Deep Learning in Scientific Computing

PINNs – applications

Spring Semester 2023

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Ben Moseley

ETH zürich

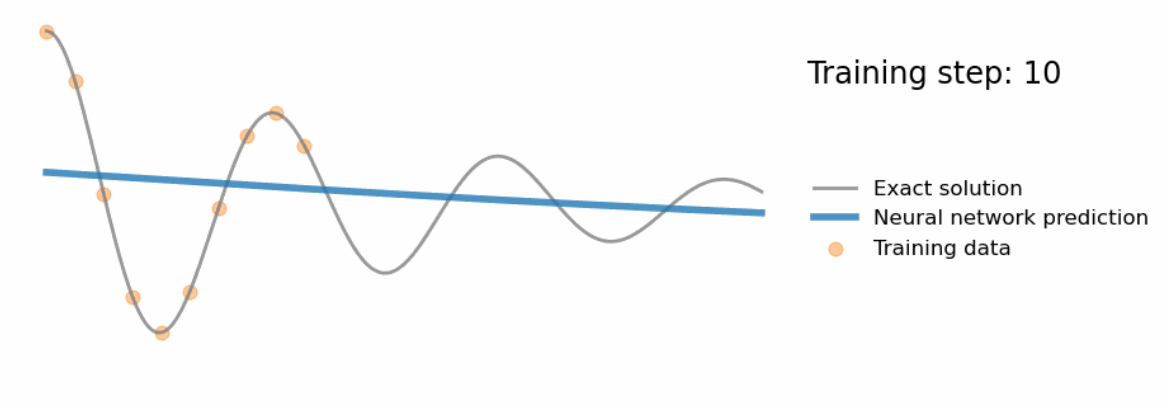
Lecture overview

- Introduction to physics-informed neural networks (PINNs): recap
- Training PINNs
- Live-coding a PINN in PyTorch
- PINN applications
  - Simulation
  - Inversion
  - Equation discovery

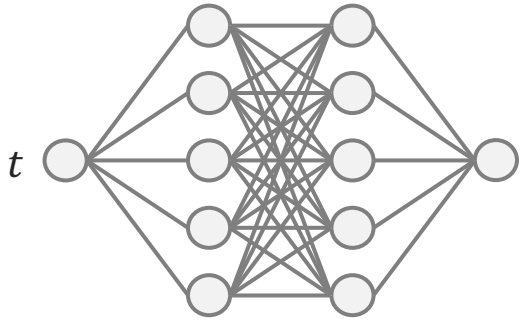
Course timeline

Tutorials		Lectures	
Tue 3:15-14:00, HG E5		Fri 12:15-14:00, HG D1.1	
21.02.		24.02.	~~Course introduction~~
28.02.	~~Intro to PyTorch~~	03.03.	~~Introduction to deep learning I~~
07.03.	~~Simple DNNs in PyTorch~~	10.03.	~~Introduction to deep learning II~~
14.03.	~~Advanced DNNs in PyTorch~~	17.03.	~~Physics-informed neural networks – introduction and theory~~
21.03.	~~PINN exercises~~	24.03.	**Physics-informed neural networks – applications**
28.03.	Implementing PINNs I	31.03.	Physics-informed neural networks – extensions
04.04.	Implementing PINNs II	07.04.	
11.04.		14.04.	
18.04.	Introduction to projects	21.04.	Neural operators – introduction and theory
25.04.	Implementing neural operators I	28.04.	Neural operators – applications
02.05.	Implementing neural operators II	05.05.	Neural operators – extensions
09.05.	Operator learning exercises	12.05.	Graph and sequence models
16.05.	Project discussions	19.05.	Differentiable physics – introduction
23.05.	Implementing autodifferentiation	26.05.	Differentiable physics and neural differential equations
30.05.	Intro to JAX	02.06.	Future trends and overview of CAMLAB

Naïve neural network



$$L(\theta) = \frac{1}{N}\sum_{i}^{N}(NN(t_i;\theta) - u_i)^2$$



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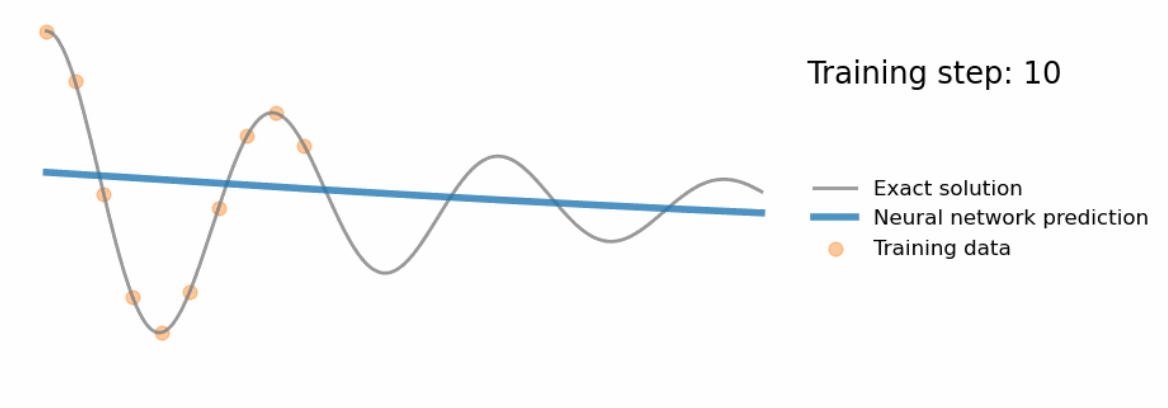

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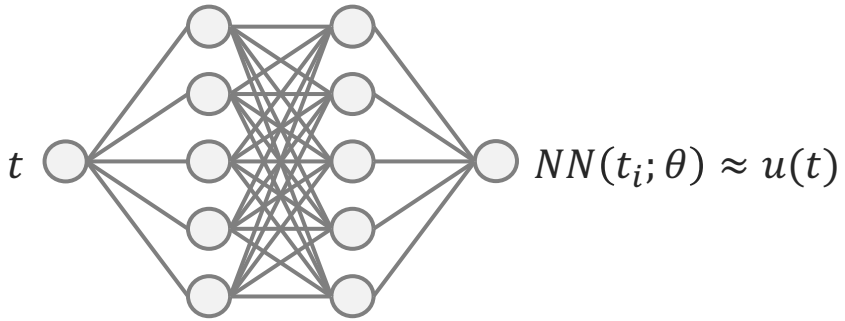

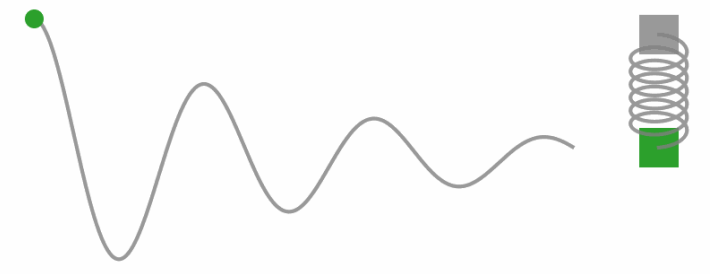

Damped harmonic oscillator

$$m\frac{d^2u}{dt^2} + \mu\frac{du}{dt} + ku = 0$$

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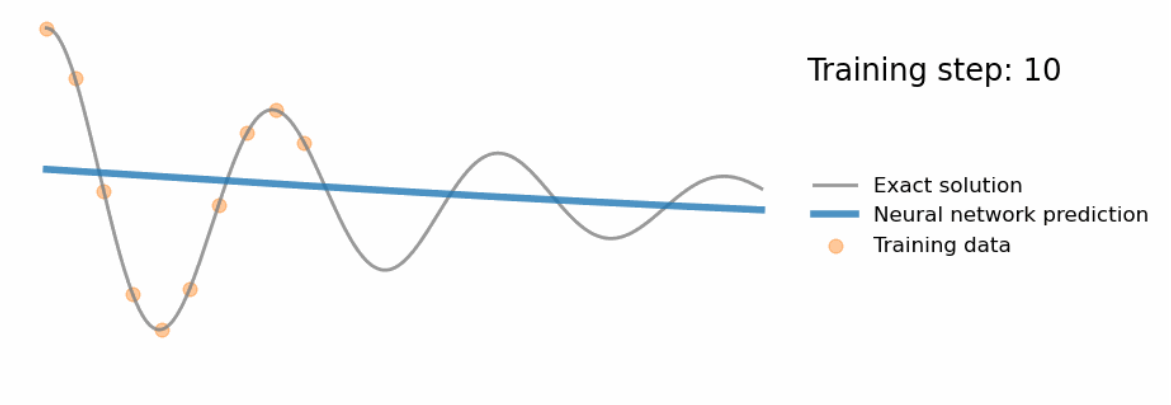

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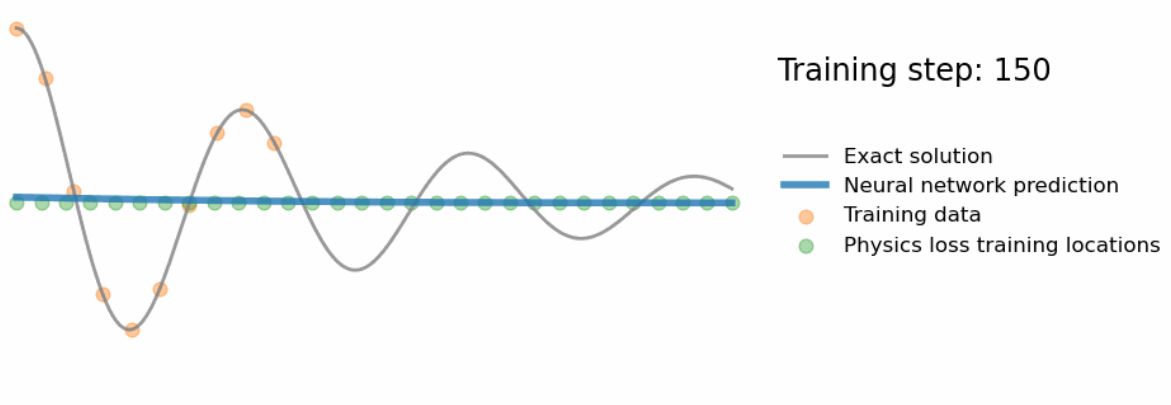
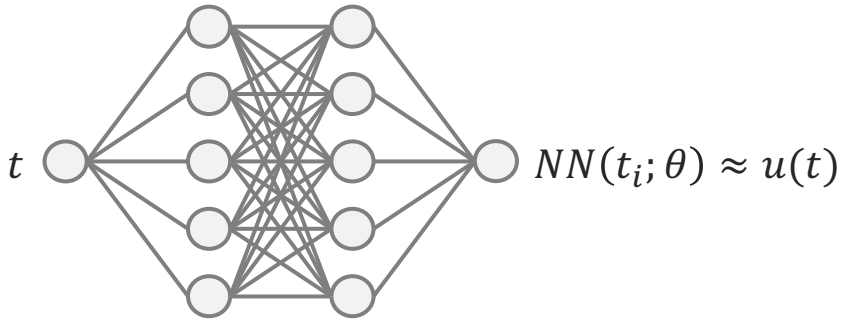
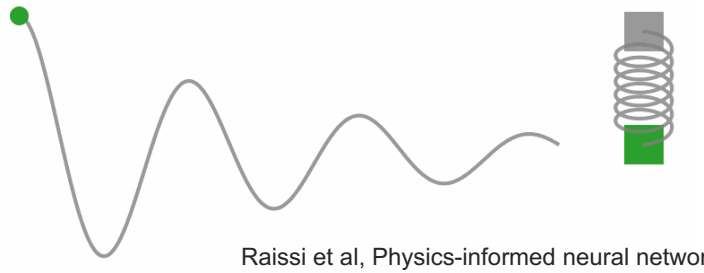
Physics-informed neural network



