

# Physics-Informed Neural Networks (PINNs)

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# Overview

- 1 The PINN Concept: Beyond Data-Only
- 2 Enforcing Boundary Conditions
- 3 Inverse Problems: Discovering Physics
- 4 Collocation Point Strategies
- 5 Adaptive Weights and Loss Balancing
- 6 Advanced Application: Burgers Equation
- 7 Discrete-Time PINNs
- 8 Variational Formulation and Energy Minimization
- 9 Practical Considerations

# Outline

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# Learning Objectives

- Understand why standard neural networks fail for physics problems
- Learn how to incorporate physics into neural network training
- Master automatic differentiation for computing derivatives
- Compare data-driven vs physics-informed approaches

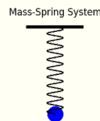
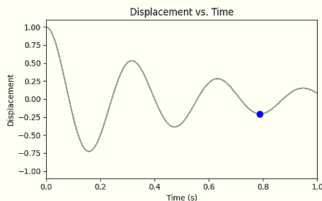
► [Open Notebook: PINN](#)

# The Problem: A Damped Harmonic Oscillator

A mass  $m$  on a spring (constant  $k$ ) with damping (coefficient  $c$ ). The displacement  $u(t)$  satisfies:

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

with initial conditions:  $u(0) = 1$ ,  $\frac{du}{dt}(0) = 0$ .



A classic physics problem to illustrate PINNs.

**The Challenge:** Reconstruct the full solution  $u(t)$  from a few sparse, noisy data points.

# Stage 1: The Data-Only Approach

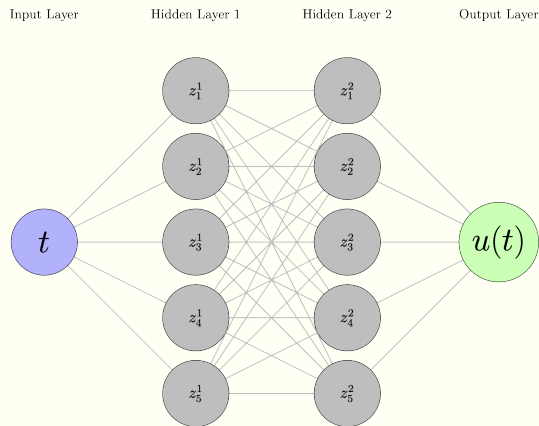
**Idea:** Train a standard neural network to fit the sparse data.

**Loss Function:** Mean Squared Error

$$\mathcal{L}_{\text{data}}(\theta) = \frac{1}{N} \sum_{i=1}^N |\hat{u}_{\theta}(t_i) - u_i|^2$$

**Architecture:**

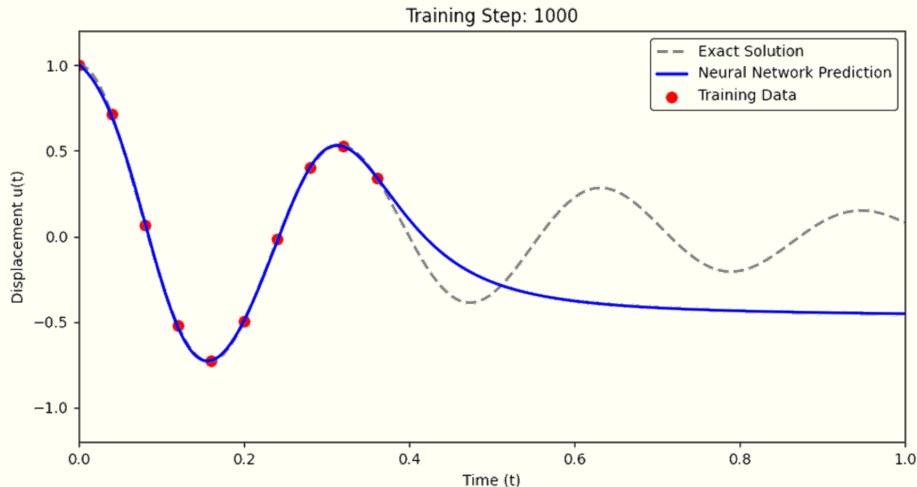
- Input: Time  $t$
- Hidden Layers: Tanh activations
- Output: Displacement  $\hat{u}_{\theta}(t)$



Standard NN for function fitting.

# The Failure of the Data-Only Approach

**Result:** The network fits the training points but fails catastrophically between them.



The network overfits to the sparse data and does not respect the underlying physics

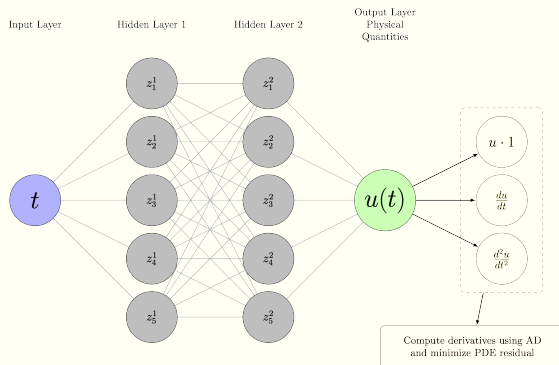
## Stage 2: Enter Physics-Informed Neural Networks

**The Key Insight:** Don't just fit data. Enforce the differential equation itself!

**Physics Residual:** We define a residual based on the ODE:

$$\mathcal{R}_\theta(t) = m \frac{d^2 \hat{u}_\theta}{dt^2} + c \frac{d \hat{u}_\theta}{dt} + k \hat{u}_\theta$$

If the solution is correct,  $\mathcal{R}_\theta(t)$  should be zero.



PINN architecture with physics loss.



