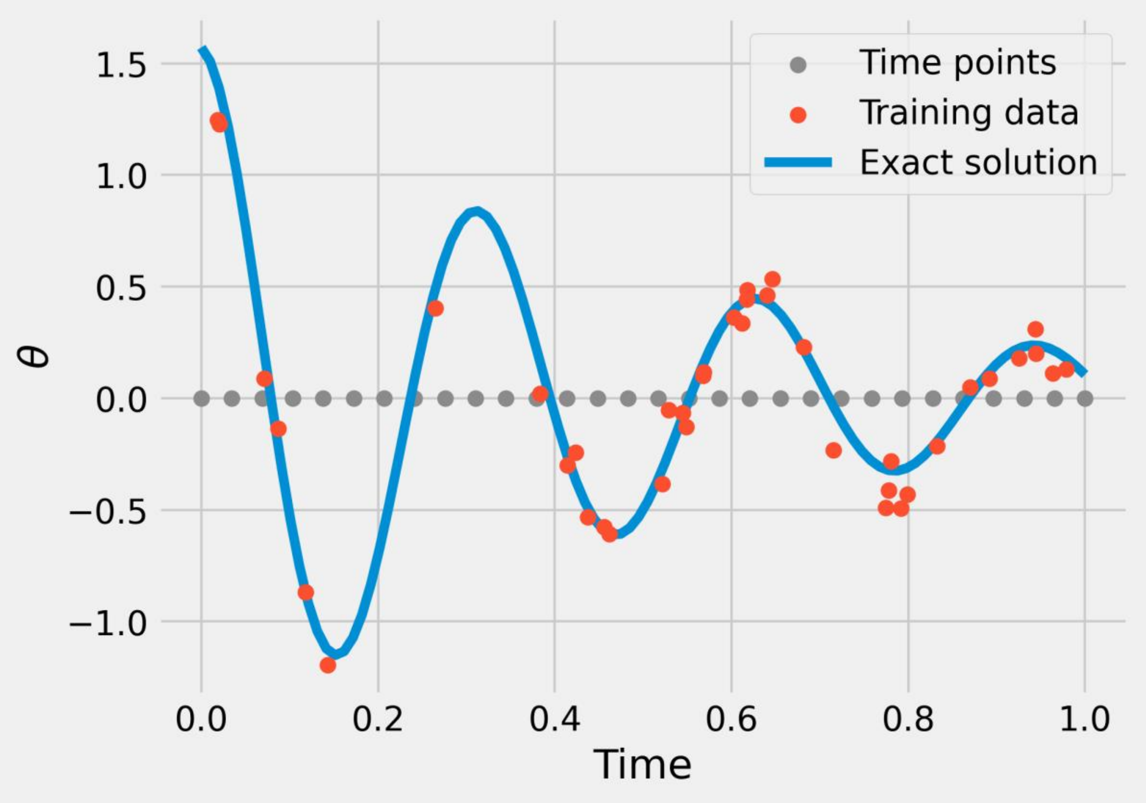
DE discovery

- Given some noisy data, what is the governing equation?

$$\frac{d^2\theta}{dt^2} + \lambda \frac{d\theta}{dt} + \omega^2\theta = 0$$

What is this value?

- Generally, this is a harder problem than the previous task



DE discovery

- Similar terms to finding DE solution
- We end up wanting to minimize the following terms:
  - $\frac{d^2\theta_{PINN}}{dt^2}(t_{\text{col}}) + \lambda\frac{d\theta_{PINN}}{dt}(t_{\text{col}}) + \omega^2\theta_{PINN}(t_{\text{col}})$ **(Physics term)**

    This is a trainable parameter!
  - $\theta_{PINN}(t_{\text{data}}) - \theta_{\text{data}}$ **(Data term)**
- **Question:** Why don't we have boundary condition terms anymore?