$$L(\theta) = \frac{1}{N}\sum_{i}^{N}(NN(t_i;\theta) - u_i)^2 + \frac{\lambda}{M}\sum_{j}^{M}\left(\left[m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k\right]NN(t_j;\theta)\right)^2$$



$$NN(t_i;\theta) \approx u(t)$$



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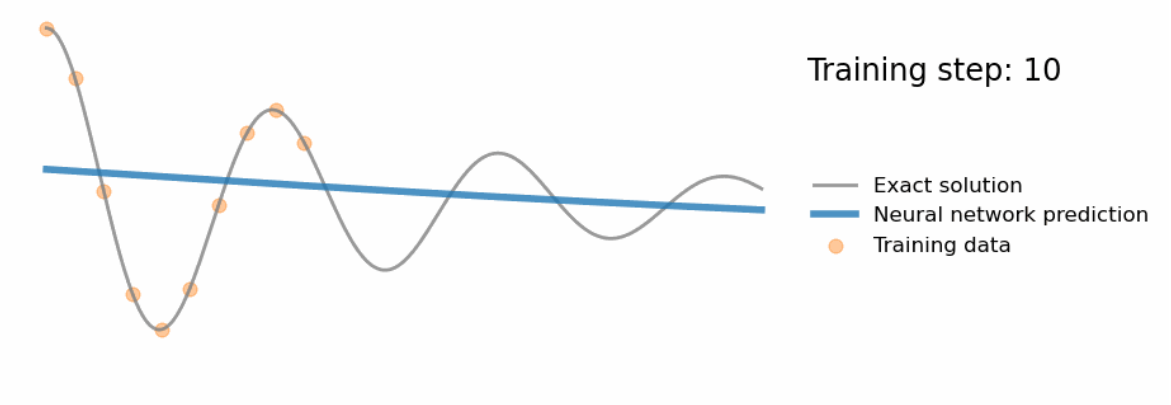

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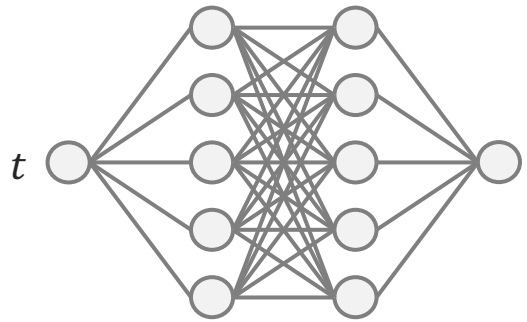

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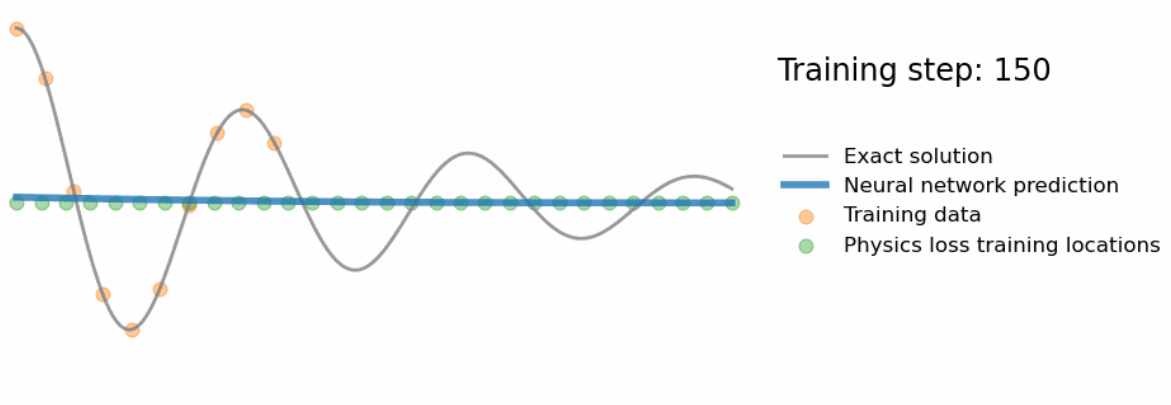
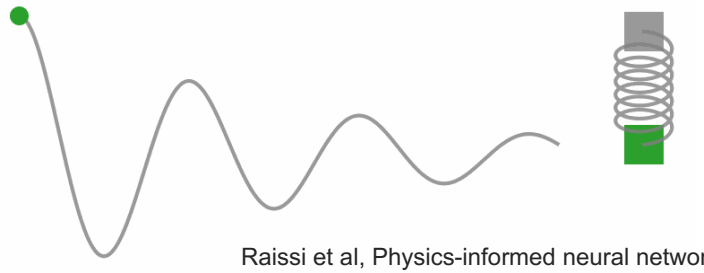


$$L(\theta) = \frac{1}{N}\sum_{i}^{N}(NN(t_i;\theta) - u_i)^2$$ Supervised loss

$$+ \frac{\lambda}{M}\sum_{j}^{M}\left(\left[m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k\right]NN(t_j;\theta)\right)^2$$ Physics loss aka PDE residual



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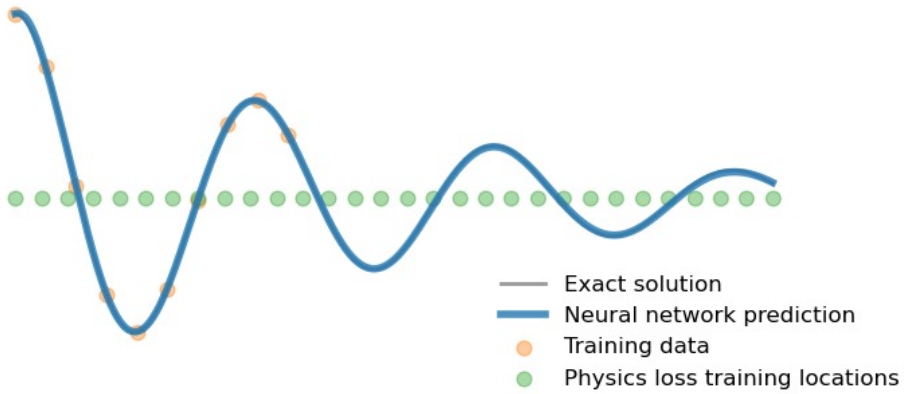
Physics-informed neural network (PINN)



From a ML perspective:

- Physics loss is an **unsupervised** regulariser, which adds prior knowledge

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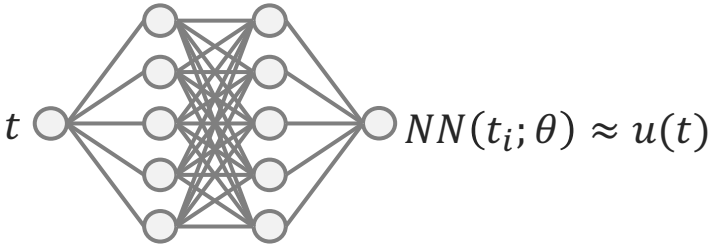

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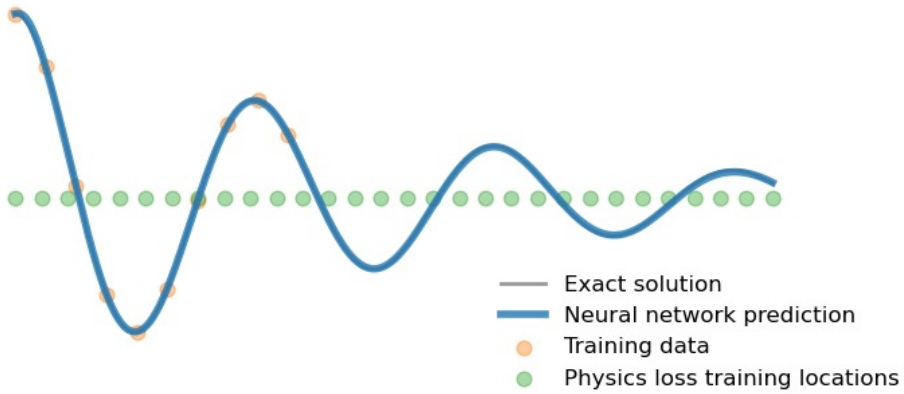

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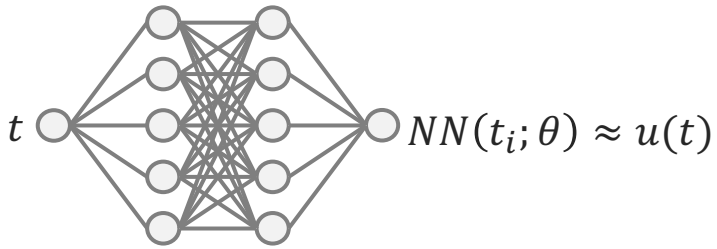

From a ML perspective:

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From a mathematical perspective:

- PINNs provide a way to solve PDEs:
  - Neural network is a mesh-free, **functional** approximation of PDE solution
  - Physics loss is used to assert solution is **consistent** with PDE
  - Supervised loss is used to assert boundary/initial conditions, to ensure solution is **unique**

PINNs are a general framework for solving PDEs

Given a PDE and its boundary/initial conditions

$$\mathcal{D}[u(x)] = f(x), \qquad x \in \Omega \subset \mathbb{R}^d$$
$$\mathcal{B}_k[u(x)] = g_k(x), \qquad x \in \Gamma_k \subset \partial\Omega$$

Where $\mathcal{D}$ is some differential operator, $\mathcal{B}_k$ are a set of boundary operators, and $u(x)$ is the solution to the PDE

PINNs train a neural network to **approximate** the solution to the PDE $NN(x;\theta) \approx u(x)$ using the following loss function:

$$L(\theta) = L_b(\theta) + L_p(\theta)$$

$$L_b(\theta) = \sum_k \frac{\lambda_k}{N_{bk}} \sum_j^{N_{bk}} \left\| \mathcal{B}_k\left[NN(x_{kj};\theta)\right] - g_k(x_{kj}) \right\|^2 \quad \textbf{Boundary loss}$$

$$L_p(\theta) = \frac{1}{N_p} \sum_i^{N_p} \left\| \mathcal{D}[NN(x_i;\theta)] - f(x_i) \right\|^2 \quad \textbf{Physics loss}$$

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For example, the 1+1D viscous Burgers' equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0$$