# The Complete PINN Loss Function

The total loss is a combination of data fit and physics enforcement.

$$\mathcal{L}_{\text{total}}(\theta) = \mathcal{L}_{\text{data}}(\theta) + \lambda \mathcal{L}_{\text{physics}}(\theta)$$

## Data Loss

Ensures the solution passes through the measurements.

$$\mathcal{L}_{\text{data}}(\theta) = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} |\hat{u}_{\theta}(t_i) - u_i|^2$$

## Physics Loss

Ensures the solution obeys the ODE at random "collocation" points.

$$\mathcal{L}_{\text{physics}}(\theta) = \frac{1}{N_{\text{colloc}}} \sum_{j=1}^{N_{\text{colloc}}} |\mathcal{R}_{\theta}(t_j)|^2$$

# The Secret Weapon: Automatic Differentiation (AD)

**Critical Question:** How do we compute  $\frac{d\hat{u}_\theta}{dt}$  and  $\frac{d^2\hat{u}_\theta}{dt^2}$ ?

**Answer:** Automatic Differentiation

AD provides **exact** derivatives of the neural network output with respect to its input, by applying the chain rule through the computational graph.

- No finite difference errors.
- Computationally efficient (especially reverse-mode AD).
- Built into modern frameworks (PyTorch, TensorFlow, JAX).

**Example:** For  $u(t) = \sin(t)$ , AD can compute  $u'(t) = \cos(t)$  and  $u''(t) = -\sin(t)$  to machine precision.

# Theoretical Foundation: UAT for Sobolev Spaces

**Classical UAT:** NNs can approximate any *continuous function*.

**Problem:** For PDEs, we need to approximate functions **and their derivatives**.

## Extended Universal Approximation Theorem

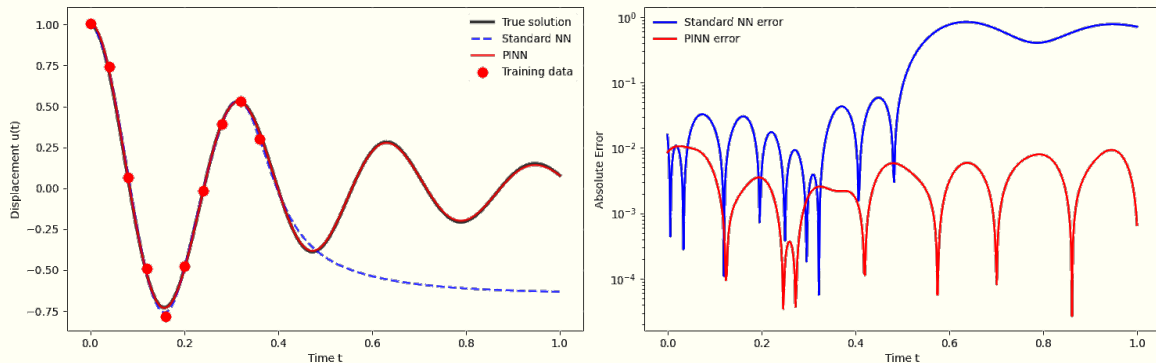
Neural networks with sufficiently smooth activation functions (e.g., tanh, not ReLU) can approximate functions in **Sobolev spaces**  $H^k(\Omega)$ .

$$\|u - \hat{u}_\theta\|_{H^k} < \epsilon$$

The Sobolev norm  $\|u\|_{H^k}^2 = \sum_{|\alpha| \leq k} \|D^\alpha u\|_{L^2}^2$  measures the error in the function and all its derivatives up to order  $k$ .

**Why this matters:** For a  $k^{th}$ -order ODE/PDE, we need an activation function that is at least  $k$  times differentiable ( $C^k$ ). For our 2nd-order oscillator, we need a  $C^2$  activation like tanh.

# The Moment of Truth: Standard NN vs. PINN



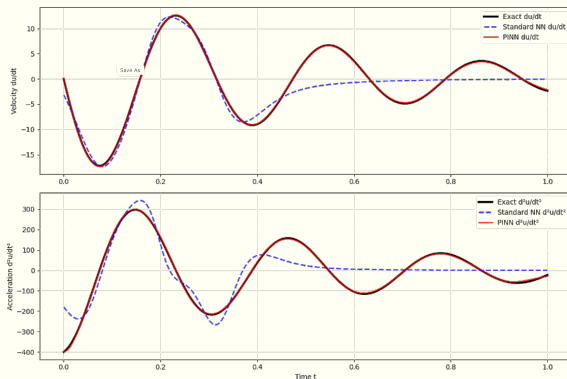
Placeholder for the comparison plot from the notebook.

## Observation:

- **Standard NN:** Fits data points, but fails to generalize.
- **PINN:** Fits data points AND follows the physics, resulting in a globally accurate solution.

# Deep Dive: Derivative and Phase Portrait Analysis

The ultimate test: Does the PINN learn physically consistent derivatives?

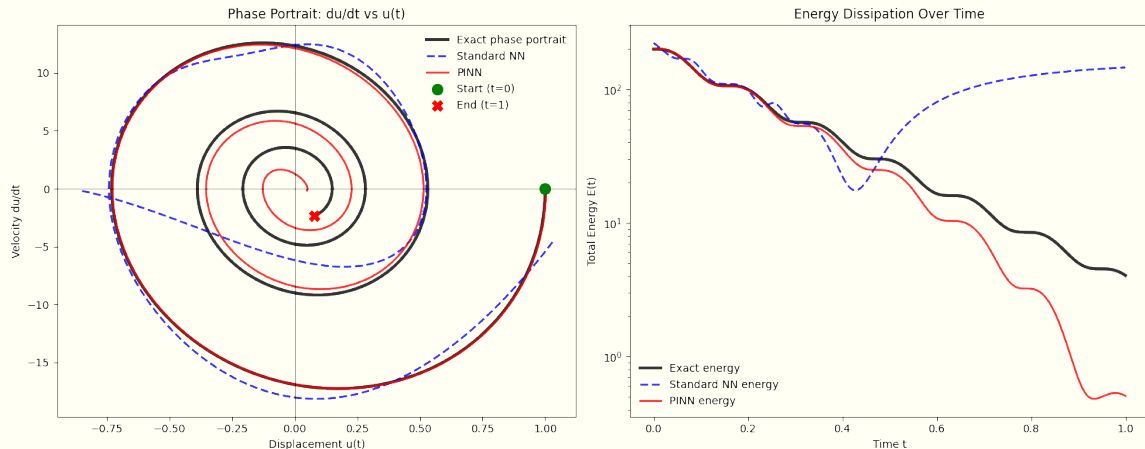


Derivative plots.