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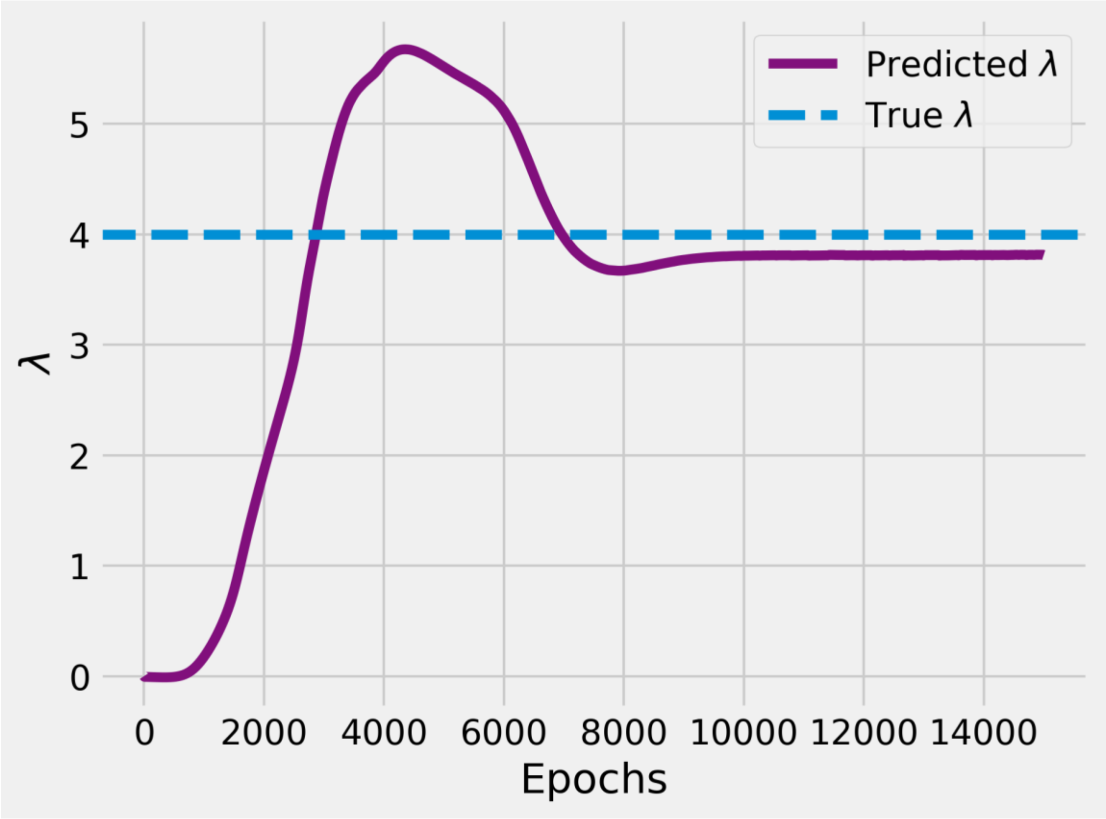
DE discovery

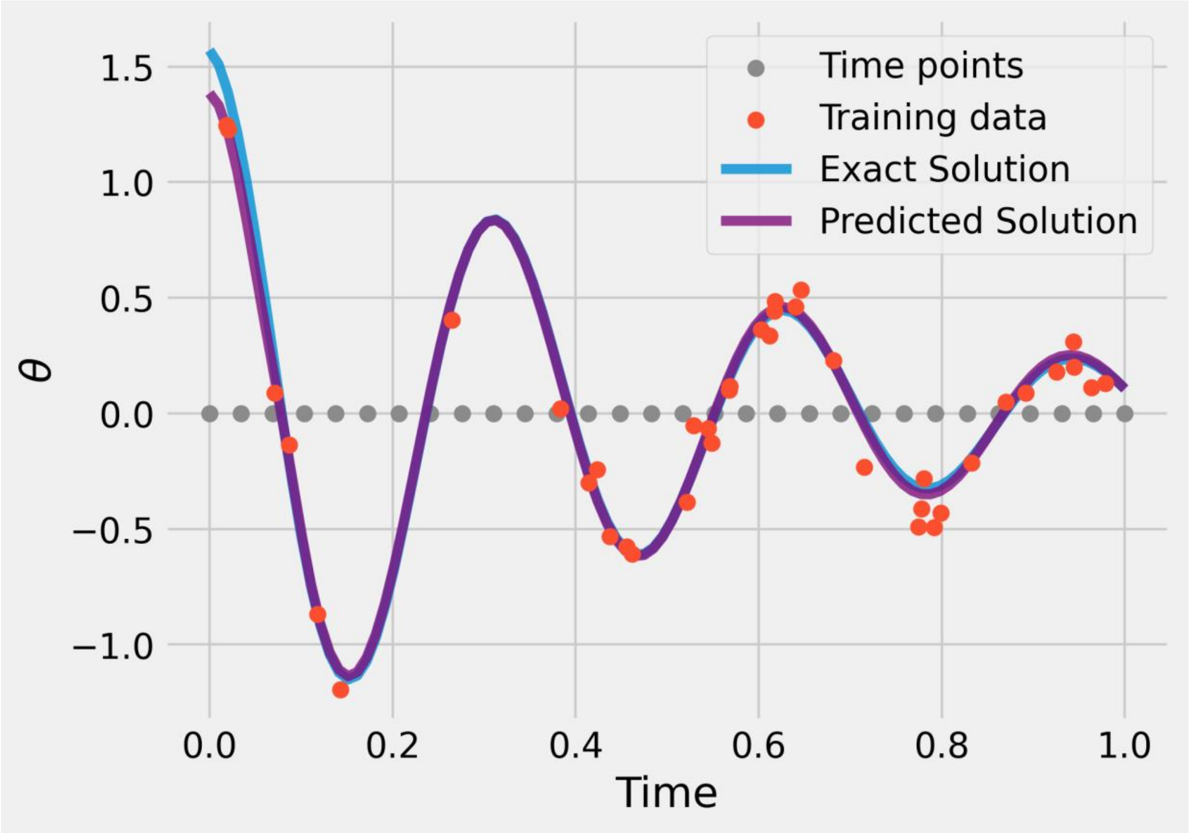
- Assuming we use MSE:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i}^{N}\left|\frac{d^2\theta_{PINN}}{dt^2}\left(t_{\mathrm{col}}^{i}\right) + \lambda\frac{d\theta_{PINN}}{dt}\left(t_{\mathrm{col}}^{i}\right) + \omega^2\theta_{PINN}\left(t_{\mathrm{col}}^{i}\right)\right|^2$$