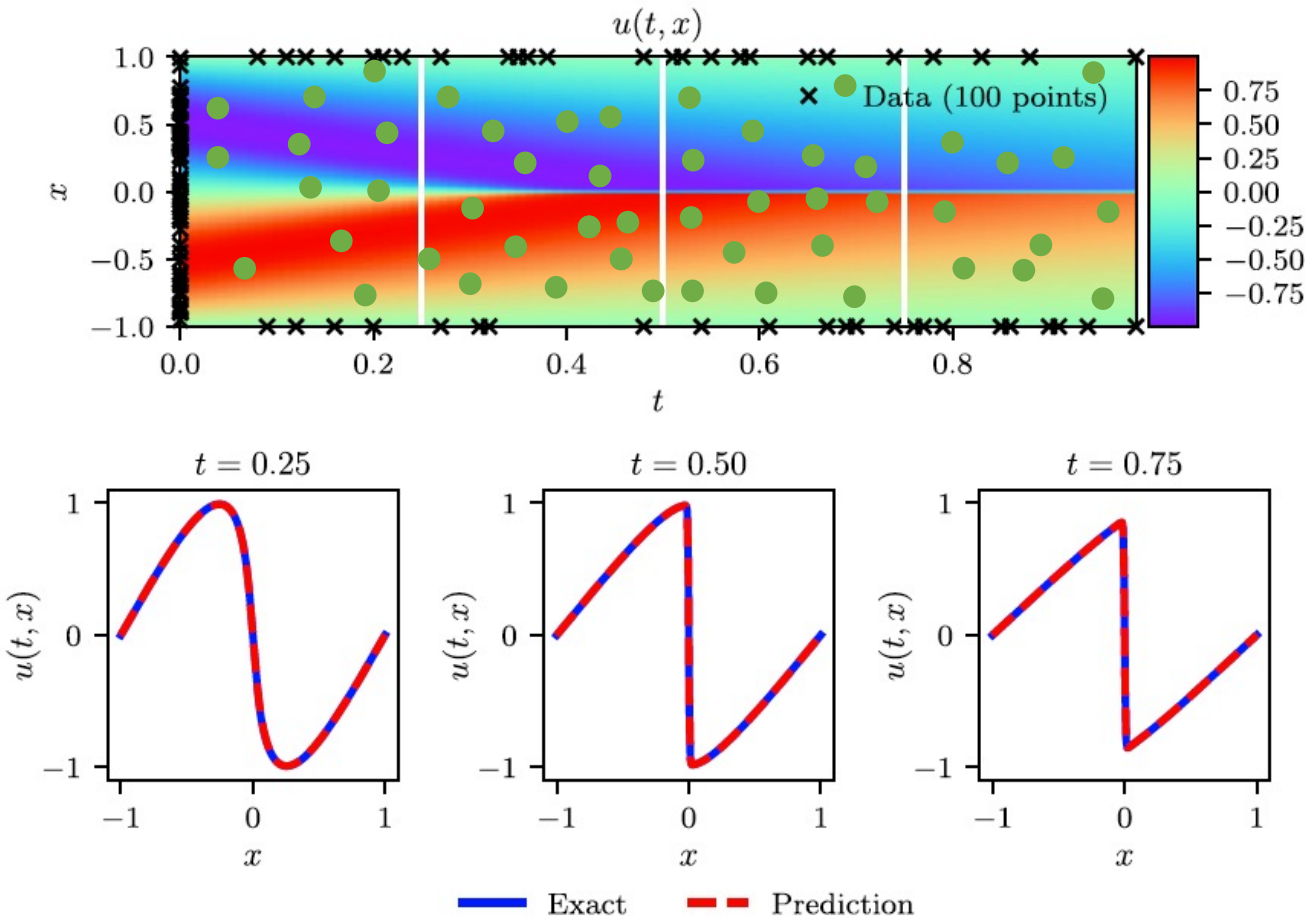
$$u(x,0) = -\sin(\pi x)$$
$$u(-1,t) = u(+1,t) = 0$$

$$NN(x,t;\theta) \approx u(x,t)$$

$$L_b(\theta) = \frac{\lambda_1}{N_{b1}} \sum_j^{N_{b1}} \left(NN\left(x_j, 0; \theta\right) + \sin(\pi x_j)\right)^2$$
$$+ \frac{\lambda_2}{N_{b2}} \sum_k^{N_{b2}} \left(NN(-1, t_k; \theta) - 0\right)^2$$
$$+ \frac{\lambda_3}{N_{b3}} \sum_l^{N_{b3}} \left(NN(+1, t_l; \theta) - 0\right)^2$$

$$L_p(\theta) = \frac{1}{N_p} \sum_i^{N_p} \left(\left(\frac{\partial NN}{\partial t} + NN\frac{\partial NN}{\partial x} - \nu\frac{\partial^2 NN}{\partial x^2} \right)(x_i, t_i; \theta) \right)^2$$

PINNs for solving viscous Burgers' equation



$$L_b(\theta) = \frac{\lambda_1}{N_{b1}} \sum_j^{N_{b1}} \left(NN(x_j, 0; \theta) + \sin(\pi x_j)\right)^2 + \frac{\lambda_2}{N_{b2}} \sum_k^{N_{b2}} (NN(-1, t_k; \theta) - 0)^2 + \frac{\lambda_3}{N_{b3}} \sum_l^{N_{b3}} (NN(+1, t_l; \theta) - 0)^2$$

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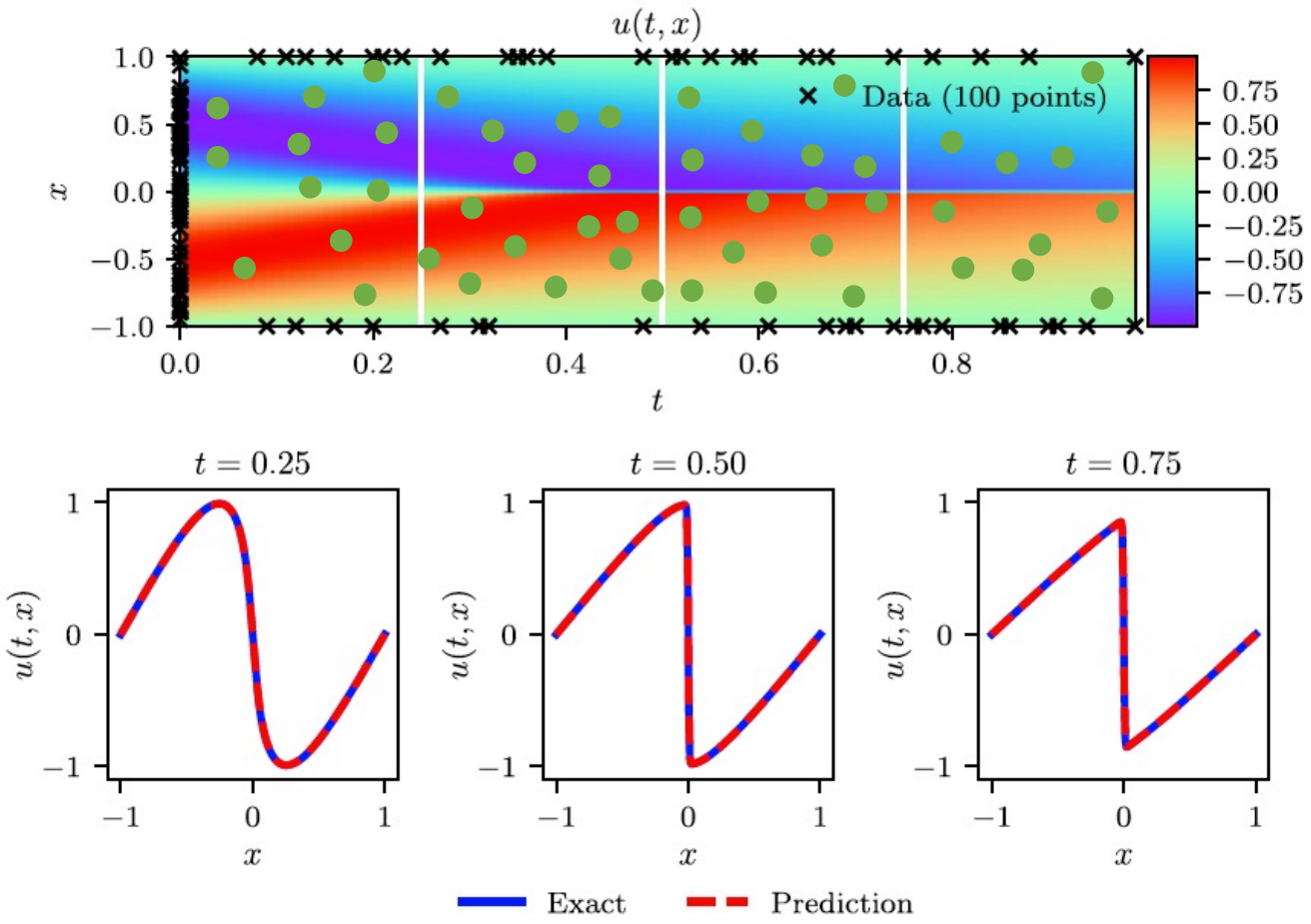

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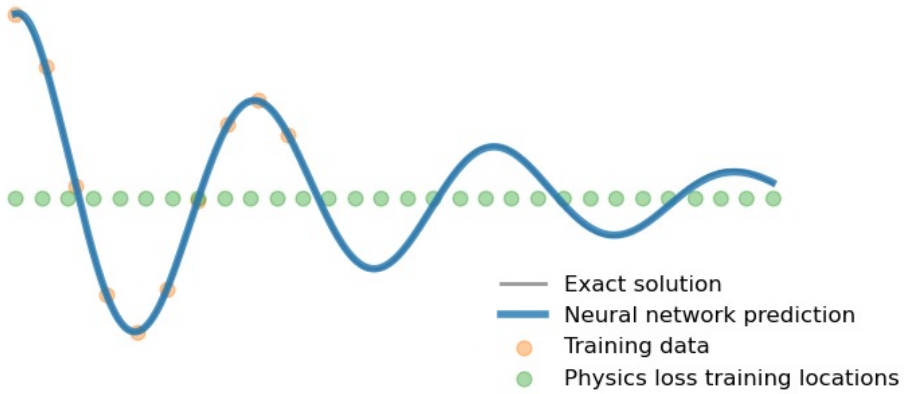
$$L_p(\theta) = \frac{1}{N_p} \sum_i^{N_p} \left(\left(\frac{\partial NN}{\partial t} + NN \frac{\partial NN}{\partial x} - \nu \frac{\partial^2 NN}{\partial x^2} \right) (x_i, t_i; \theta) \right)^2$$

$\nu = 0.01/\pi$
$N_p = 10{,}000$ (Latin hypercube sampling)
$N_{b1} + N_{b2} + N_{b3} = 100$
Fully connected network with 9 layers, 20 hidden units (3021 free parameters)
Tanh activation function
L-BFGS optimiser

PINN training loop



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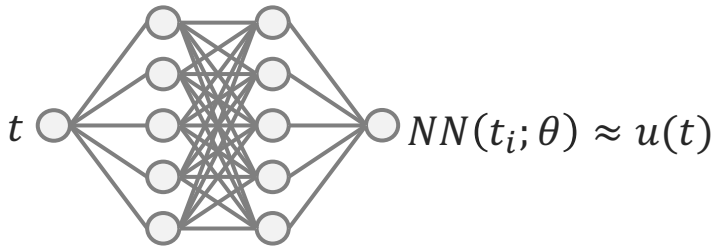


Training loop:

1. Sample boundary/ physics training points
2. Compute network outputs
3. Compute 1st and 2nd order gradient of network output **with respect to network input**
4. Compute loss
5. Compute gradient of loss function **with respect to network parameters**
6. Take gradient descent step

How can we compute the gradients (e.g. $\frac{dNN}{dt}$ and $\frac{dL}{d\theta}$) required in steps 3 and 5?