**Result:** The PINN learns the correct velocity ( $du/dt$ ) and acceleration ( $d^2u/dt^2$ ).

# Deep Dive: Derivative and Phase Portrait Analysis

The ultimate test: Does the PINN learn physically consistent derivatives?



Phase portrait plots.

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# The 1D Poisson Problem

We now tackle a boundary value problem, the 1D Poisson equation:

$$\frac{d^2 u}{dx^2} + \pi \sin(\pi x) = 0, \quad \text{for } x \in [0, 1]$$

with Dirichlet boundary conditions (BCs):

$$u(0) = 0 \quad \text{and} \quad u(1) = 0$$

**Goal:** Train a PINN to find the solution using only the governing equation and its BCs.

► Open Notebook: 1D Poisson



# Method 1: Soft Constraints

Treat the boundary conditions as another component of the loss function.

**Total Loss:**

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{PDE}} + \lambda_{BC} \mathcal{L}_{BC}$$

## Boundary Loss

A mean squared error term that penalizes violations of the BCs.

$$\mathcal{L}_{BC} = \frac{1}{N_{BC}} \sum_{i=1}^{N_{BC}} |\hat{u}_{\theta}(x_i) - u_{BC}|^2$$

## Pros & Cons

- + **Flexible:** Easy to implement for any type of BC (Dirichlet, Neumann, etc.).
- **Approximate:** Satisfaction is not guaranteed, only encouraged.
- **Tuning:** Requires careful tuning of the weight  $\lambda_{BC}$ .

## Method 2: Hard Constraints

Modify the network architecture to satisfy the BCs *by construction*.

For our problem with  $u(0) = 0$  and  $u(1) = 0$ , we can define a trial solution  $\tilde{u}(x)$ :

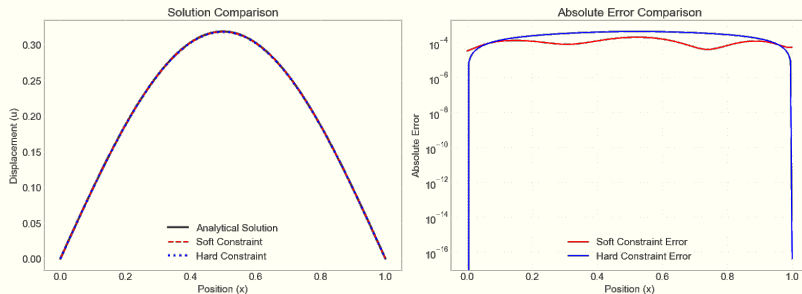
$$\tilde{u}(x) = \underbrace{x(1-x)}_{D(x)} \cdot \underbrace{\text{NN}(x; \theta)}_{\text{Network Output}}$$

The distance function  $D(x)$  is zero at the boundaries, forcing  $\tilde{u}(x)$  to be zero there, regardless of the network's output.

### Pros & Cons

- + **Exact:** BCs are satisfied perfectly.
- + **Simpler Loss:** No need for  $\mathcal{L}_{BC}$  or  $\lambda_{BC}$ , leading to more stable training.
- **Inflexible:** Requires designing a specific trial function for the problem's geometry and BCs, which can be difficult for complex cases.

# Comparison: Soft vs. Hard Constraints



## Conclusion:

- Both methods achieve high accuracy.
- The hard constraint method shows slightly lower error and, by design, has zero error at the boundaries.
- For simple geometries and Dirichlet BCs, **hard constraints are often superior**.
- For complex problems, **soft constraints offer greater versatility**.

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# Forward vs. Inverse Problems

## Forward Problem

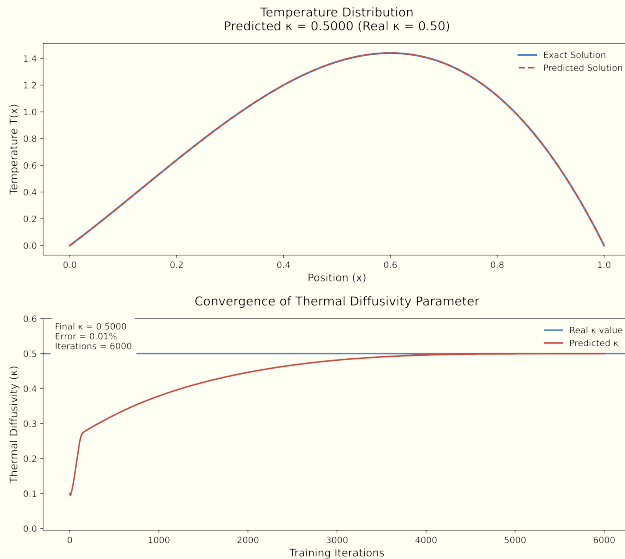
- **Given:** Full physical model (equations + parameters).
- **Find:** The solution  $u(x, t)$ .
- *Example: Simulate temperature given thermal conductivity.*

## Inverse Problem

- **Given:** Sparse measurements of the solution  $u(x, t)$ .
- **Find:** Unknown physical parameters in the model.
- *Example: Infer thermal conductivity from temperature measurements.*

► [Open Notebook: Inverse Heat](#)

# Forward vs. Inverse Problems



# The PINN Approach to Inverse Problems

**The Key Insight:** Treat the unknown physical parameters as additional trainable variables in the network.

**Problem:** 1D steady-state heat conduction.

$$-k \frac{d^2 T}{dx^2} = f(x)$$

Here, the thermal diffusivity  $k$  is **unknown**.