$$+\frac{1}{M}\sum_{i}^{M}\left|\theta_{PINN}\left(t_{\mathrm{data}}^{j}\right) - \theta_{\mathrm{data}}^{j}\right|^2$$

DE discovery





Pop quiz ☺

Given the following, what is the correct MSE loss if we want to find the solution for u?

$$\frac{\partial u}{\partial t} = c^2\left(\frac{\partial^2 u}{\partial x^2}\right)$$

$$u(0,t) = 1$$

a) $\frac{1}{N}\sum_i^N \left|\frac{\partial u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial t} + c^2\left(\frac{\partial^2 u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial x^2}\right)\right|^2 + |u_{PINN}(0, t_{\text{BC}})|^2$

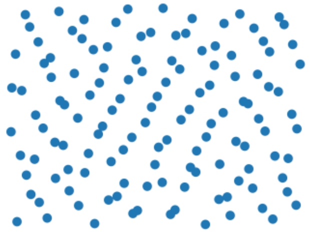
b) $\frac{1}{N}\sum_i^N \left|\frac{\partial u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial t} + c^2\left(\frac{\partial^2 u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial x^2}\right)\right|^2 + \frac{1}{M}\sum_i^M \left|u_{PINN}(0, t_{\text{BC}}^j)\right|^2$

c) $\frac{1}{N}\sum_i^N \left|\frac{\partial u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial t} - c^2\left(\frac{\partial^2 u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial x^2}\right)\right|^2 + \frac{1}{M}\sum_i^M \left|u_{PINN}(0, t_{\text{BC}}^j) + 1\right|^2$

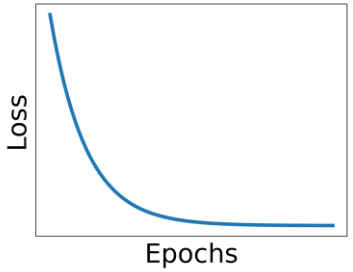
d) $\frac{1}{N}\sum_i^N \left|\frac{\partial u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial t} - c^2\left(\frac{\partial^2 u_{PINN}(x_{\text{col}}^i, t_{\text{col}}^i)}{\partial x^2}\right)\right|^2 + \frac{1}{M}\sum_i^M \left|u_{PINN}(0, t_{\text{BC}}^j) - 1\right|^2$

Questions in PINN research

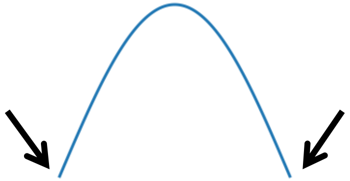
How do we choose collocation points?



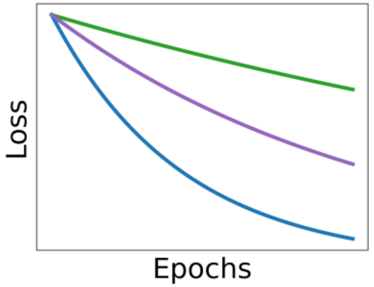
What are the convergence properties of PINNs?



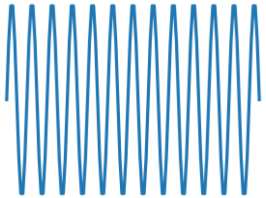
How do we enforce boundary conditions?