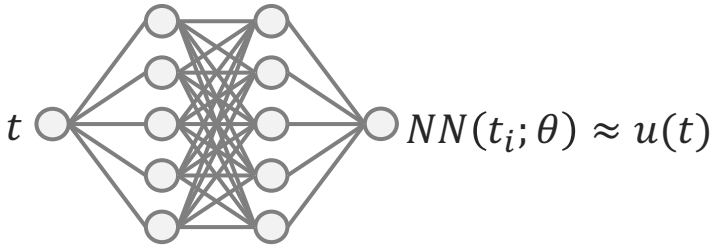
Gradient computation for PINNs

Assume network is a MLP, e.g.:

$$NN(t;\theta) = W_3(\sigma(W_2\sigma(W_1 t + \boldsymbol{b_1}) + \boldsymbol{b_2}) + b_3 \approx u(x)$$

Analogous to backpropagation, we can use the multivariate **chain rule** to compute gradients with respect to network **inputs**:

$$NN(t;\theta) = f \circ \boldsymbol{g} \circ \boldsymbol{h}(t;\theta)$$
$$f = W_3\sigma(\boldsymbol{g}) + b_3$$
$$\boldsymbol{g} = W_2\sigma(\boldsymbol{h}) + \boldsymbol{b_2}$$
$$\boldsymbol{h} = W_1 t + \boldsymbol{b_1}$$



$$\frac{\partial NN}{\partial t} = \frac{\partial f}{\partial \boldsymbol{g}}\frac{\partial \boldsymbol{g}}{\partial \boldsymbol{h}}\frac{\partial \boldsymbol{h}}{\partial t}$$

$$\frac{\partial NN}{\partial t} = W_3\,\mathrm{diag}(\sigma'(\boldsymbol{g}))W_2\,\mathrm{diag}\big(\sigma'(\boldsymbol{h})\big)W_1$$

(see Lecture 2: Introduction to Deep Learning Part I)

Extending computational graph

Computing gradients can simply be thought of as **extending** the network's computational graph:

$$NN(t;\theta) = W_3(\sigma(W_2\sigma(W_1 t + \boldsymbol{b_1}) + \boldsymbol{b_2}) + b_3$$

$$\begin{aligned} f &= W_3\sigma(\boldsymbol{g}) + b_3 \\ \boldsymbol{g} &= W_2\sigma(\boldsymbol{h}) + \boldsymbol{b_2} \\ \boldsymbol{h} &= W_1 t + \boldsymbol{b_1} \end{aligned}$$

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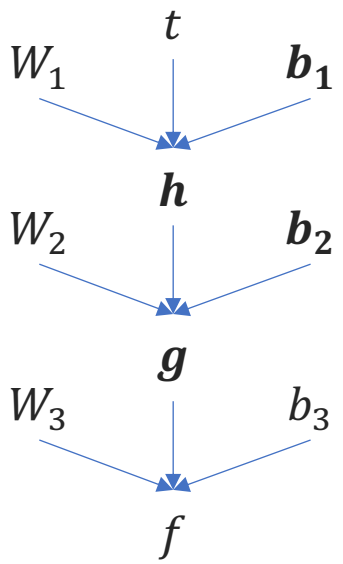

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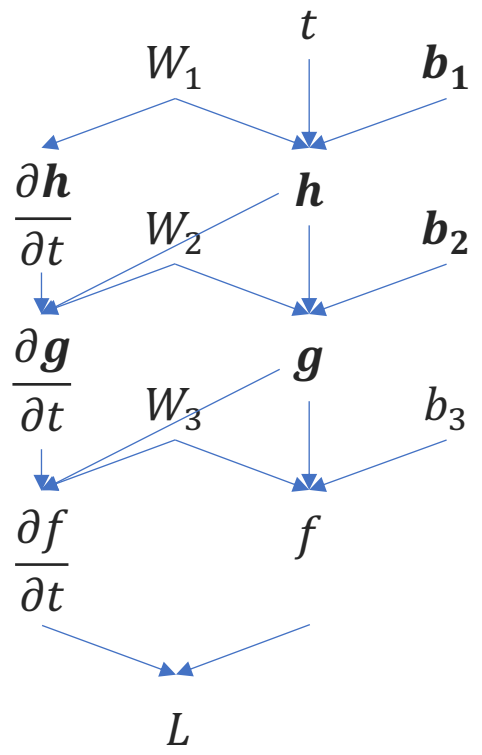

(Forward-mode differentiation)

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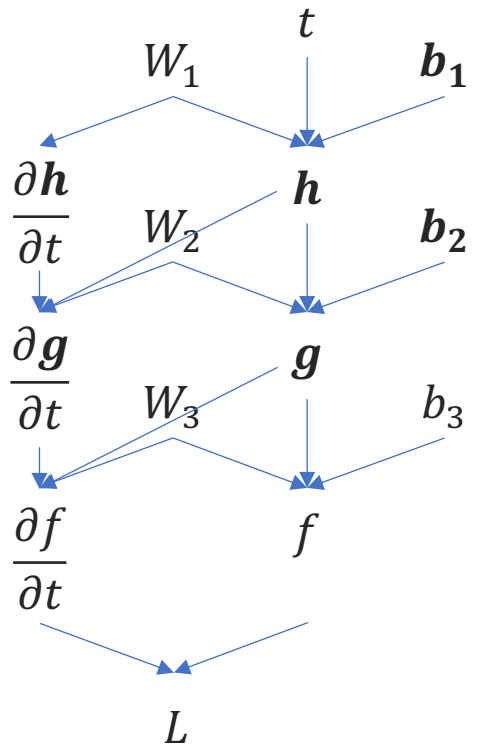
We can recursively apply **autodifferentiation** to compute gradients and extend the graph



(Forward-mode differentiation)

PINN training loop

Training loop:

1. Sample boundary/ physics training points
2. Compute network outputs
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4. Compute loss
5. Compute gradient of loss function **with respect to network parameters <= apply autodiff on extended graph**
6. Take gradient descent step

We can recursively apply **autodifferentiation** to compute gradients and extend the graph

```
# PINN training psuedocode

#2.
t.requires_grad_(True)# tells PyTorch to start tracking graph
theta.requires_grad_(True)
u = NN(t, theta)

#3.
dudt = torch.autograd.grad(u, t, torch.ones_like(u),
                           create_graph=True)[0]
d2udt2 = torch.autograd.grad(dudt, t, torch.ones_like(u),
                             create_graph=True)[0]

#4.
physics_loss = torch.mean((m*d2udt2 + mu*dudt + k*u)**2)
loss = physics_loss + lambda_*boundary_loss

#5.
dtheta = torch.autograd.grad(loss, theta)[0]
```

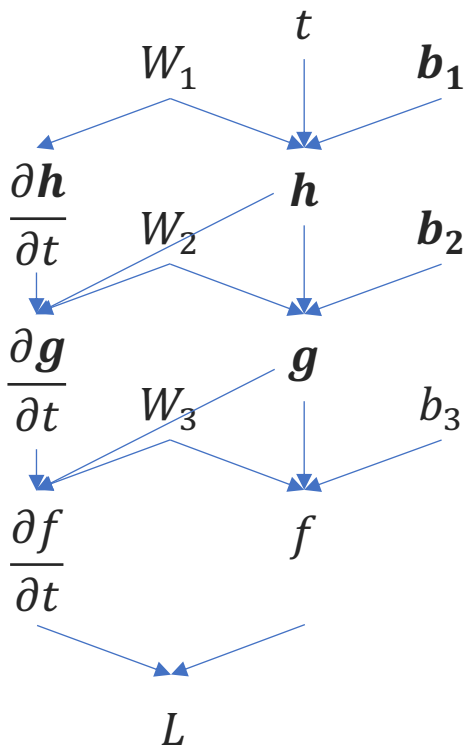
Live-coding a PINN in PyTorch

Computational cost of higher order derivatives

⚠ Note, gradient computation roughly doubles the size of the computational graph*

⇒ The cost of evaluating $\frac{\partial^n NN}{\partial t^n}$ grows exponentially with n (!)

⇒ Most time is spent computing gradients, not the forward pass, when training PINNs



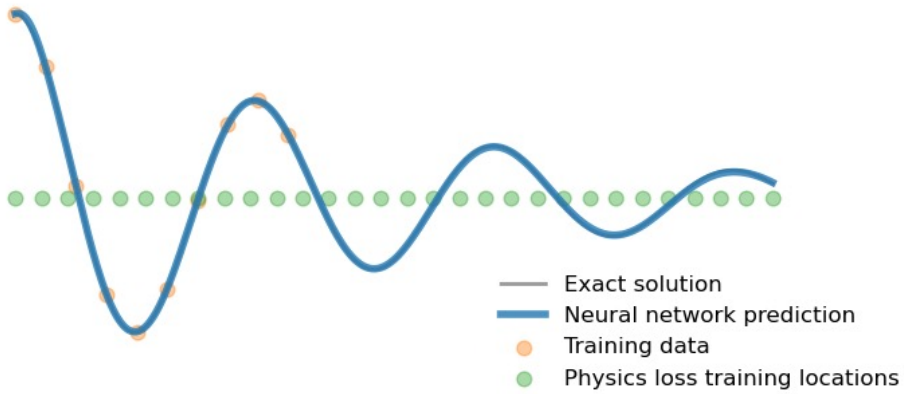
*More precisely, given some $f: \mathbb{R}^n \to \mathbb{R}^m$, its Jacobian $J \in \mathbb{R}^{m \times n}$ and some vector $v \in \mathbb{R}^n$

$$TIME\{f, Jv\} \leq \omega \, TIME\{f\}$$

With a constant $\omega \in [2, 2.5]$ using autodifferentiation

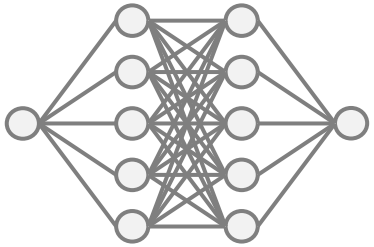
For detailed derivation, see eg: Griewank and Walther, Evaluating Derivatives, Ch 3.1, SIAM (2008))

Other important training considerations



$$L(\theta) = \frac{1}{N}\sum_{i}^{N}(NN(t_i;\theta) - u_i)^2$$ Supervised loss

$$+ \frac{\lambda}{M}\sum_{j}^{M}\left(\left[m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k\right]NN(t_j;\theta)\right)^2$$ Physics loss



- λ is added as a hyperparameter to control the balance of each loss term (note: units of each loss term are not the same!)
- "Enough" collocation points t_j must be chosen so that the learned solution is accurate across the full domain
- Similarly, "enough" boundary points must be chosen such that the learned solution is unique
- Training points are usually uniformly, randomly or quasirandomly sampled
- PINNs still suffer from approximation, estimation and optimisation error (just like normal neural networks, see Lecture 2: Introduction to Deep Learning Part II)!