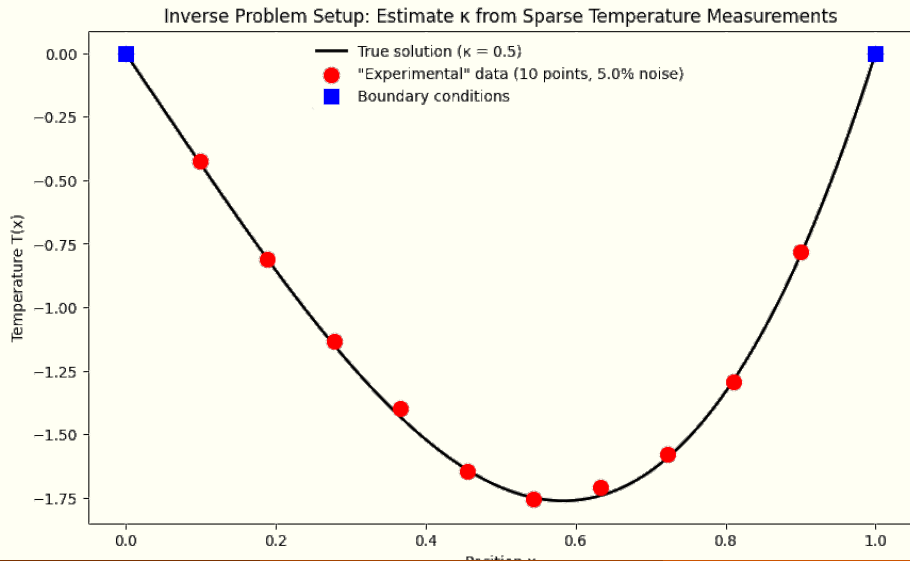
**PINN Framework:**

- The neural network learns the temperature field:  $\hat{T}_\theta(x)$ .
- A new trainable parameter is introduced:  $\hat{k}$ .
- The optimizer updates both the network weights  $\theta$  and the parameter  $\hat{k}$  simultaneously.

**Loss Function:**  $\mathcal{L}(\theta, \hat{k}) = \mathcal{L}_{\text{data}} + \mathcal{L}_{\text{PDE}} + \mathcal{L}_{\text{BC}}$  where the physics loss now includes the trainable parameter  $\hat{k}$ :

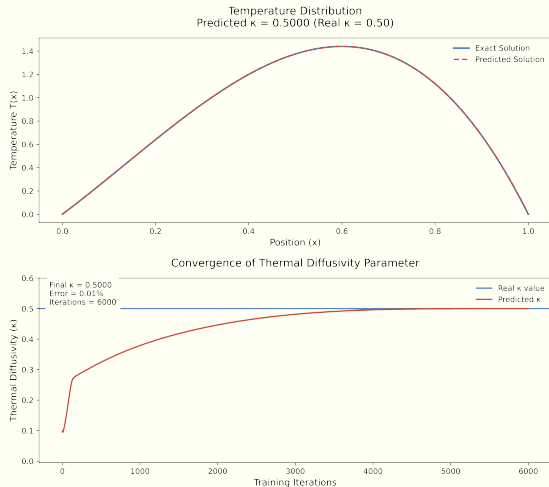
$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_f} \sum \left| -\hat{k} \frac{d^2 \hat{T}_\theta}{dx^2}(x_j) - f(x_j) \right|^2$$

# Implementation: Parameter Estimation





# Results: Parameter Recovery



- The estimated parameter  $\hat{\kappa}$  converges to the true value.
- The PINN simultaneously reconstructs the full, continuous temperature field accurately.
- This is achieved from very sparse and noisy data, showcasing the regularizing effect of the physics loss.

## Parameter convergence and temperature field

# Summary: Why PINNs are Powerful

## 1. Regularization Effect:

- Physics constraints prevent overfitting and guide the solution in data-sparse regions.

## 2. Data Efficiency:

- Physics provides a strong inductive bias, allowing PINNs to learn from very few measurements.

## 3. Accurate Derivatives:

- Automatic differentiation provides exact derivatives, which are learned correctly as a consequence of enforcing the physics.

## 4. Versatility:

- The same framework can solve forward problems, inverse problems, and handle various boundary conditions.

**PINNs = Universal Function Approx. + Physics Constraints + Auto. Diff.**

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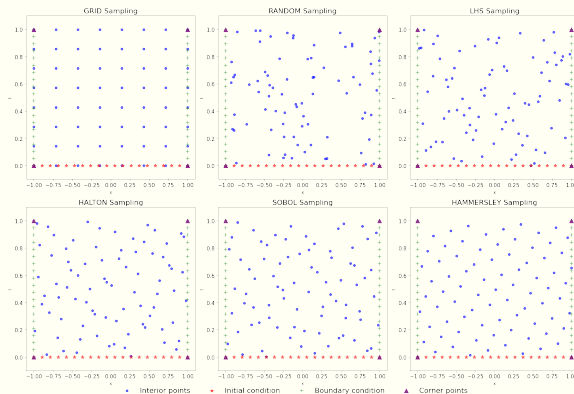
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# Collocation Points: Where to Enforce Physics

## What are collocation points?

- Points where we evaluate PDE residual
- Do not need measurement data
- Distributed throughout domain
- More points  $\rightarrow$  better physics enforcement