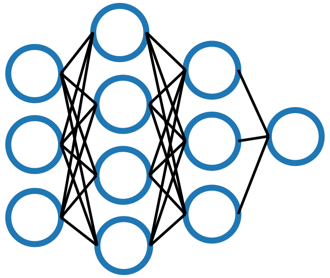
How do we handle competing loss objectives?



How do we handle high frequency solutions?



What architecture should we use?



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Summary

- PINNs incorporate physical constraints to train NNs and fall under the category of ‘Scientific machine learning’
- PINNs can be used to find solutions of DEs or even determine the DE itself
- They can be applied to many practical fields and can have some advantages over traditional numerical methods
- There are still open questions in PINN research making it an exciting and dynamic field!

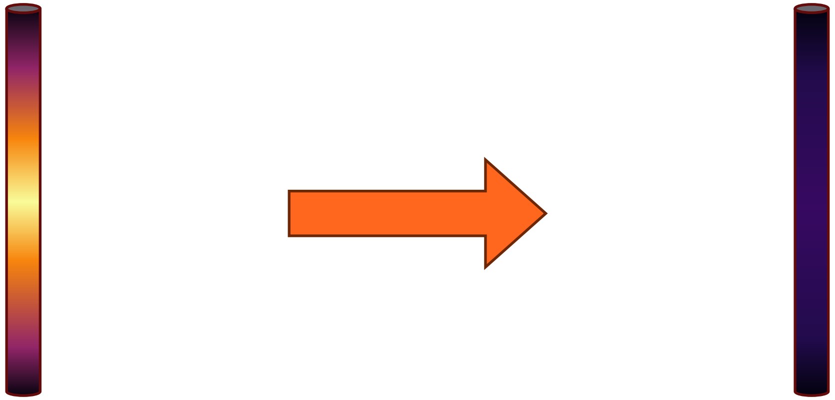
Next class:

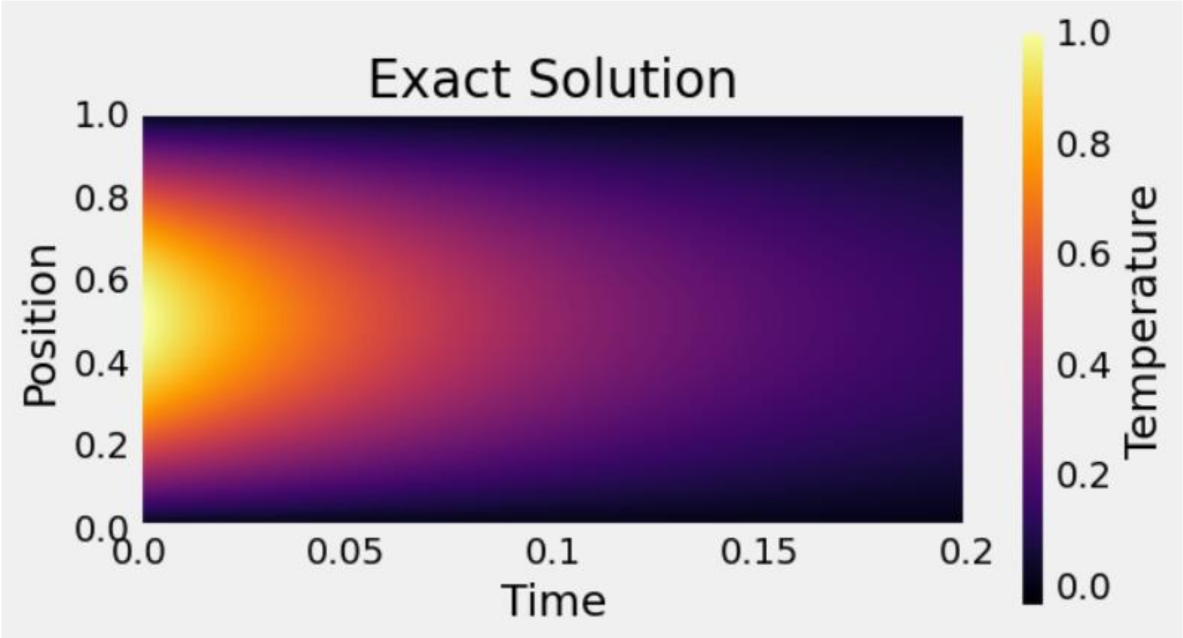
- Solving the following problem:

$$\frac{\partial u}{\partial t} = c^2\left(\frac{\partial^2 u}{\partial x^2}\right)$$

$$u(0,t) = u(1,t) = 0$$

$$u(x,0) = \sin(x)$$





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Thank you!

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