Lecture overview

- Introduction to physics-informed neural networks (PINNs): recap
- Training PINNs
- Live-coding a PINN in PyTorch
- PINN applications
  - Simulation
  - Inversion
  - Equation discovery

5 min break

Lecture overview

- Introduction to physics-informed neural networks (PINNs): recap
- Training PINNs
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- PINN applications
  - Simulation
  - Inversion
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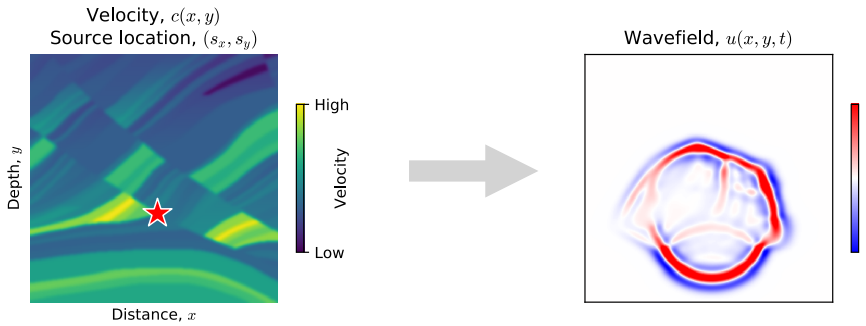
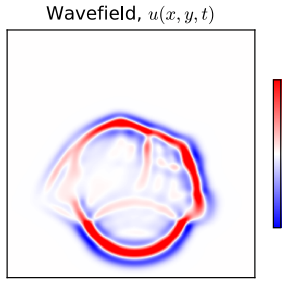
PINN applications

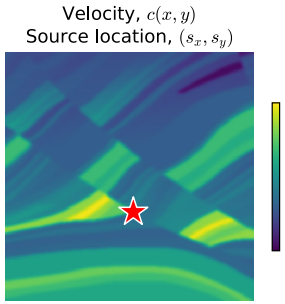


Forward simulation

Estimate wavefield $u(x, y, t)$
Given velocity $c(x, y)$
and source location (s_x, s_y)

$$b = F(a)$$

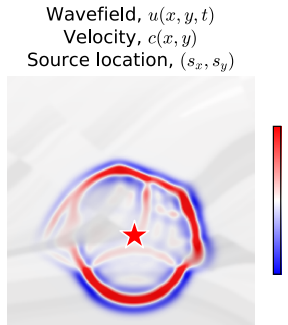




Inversion

Estimate velocity $c(x, y)$
and source location (s_x, s_y)
Given wavefield $u(x, y, t)$

$$b = F(a)$$



Wave equation

$$\nabla^2 u - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = f$$

Equation discovery

Estimate governing equation
Given wavefield $u(x, y, t)$,
velocity $c(x, y)$,
and source location (s_x, s_y)

$$b = F(a)$$

PINNs can be used to solve **forward**, **inverse** and **equation discovery** tasks related to PDEs

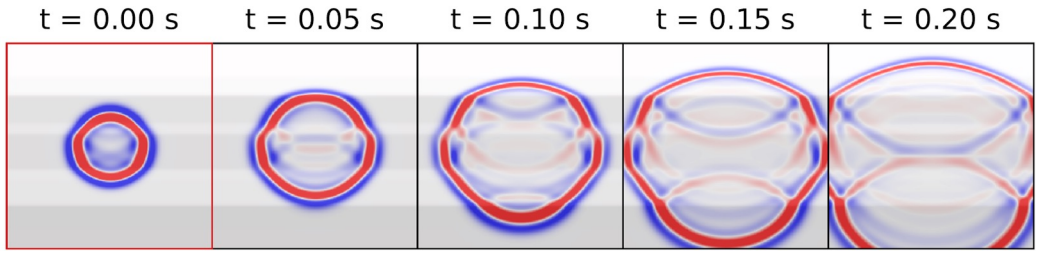
a = set of input conditions

F = physical model of the system

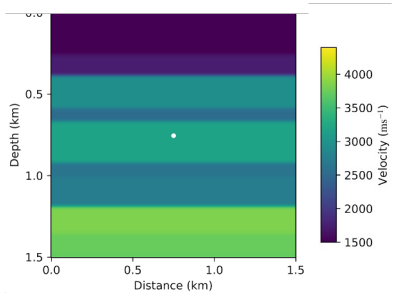
b = resulting properties given F and a

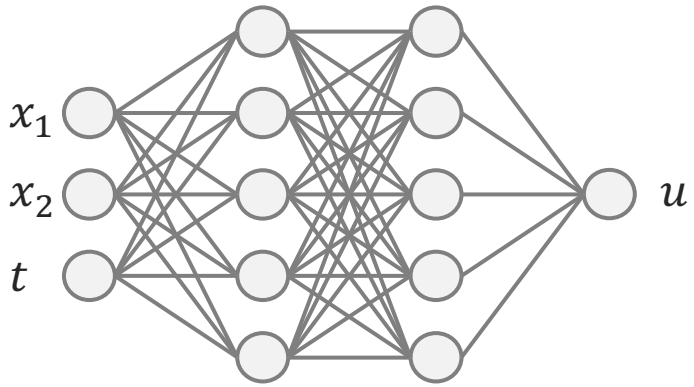
PINNs for solving wave equation

Ground truth FD simulation



Velocity model, $c(x)$





Moseley et al, Solving the wave equation with physics-informed deep learning, ArXiv (2020)

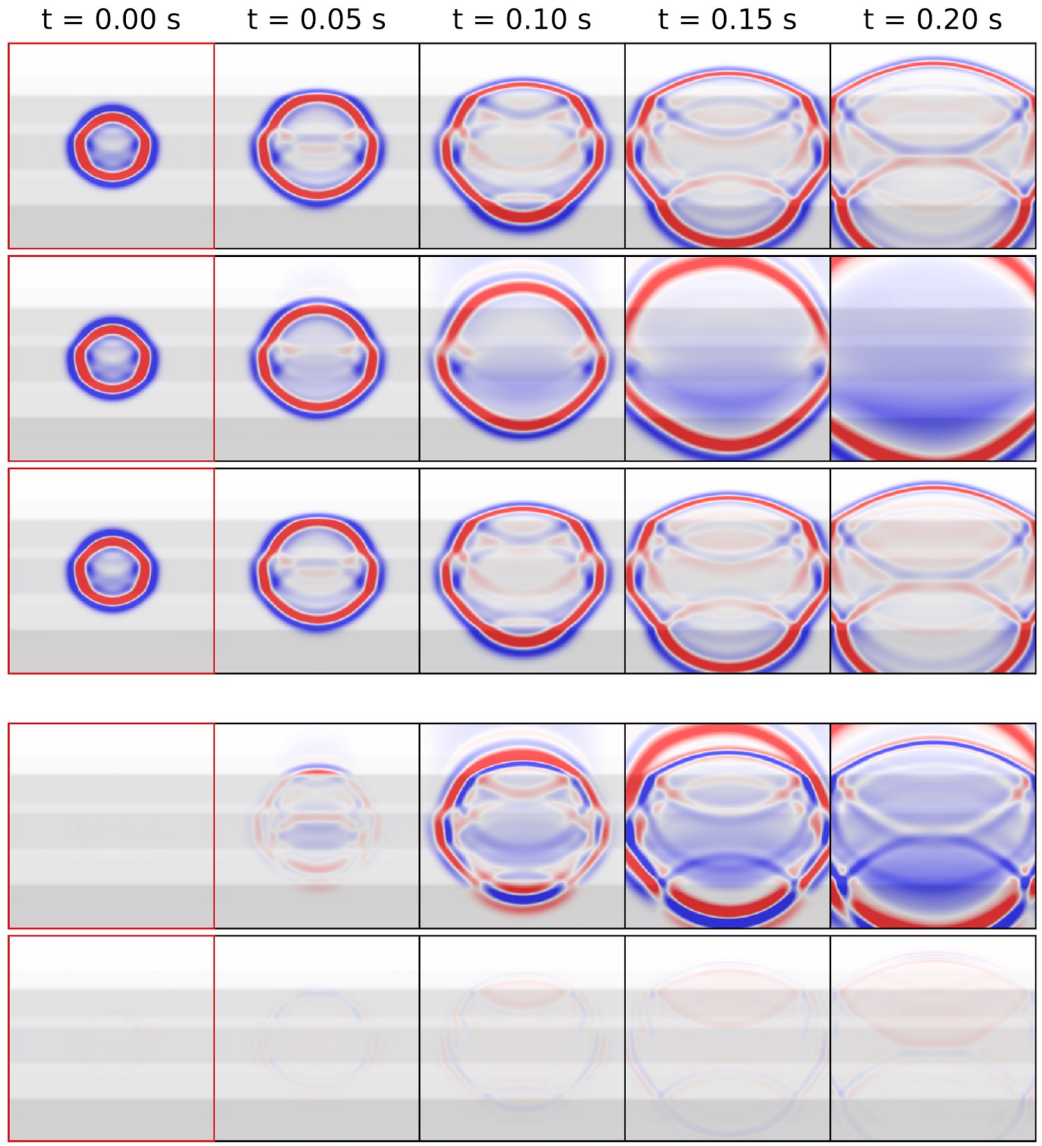
$$L_b(\theta) = \frac{\lambda}{N_b}\sum_{j}^{N_b}\left(NN(x_j, t_j; \theta) - u_{FD}(x_j, t_j)\right)^2$$

Boundary data from FD simulation (first 0.02 seconds)

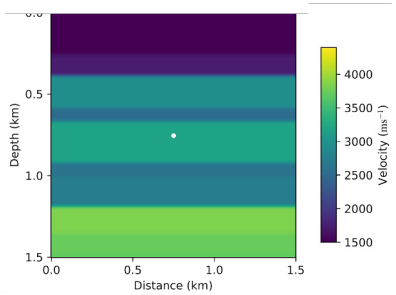
$$L_p(\theta) = \frac{1}{N_p}\sum_{i}^{N_p}\left(\left[\nabla^2 - \frac{1}{c(x_i)^2}\frac{\partial^2}{\partial t^2}\right] NN(x_i, t_i; \theta)\right)^2$$

Collocation points randomly sampled over entire domain (up to 0.2 seconds)

PINNs for solving wave equation



Velocity model, $c(x)$



Moseley et al, Solving the wave equation with physics-informed deep learning, ArXiv (2020)

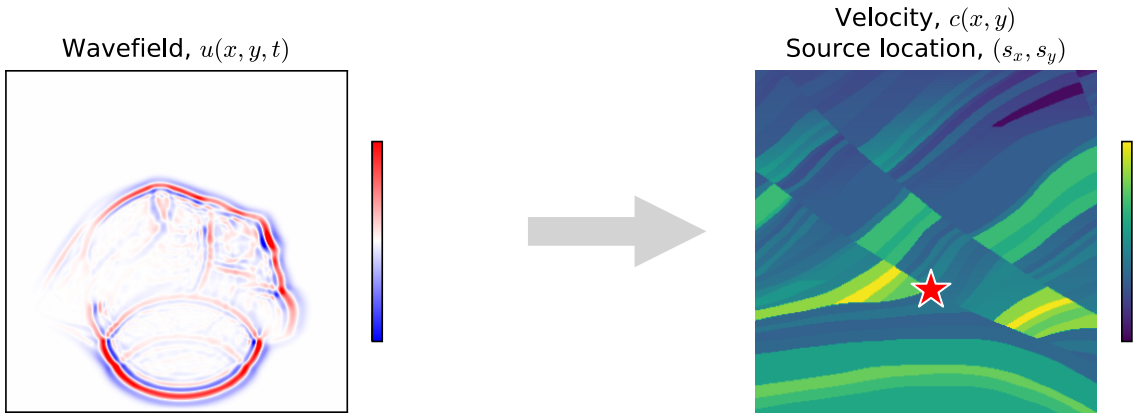
Mini-batch size $N_b = N_p = 500$ (random sampling)
Fully connected network with 10 layers, 1024 hidden units
Softplus activation
Adam optimiser

Training time: **~1 hour**

What is an inverse problem?