**Key question:** How should we distribute these points for optimal performance?



Different collocation sampling strategies

# Collocation Sampling Strategies

## Uniform Grid:

- Simple to implement
- Good coverage
- Curse of dimensionality

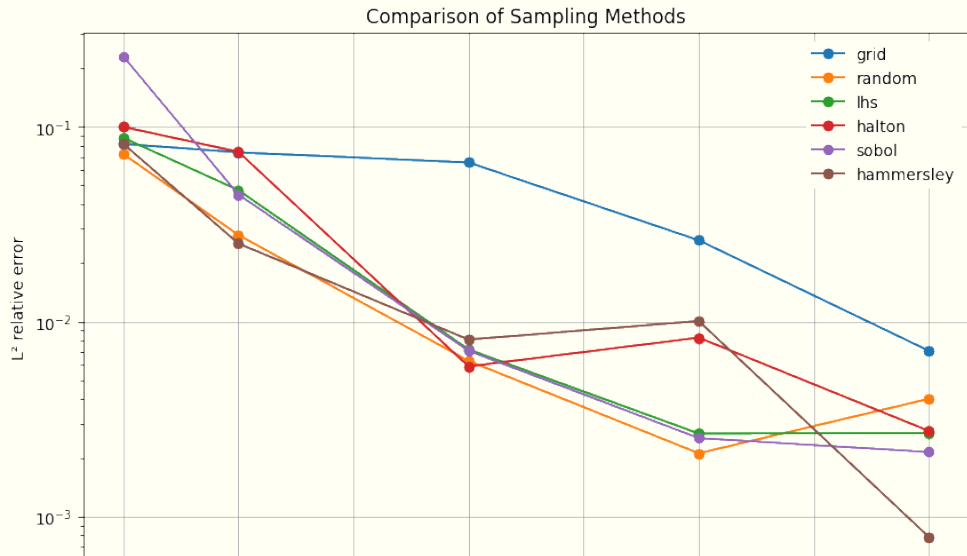
## Random (Monte Carlo):

- Dimension-independent
- May cluster/leave gaps
- Easy to add points

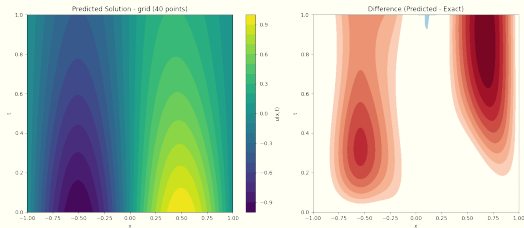
## Quasi-Random:

- Better coverage than random
- Low discrepancy sequences
- Hammersley, Sobol, Halton

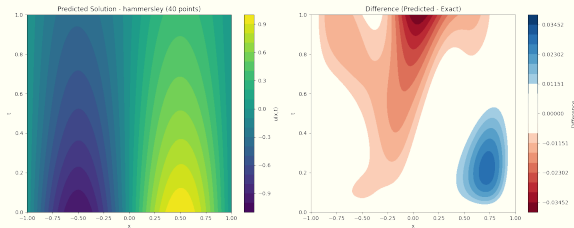
# Collocation Sampling Strategies



# Impact of Collocation Strategy



Error with uniform grid sampling



Error with Hammersley sampling

## Observations:

- Quasi-random sampling often outperforms uniform/random
- Better space-filling properties lead to lower errors
- Particularly important in higher dimensions

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# The Loss Balancing Challenge

## The Problem

Different loss terms can have vastly different magnitudes and gradients

**Total PINN loss:**

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda_{\text{PDE}}\mathcal{L}_{\text{PDE}} + \lambda_{\text{BC}}\mathcal{L}_{\text{BC}} + \lambda_{\text{IC}}\mathcal{L}_{\text{IC}}$$

**Challenges:**

- Data loss: Often  $O(10^{-3})$  to  $O(10^{-1})$
- PDE residual: Can be  $O(10^2)$  to  $O(10^4)$  initially
- Boundary conditions: Variable scale
- Poor balance  $\rightarrow$  training instability or failure

**Question:** How to choose  $\lambda$  values optimally?

# Gradient-Based Adaptive Weighting

**Key idea:** Balance the gradients of different loss terms

**Algorithm (Wang et al., 2021):**

- 1 Compute gradient statistics:

$$\bar{g}_i = \frac{1}{|\theta|} \sum_{\theta} |\nabla_{\theta} \mathcal{L}_i|$$

- 2 Update weights to balance gradients:

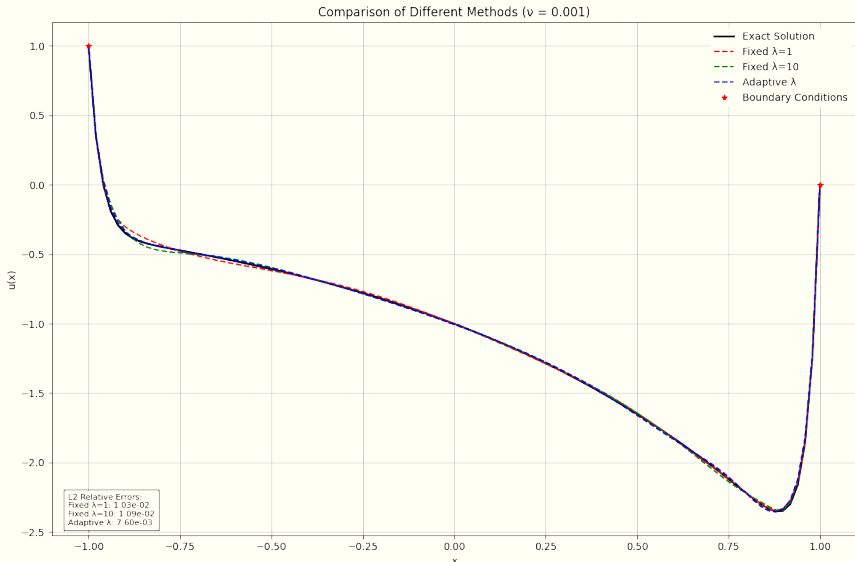
$$\lambda_i^{(k+1)} = \lambda_i^{(k)} \cdot \left( \frac{\max_j \bar{g}_j}{\bar{g}_i} \right)^{\alpha}$$