Wave equation:

$$\nabla^2 u - \frac{1}{c(x)^2}\frac{\partial^2 u}{\partial t^2} = 0$$



$b =$ observed wavefield $u(x, t)$

$a =$ velocity model $c(x)$ source location

- Fundamentally, inverse problems are **search** problem
- It is often useful to frame them as an optimisation problem, for example:

$$\min_{\hat{a}} \|b - F(\hat{a})\|^2$$

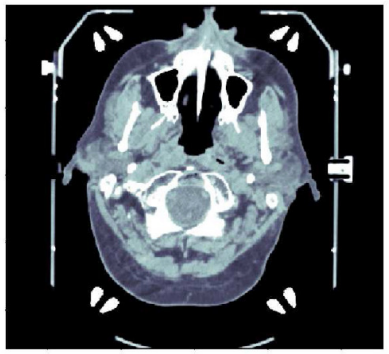
$$b = F(a)$$

$a =$ set of input conditions

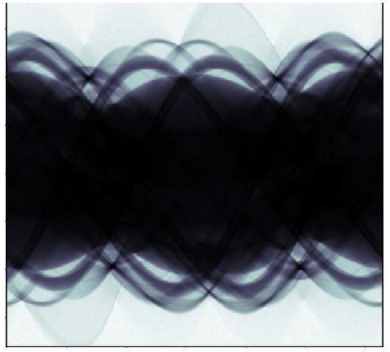
$F =$ physical model of the system

$b =$ resulting properties given F and a

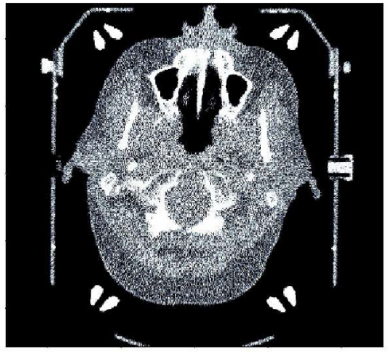
Challenges of inverse problems



Ground truth computed tomography image

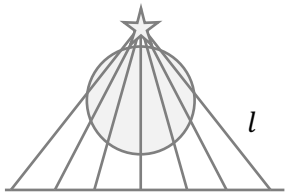


Resulting tomographic data (sinogram)



Result of inverse algorithm (filtered back-projection)

$a(x)$ $\quad F(a)(l) = I_0 \exp(-\int_l a(x)\,dx))$ $\quad \hat{a}(x)$



Adler et al, Solving ill-posed inverse problems using iterative deep neural networks, Inverse Problems (2017)

Typically, inverse problems are **incredibly challenging** to solve because:

- They are usually **ill-posed** (not enough information for a unique solution)
- Observed real-world data is usually **noisy** and **sparse**
- Often require forward modelling to be carried out thousands of times – making them extremely **computationally demanding**

PINNs for inversion

PINNs for solving **forward** simulation:

$$L(\theta) = L_b(\theta) + L_p(\theta)$$

$$L_b(\theta) = \sum_k \frac{\lambda_k}{N_{bk}} \sum_j^{N_{bk}} \left\| \mathcal{B}_k\left[NN(x_{kj};\theta)\right] - g_k(x_{kj}) \right\|^2 \text{ Boundary loss}$$

$$L_p(\theta) = \frac{1}{N_p} \sum_i^{N_p} \| \mathcal{D}[NN(x_i;\theta)] - f(x_i) \|^2 \text{ Physics loss}$$

For example:

$$D = \left[\nabla^2 - \frac{1}{c(x)^2} \frac{\partial^2}{\partial t^2} \right]$$
$$f = 0$$

PINNs for inversion

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For example:

$$D = \left[\nabla^2 - \frac{1}{c(x)^2}\frac{\partial^2}{\partial t^2}\right]$$
$$f = 0$$

PINNs for solving **inverse** problems:

$$L(\theta, \phi) = L_p(\theta, \phi) + L_d(\theta)$$

$$L_p(\theta, \phi) = \frac{1}{N_p} \sum_i^{N_p} \|\mathcal{D}[NN(x_i;\theta);\phi] - f(x_i)\|^2 \text{ Physics loss}$$

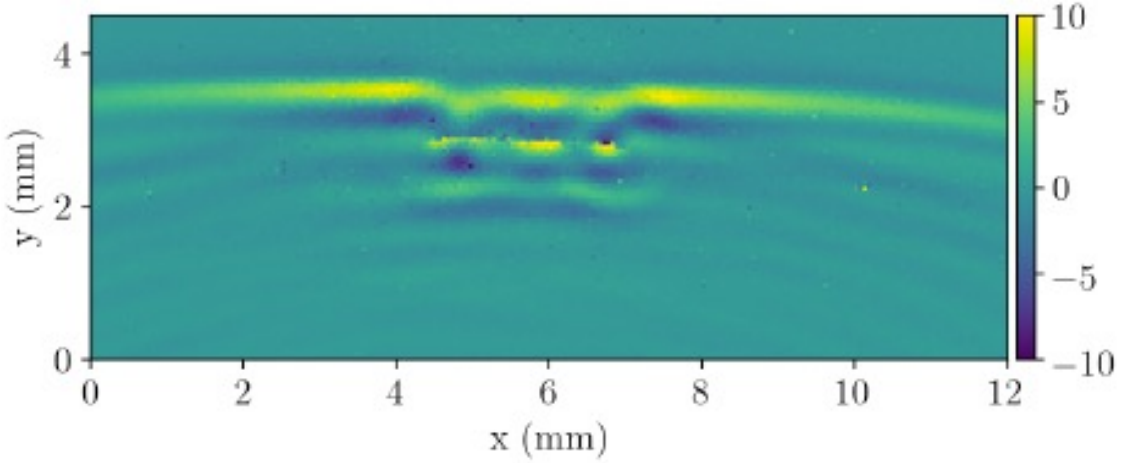
$$L_d(\theta) = \frac{\lambda}{N_d} \sum_l^{N_d} \|NN(x_l;\theta) - u_l\|^2 \quad \textbf{Data loss}$$

Where ϕ are unknown, underlying PDE parameters we wish to invert for, and $\{x_l, u_l\}$ are a set of (potentially noisy) observational data

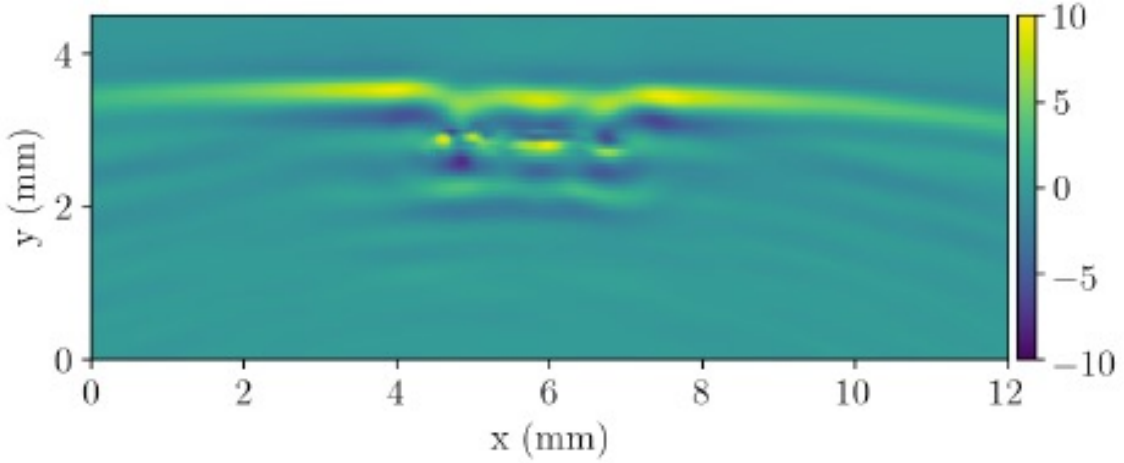
We **simultaneously** learn θ and ϕ when training the PINN

PINNs for wave equation

Shukla et al, Physics-Informed Neural Network for Ultrasound Nondestructive Quantification of Surface Breaking Cracks, Journal of Nondestructive Evaluation (2020)



(a) Actual data at $t = 12.38\ \mu s$.

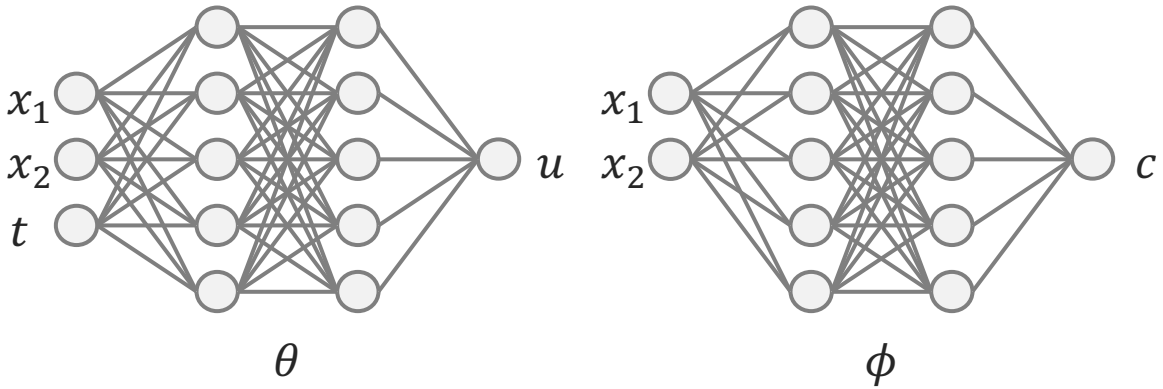


(b) Data recovered from PINN simulation at $t = 12.38\ \mu s$.

$$L_p(\theta, \phi) = \frac{1}{N_p} \sum_i^{N_p} \left(\left[\nabla^2 - \frac{1}{c(x_i; \phi)^2} \frac{\partial^2}{\partial t^2} \right] NN(x_i, t_i; \theta) \right)^2$$