- 3 Apply exponential moving average for stability

**Benefits:**

- Prevents gradient imbalance
- Improves convergence speed
- Reduces manual tuning

# Adaptive Weights in Action



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# The Burgers Equation: A Nonlinear PDE Challenge

**Viscous Burgers equation:**

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

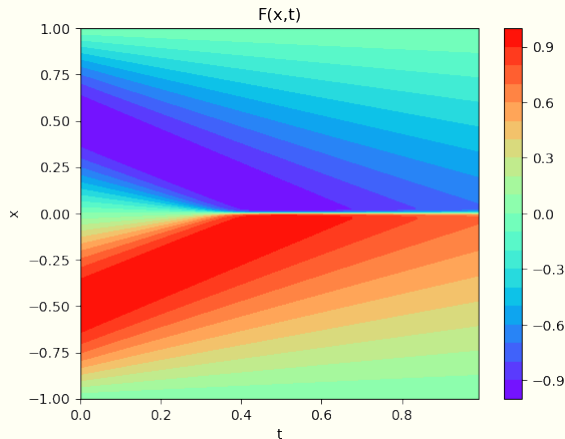
**Domain:**  $(x, t) \in [-1, 1] \times [0, 1]$

**Initial condition:**

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

**Boundary conditions:**

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



Burgers equation solution showing shock formation

# PINN for Burgers Equation

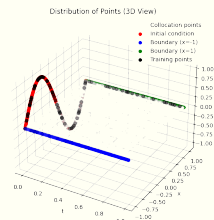
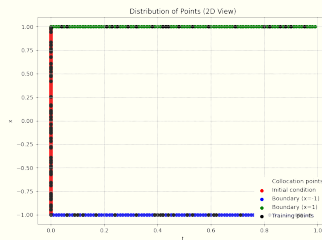
## Network architecture:

- Input:  $(x, t)$
- Output:  $u(x, t)$
- Hidden layers:  $8 \times 20$  neurons
- Activation: Tanh

## Loss function:

$$\mathcal{L} = \mathcal{L}_{\text{PDE}} + \mathcal{L}_{\text{IC}} + \mathcal{L}_{\text{BC}}$$

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_f} \sum \left| \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} \right|^2$$

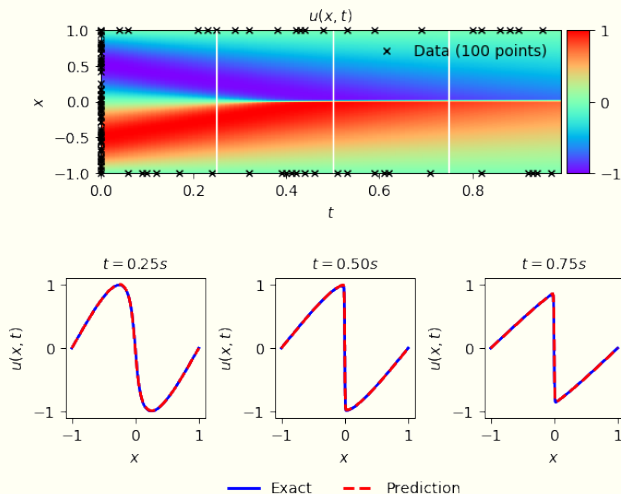


Collocation points for Burgers equation

# Burgers Equation: Forward Problem Results

## Performance metrics:

- Relative  $L^2$  error:  $< 1\%$
- Training time: 5 minutes on GPU
- No mesh required
- Captures shock accurately



# Inverse Problem: Parameter Discovery in Burgers

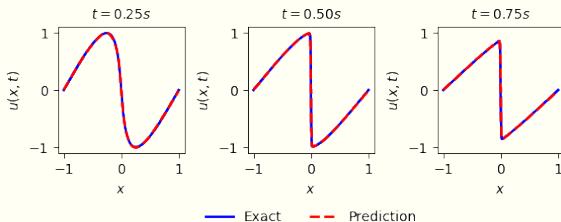
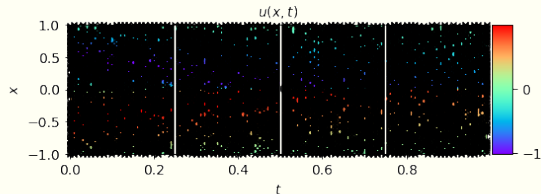
## Problem setup:

- Unknown viscosity  $\nu$
- Sparse measurements of  $u(x, t)$
- Goal: Recover  $\nu$  and full solution

## Modified loss:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda \mathcal{L}_{\text{PDE}}(\nu)$$

where  $\nu$  is a trainable parameter



Inverse problem: recovering solution from sparse



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# Why Discrete-Time PINNs?

## Limitations of Continuous-Time Approach:

- **Computational Cost:**  $O(N_x \times N_t)$  collocation points
- **Memory Issues:** Storing entire space-time solution
- **Training Difficulty:** Long-time behavior hard to capture
- **Stiff Problems:** Need very dense time sampling

**Example:** For Burgers equation on  $[-1, 1] \times [0, 10]$ :

- Continuous:  $100 \times 1000 = 100,000$  collocation points
- Discrete: 100 spatial points per time step

## Solution

Use time-stepping methods within PINN framework to evolve solution sequentially

# Continuous vs Discrete Time Approaches

## Continuous-Time PINNs:

- Treat time as another input:  
 $(x, t) \rightarrow u(x, t)$
- Learn entire space-time solution
- Many collocation points in time
- Can become expensive for long simulations

## Discrete-Time PINNs:

- Leverage classical time-stepping schemes
- Learn mapping from  $t^n \rightarrow t^{n+1}$
- Only spatial collocation needed
- More efficient for long time simulations

**Key Idea:** Integrate Runge-Kutta methods within the PINN framework

# Runge-Kutta Time-Stepping Foundation

For time-dependent PDEs in semi-discrete form:

$$\frac{du}{dt} = \mathcal{N}[u](t)$$

A  $q$ -stage Runge-Kutta method computes:

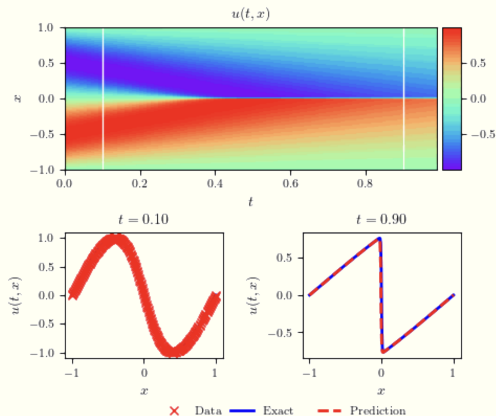
$$U^i = u^n + \Delta t \sum_{j=1}^q a_{ij} \mathcal{N}[U^j], \quad i = 1, \dots, q$$

$$u^{n+1} = u^n + \Delta t \sum_{j=1}^q b_j \mathcal{N}[U^j]$$

Where:

- $U^i$ : intermediate stage values
- $\{a_{ij}\}, \{b_j\}, \{c_j\}$ : RK coefficients (Butcher tableau)
- Implicit if  $a_{ij} \neq 0$  for  $j \geq i$

# Discrete-Time PINN Architecture



Network outputs  $q$  intermediate stages and final solution at  $t^{n+1}$

Network output:  $\mathcal{NN}(x; \theta) = [U_{NN}^1, \dots, U_{NN}^q, u_{NN}^{n+1}]^T$

# Training Discrete-Time PINNs

**Loss Function:** Enforce consistency with RK scheme

The RK equations provide multiple estimates of  $u^n(x)$ :

$$u^n(x) \approx U_{NN}^i(x) - \Delta t \sum_{j=1}^q a_{ij} \mathcal{N}[U_{NN}^j](x), \quad i = 1, \dots, q$$

$$u^n(x) \approx u_{NN}^{n+1}(x) - \Delta t \sum_{j=1}^q b_j \mathcal{N}[U_{NN}^j](x)$$

**Total Loss:**

$$\mathcal{L}(\theta) = \frac{1}{N_n(q+1)} \sum_{i=1}^{q+1} \sum_{k=1}^{N_n} |u_{i,NN}^n(x_k) - u^n(x_k)|^2$$

- All estimates should equal the known  $u^n(x)$
- Minimizing discrepancy enforces the physics
- Spatial derivatives computed via AD

# Algorithm: Single-Step Discrete-Time PINN

- 1: **Input:** Solution  $u^n(x)$  at time  $t^n$ , time step  $\Delta t$
- 2: **Input:** RK coefficients  $\{a_{ij}\}, \{b_j\}$  for  $q$  stages
- 3: Initialize network  $\mathcal{NN}(x; \theta) : x \rightarrow [U^1, \dots, U^q, u^{n+1}]$
- 4: **while** not converged **do**
- 5:   Sample spatial points  $\{x_k\}_{k=1}^{N_n}$  and-  $[U_{NN}^1, \dots, U_{NN}^q, u_{NN}^{n+1}] \leftarrow \mathcal{NN}(x_k; \theta)$
- 6:   **for**  $j = 1$  to  $q$  **do**
- 7:     Compute  $\mathcal{N}[U_{NN}^j] = -U_{NN}^j \frac{\partial U_{NN}^j}{\partial x} + \nu \frac{\partial^2 U_{NN}^j}{\partial x^2}$
- 8:   **end for**
- 9:   **for**  $i = 1$  to  $q$  **do**
- 10:      $u_{i,est}^n = U_{NN}^i - \Delta t \sum_j a_{ij} \mathcal{N}[U_{NN}^j]$
- 11:   **end for**
- 12:    $u_{q+1,est}^n = u_{NN}^{n+1} - \Delta t \sum_j b_j \mathcal{N}[U_{NN}^j]$  and  $\mathcal{L} = \frac{1}{(q+1)N_n} \sum_{i,k} |u_{i,est}^n(x_k) - u^n(x_k)|^2$
- 13:   Update  $\theta$  using gradient descent on  $\mathcal{L}$
- 14: **end while**
- 15: **Output:**  $u^{n+1}(x) = u_{q+1,est}^{n+1}(x; \theta^*)$

# Algorithm: Adaptive Time-Stepping

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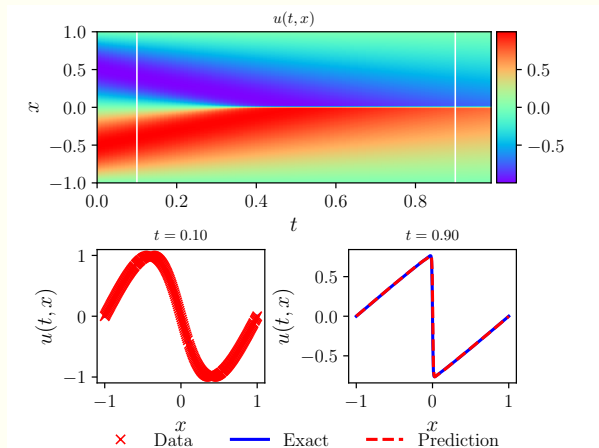
**Algorithm** Adaptive Discrete-Time PINN

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- 1: **Input:** Initial  $u^0(x)$ , target time  $T$ , tolerance  $\epsilon$
- 2: Initialize  $t = 0$ ,  $\Delta t = \Delta t_0$
- 3: **while**  $t < T$  **do**
- 4:   Train PINN for step  $t \rightarrow t + \Delta t$  (Algorithm 1)
- 5:   Compute error estimate  $E$  using embedded RK method:
- 6:      $E = \|u_{high}^{n+1} - u_{low}^{n+1}\|_2$
- 7:   **if**  $E < \epsilon$  **then**
- 8:     Accept step:  $u^{n+1} = u_{high}^{n+1}$ ;  $t = t + \Delta t$
- 9:     Adjust:  $\Delta t_{new} = 0.9\Delta t(\epsilon/E)^{1/p}$
- 10:   **else**
- 11:     Reject step, retrain with smaller  $\Delta t$  and update  $\Delta t = 0.5\Delta t$
- 12:   **end if**
- 13:    $\Delta t = \min(\Delta t_{new}, T - t)$
- 14: **end while**