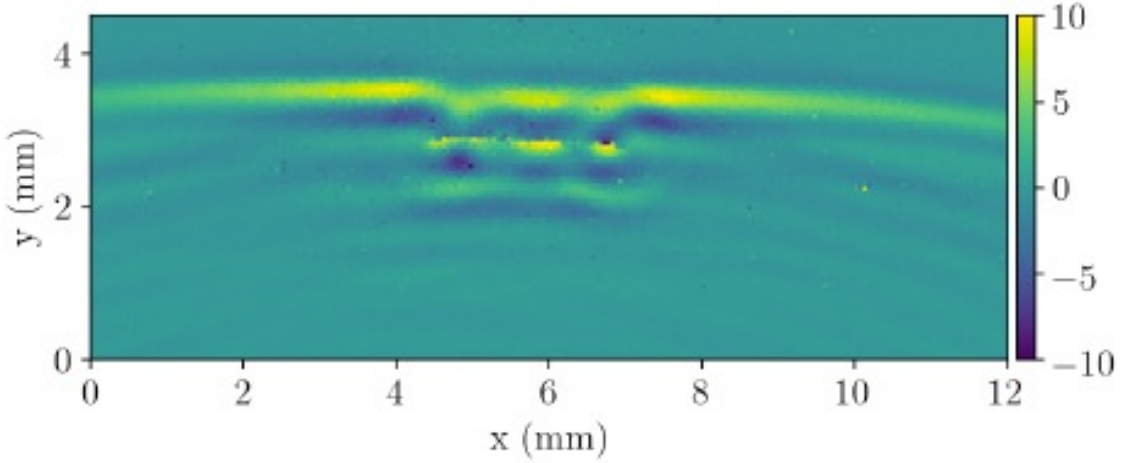
$$L_d(\theta) = \frac{\lambda}{N_d} \sum_l^{N_d} (NN(x_l, t_l; \theta) - u_{obs\,l})^2$$

Treat velocity model as **another** neural network, and simultaneously learn it

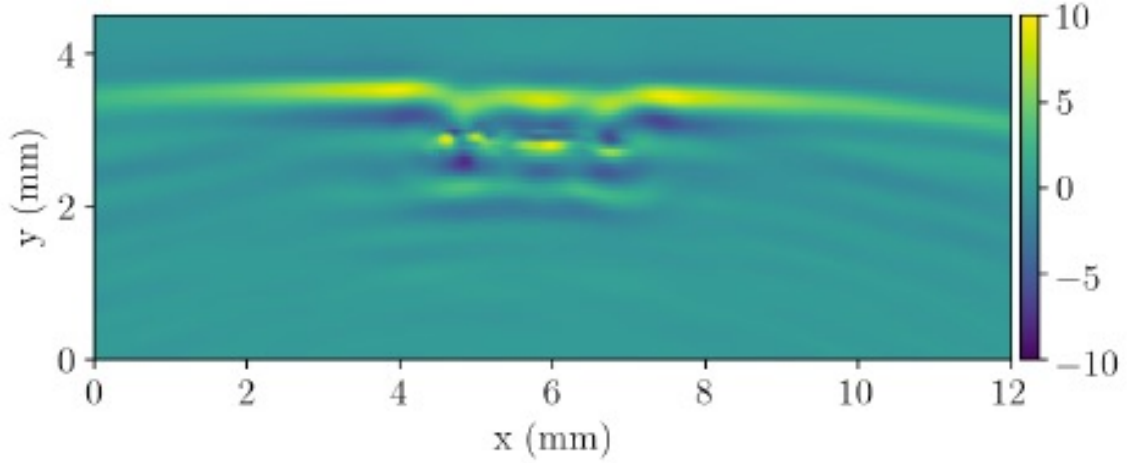


PINNs for wave equation

Shukla et al, Physics-Informed Neural Network for Ultrasound Nondestructive Quantification of Surface Breaking Cracks, Journal of Nondestructive Evaluation (2020)



(a) Actual data at $t = 12.38\ \mu s$.

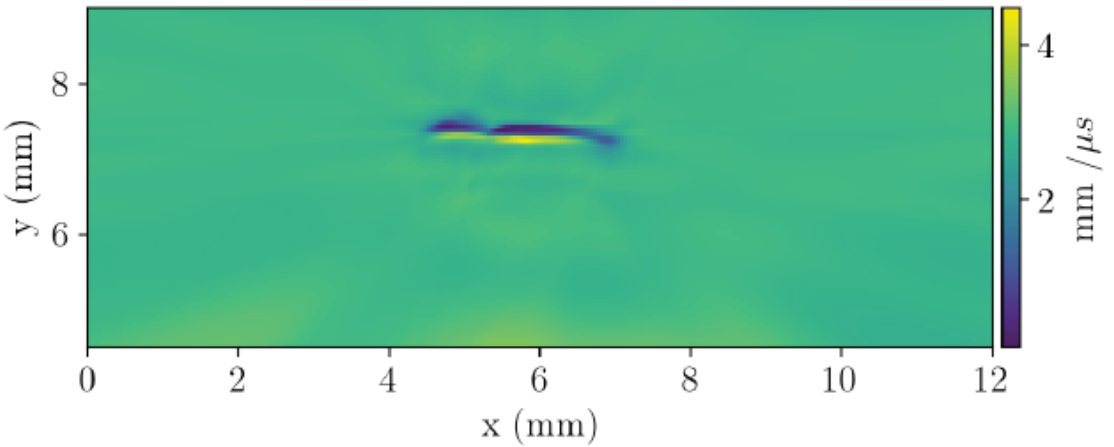


(b) Data recovered from PINN simulation at $t = 12.38\ \mu s$.

$$L_p(\theta, \phi) = \frac{1}{N_p} \sum_i^{N_p} \left(\left[\nabla^2 - \frac{1}{c(x_i; \phi)^2} \frac{\partial^2}{\partial t^2} \right] NN(x_i, t_i; \theta) \right)^2$$

$$L_d(\theta) = \frac{\lambda}{N_d} \sum_l^{N_d} (NN(x_l, t_l; \theta) - u_{obs\,l})^2$$

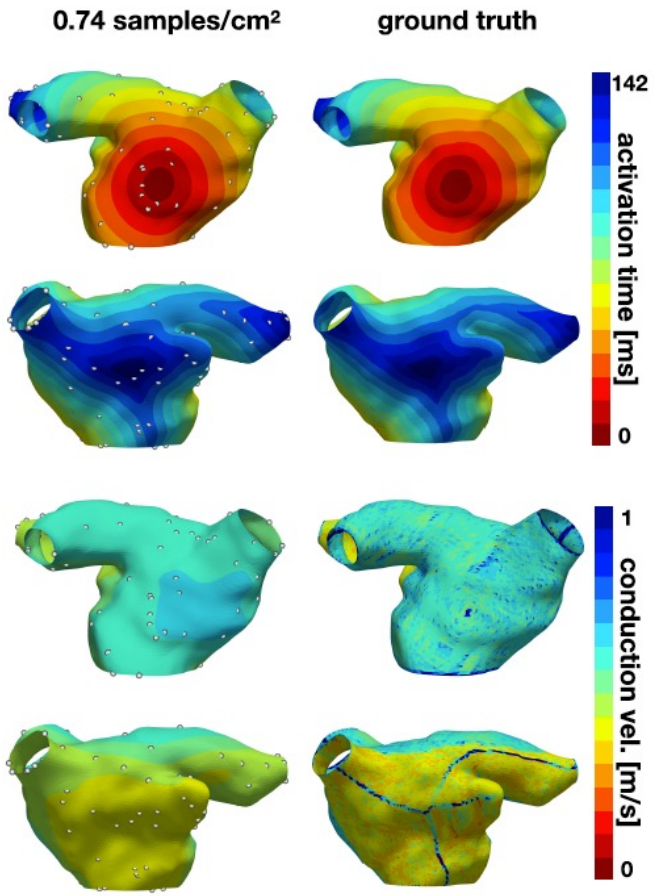
Treat velocity model as **another** neural network, and simultaneously learn it

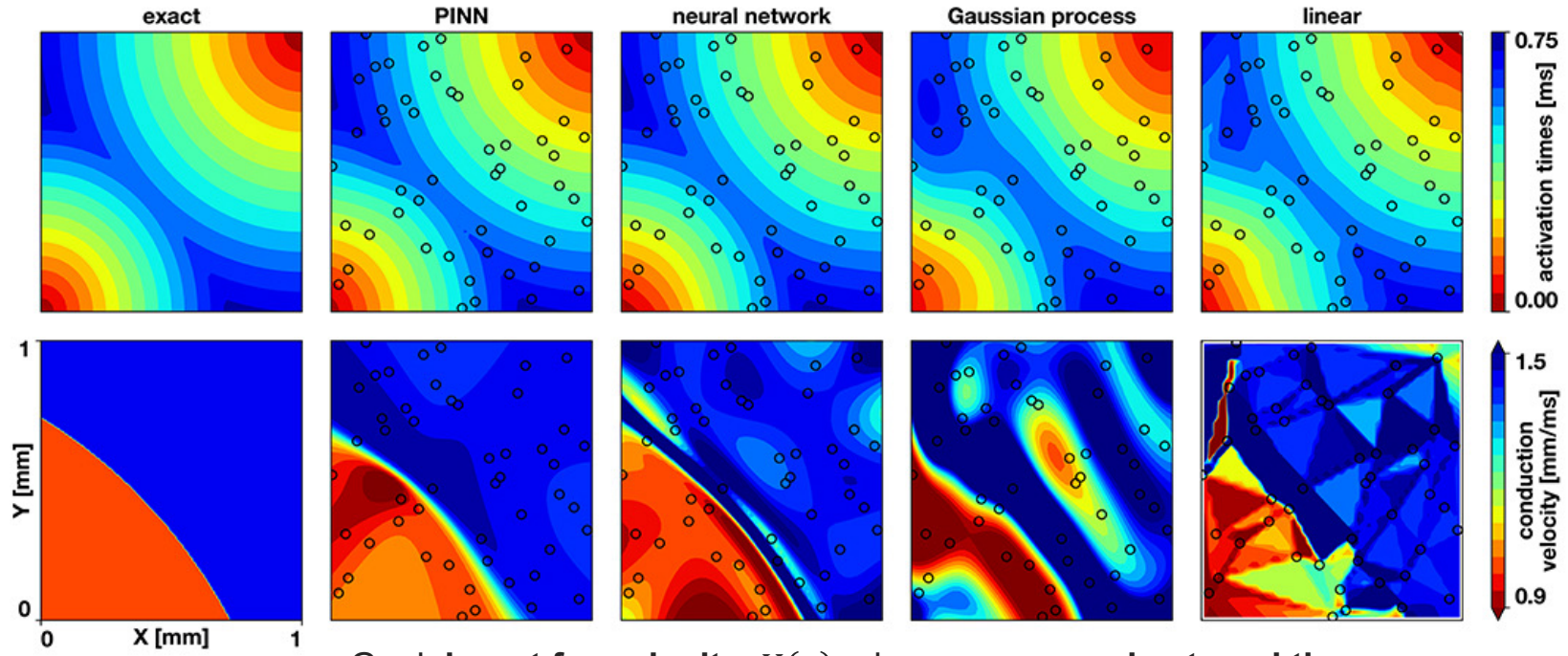


(d) Speed $v(x, y)$ recovered from PINN simulation.

Live-coding a PINN in PyTorch

PINNs for cardiac activation mapping





Goal: **invert for velocity**, $V(x)$, given **sparse, noisy travel time** measurements T_{obs}

Eikonal equation: $\|\nabla T(x)\| = 1/V(x)$

$$L_p(\theta, \phi) = \frac{1}{N_p} \sum_i^{N_p} (\|\nabla NN(x_i; \theta)\| V(x_i; \phi) - 1)^2$$

$$L_d(\theta) = \frac{\lambda}{N_d} \sum_l^{N_d} (NN(x_l; \theta) - T_{obs\,l})^2$$

Sahli Costabal et al, Physics-Informed Neural Networks for Cardiac Activation Mapping, Frontiers in Physics (2020)

PINNs for equation discovery

PINNs for solving **inverse** problems:

$$L(\theta, \phi) = L_p(\theta, \phi) + L_d(\theta)$$

$$L_p(\theta, \phi) = \frac{1}{N_p} \sum_i^{N_p} \|\mathcal{D}[NN(x_i; \theta); \phi] - f(x_i)\|^2 \quad \text{Physics loss}$$

$$L_d(\theta) = \frac{\lambda}{N_d} \sum_l^{N_d} \|NN(x_l; \theta) - u_l\|^2 \quad \text{Data loss}$$

Where $\{x_l, u_l\}$ are a set of (potentially noisy) observational data

But how do we learn the **entire** differential operator $\mathcal{D}$, rather than its parameters ϕ?

PINNs for equation discovery

How do we learn an **entire** differential operator $\mathcal{D}$?

Build a **library** of n operators, such as:

$$\phi = (1, \partial_x, \partial_t, \partial_{xx}, \partial_{tt}, \partial_{xt})^T$$

Then assume the differential operator can be represented as

$$\mathcal{D} = \Lambda\phi$$

Where Λ is a (sparse) matrix of shape (d_u, n)

E.g. for 1D damped harmonic oscillator:

$$\mathcal{D} = \begin{pmatrix} k & \mu & m & 0 \end{pmatrix} \begin{pmatrix} 1 \\ d_t \\ d_{tt} \\ d_{ttt} \end{pmatrix}$$

$$= m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k$$

PINNs for equation discovery

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$$= m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k$$

PINNs for **equation discovery**:

$$L(\theta, \Lambda) = L_p(\theta, \Lambda) + L_d(\theta)$$

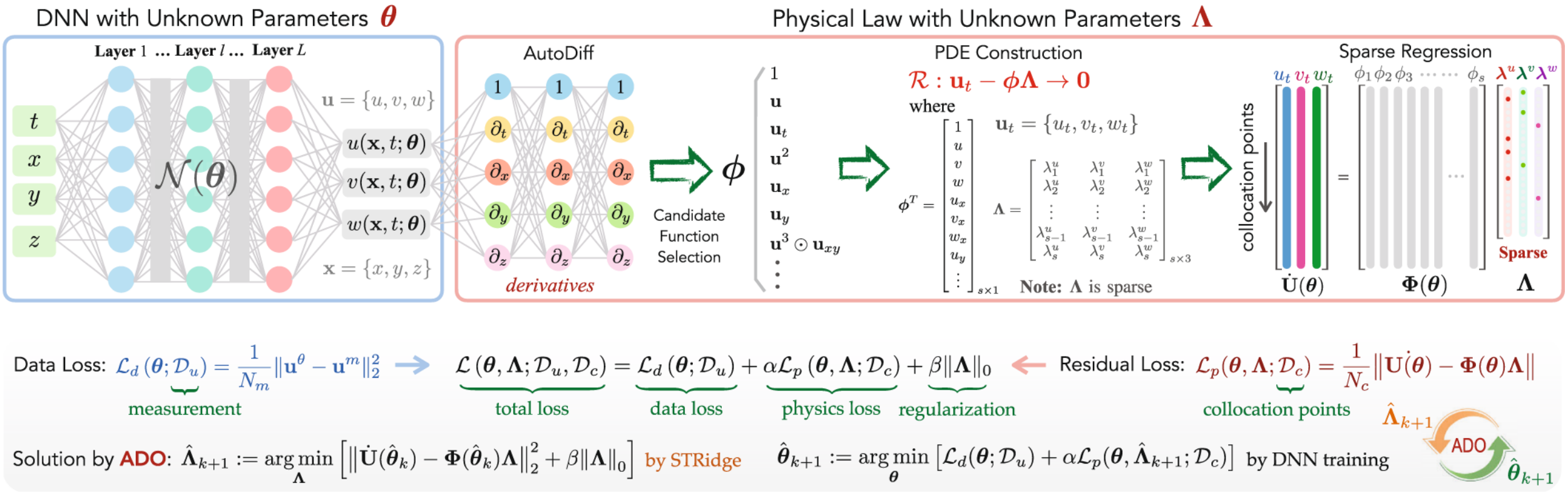
$$L_p(\theta, \Lambda) = \frac{1}{N_p}\sum_i^{N_p} \|\Lambda\phi[NN(x_i;\theta)]\|^2 + \|\Lambda\|^2 \quad \text{Physics loss}$$

$$L_d(\theta) = \frac{\lambda}{N_d}\sum_l^{N_d} \|NN(x_l;\theta) - u_l\|^2 \quad \text{Data loss}$$

Where Λ are treated as **learnable** parameters and $\{x_l, u_l\}$ are a set of (potentially noisy) observational data

Typically, some regularization / prior on Λ (e.g. sparsity) is needed, as this optimisation problem can be very **ill-posed**

PINNs for equation discovery



Data Loss: $\mathcal{L}_d(\boldsymbol{\theta}; \mathcal{D}_u) = \frac{1}{N_m}\|\mathbf{u}^\theta - \mathbf{u}^m\|_2^2$ (measurement)

$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\Lambda}; \mathcal{D}_u, \mathcal{D}_c) = \mathcal{L}_d(\boldsymbol{\theta}; \mathcal{D}_u) + \alpha\mathcal{L}_p(\boldsymbol{\theta}, \boldsymbol{\Lambda}; \mathcal{D}_c) + \beta\|\boldsymbol{\Lambda}\|_0$ (total loss = data loss + physics loss + regularization)

Residual Loss: $\mathcal{L}_p(\boldsymbol{\theta}, \boldsymbol{\Lambda}; \mathcal{D}_c) = \frac{1}{N_c}\|\dot{\mathbf{U}}(\boldsymbol{\theta}) - \boldsymbol{\Phi}(\boldsymbol{\theta})\boldsymbol{\Lambda}\|$ (collocation points)

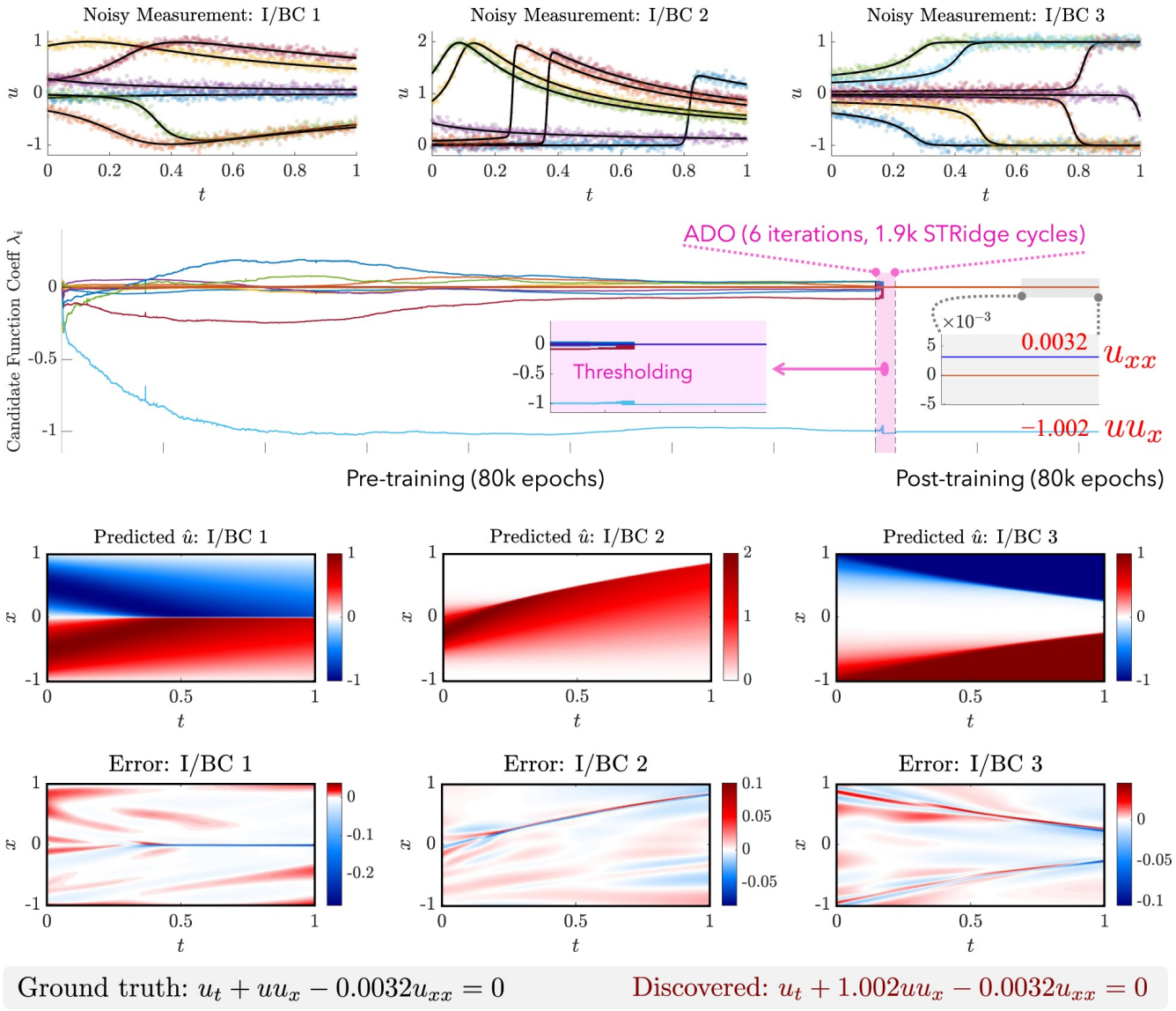
Solution by **ADO**: $\hat{\boldsymbol{\Lambda}}_{k+1} := \arg\min_{\boldsymbol{\Lambda}} \left[\|\dot{\mathbf{U}}(\hat{\boldsymbol{\theta}}_k) - \boldsymbol{\Phi}(\hat{\boldsymbol{\theta}}_k)\boldsymbol{\Lambda}\|_2^2 + \beta\|\boldsymbol{\Lambda}\|_0\right]$ by STRidge

$\hat{\boldsymbol{\theta}}_{k+1} := \arg\min_{\boldsymbol{\theta}} \left[\mathcal{L}_d(\boldsymbol{\theta}; \mathcal{D}_u) + \alpha\mathcal{L}_p(\boldsymbol{\theta}, \hat{\boldsymbol{\Lambda}}_{k+1}; \mathcal{D}_c)\right]$ by DNN training

- Trains by alternating between updating Λ and θ

Chen et al, Physics-informed learning of governing equations from scarce data, Nature communications (2021)

PINNs for equation discovery



- PINN “discovering” Burgers’ equation
- By combining datasets sampled under three different I/BCs with 10% noise

Chen et al, Physics-informed learning of governing equations from scarce data, Nature communications (2021)