# Discrete-Time Results: Burgers Equation



## Key Results:

- High accuracy with large time steps
- Stable evolution over long times
- Captures shock formation accurately

Discrete-time PINN prediction for Burgers equation using implicit Runge-Kutta

# Advantages of Discrete-Time PINNs

## Computational Efficiency:

- Loss evaluated only over spatial domain
- No time-dimension collocation points
- Drastically reduced training points

## Stability:

- Implicit RK schemes (e.g., Gauss-Legendre)
- Stable for large time steps
- Essential for stiff problems

## Accuracy Control:

- High-order temporal accuracy via stages
- Adding stages only increases output layer
- Less costly than deeper networks

## Leverages Numerical Analysis:

- Decades of research on time-stepping
- Proven stability properties
- Well-understood error bounds

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# From Strong Form to Energy Minimization

Many physical systems are governed by variational principles:

## Principle of Minimum Potential Energy

The true solution  $u(\mathbf{x})$  minimizes the total potential energy functional  $\Pi(u)$

**Total Potential Energy:**

$$\Pi(u) = \underbrace{\int_{\Omega} \Psi(\epsilon(u)) d\Omega}_{\text{Internal Energy}} - \underbrace{\int_{\Omega} f \cdot u d\Omega}_{\text{Body Forces}} - \underbrace{\int_{\Gamma_N} t \cdot u d\Gamma}_{\text{Surface Traction}}$$

**Deep Ritz Method:** Train PINN by minimizing energy instead of PDE residual

# Deriving the Energy Formulation

Starting from the strong form (equilibrium equations):

$$\nabla \cdot \sigma + f = 0 \text{ in } \Omega$$

**Step 1:** Multiply by test function  $v$  and integrate:

$$\int_{\Omega} (\nabla \cdot \sigma) \cdot v \, d\Omega + \int_{\Omega} f \cdot v \, d\Omega = 0$$

**Step 2:** Apply integration by parts:

$$- \int_{\Omega} \sigma : \nabla v \, d\Omega + \int_{\Gamma} (\sigma \cdot n) \cdot v \, d\Gamma + \int_{\Omega} f \cdot v \, d\Omega = 0$$

**Step 3:** For  $v = \delta u$  (virtual displacement), this becomes:

$$\delta \Pi = 0 \quad \Rightarrow \quad \text{Stationarity of } \Pi(u)$$

# Implementation: Strain Energy Density

For linear elasticity with Lamé parameters  $\lambda, \mu$ :

**Strain energy density:**

$$\Psi(\epsilon) = \frac{\lambda}{2}(\text{tr}(\epsilon))^2 + \mu \text{tr}(\epsilon^2)$$

Expanding:

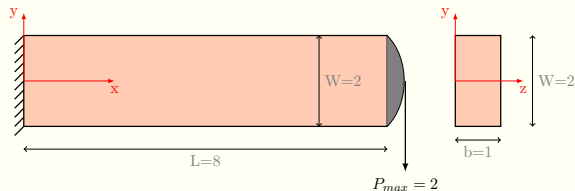
$$\Psi = \frac{\lambda}{2}(\epsilon_{xx} + \epsilon_{yy})^2 + \mu(\epsilon_{xx}^2 + \epsilon_{yy}^2 + 2\epsilon_{xy}^2)$$

```
def strain_energy_density(epsilon_xx, epsilon_yy, epsilon_xy):  
    # First term: lambda*(trace)^2  
    psi_1 = 0.5 * lambda_ * (epsilon_xx + epsilon_yy)**2  
  
    # Second term: mu*tr(epsilon^2)  
    psi_2 = mu * (epsilon_xx**2 + epsilon_yy**2 + 2*epsilon_xy**2)  
  
    return psi_1 + psi_2
```

# Computing Total Potential Energy

```
def potential_energy(x_colloc, y_colloc, x_bound, y_bound):  
    # Compute strains at collocation points  
    epsilon_xx, epsilon_yy, epsilon_xy = strain(x_colloc, y_colloc)  
  
    # Strain energy density  
    psi = strain_energy_density(epsilon_xx, epsilon_yy, epsilon_xy)  
  
    # Numerical integration over domain  
    dx = L / (Nx - 1)  
    dy = W / (Ny - 1)  
    internal_energy = (psi * dx * dy).sum()  
  
    # External work on boundary  
    u_bound = net_u(x_bound, y_bound)  
    v_bound = net_v(x_bound, y_bound)  
    t_x = traction_x(y_bound)  
    t_y = traction_y(y_bound)  
  
    external_work = ((t_x * u_bound + t_y * v_bound) * dy).sum()  
  
    # Total potential energy  
    return internal_energy - external_work
```

# Example: 2D Cantilever Beam



Cantilever beam: fixed at  $x = 0$ , loaded at  $x = L$

## Problem Setup:

- Linear elasticity
- Fixed end:  $u(0, y) = g_u(y)$ ,  
 $v(0, y) = g_v(y)$
- Free end: traction  $\mathbf{t}$

## Approach:

- Strong BC enforcement
- Energy minimization



# Strong BC Enforcement with Trial Functions

**Problem:** Enforce  $u(x=0, y) = g_u(y)$  and  $v(x=0, y) = g_v(y)$

**Solution:** Construct trial functions that satisfy BCs by design

$$\tilde{u}(x, y) = g_u(y) + \mathcal{D}(x) \cdot \hat{u}_{NN}(x, y)$$

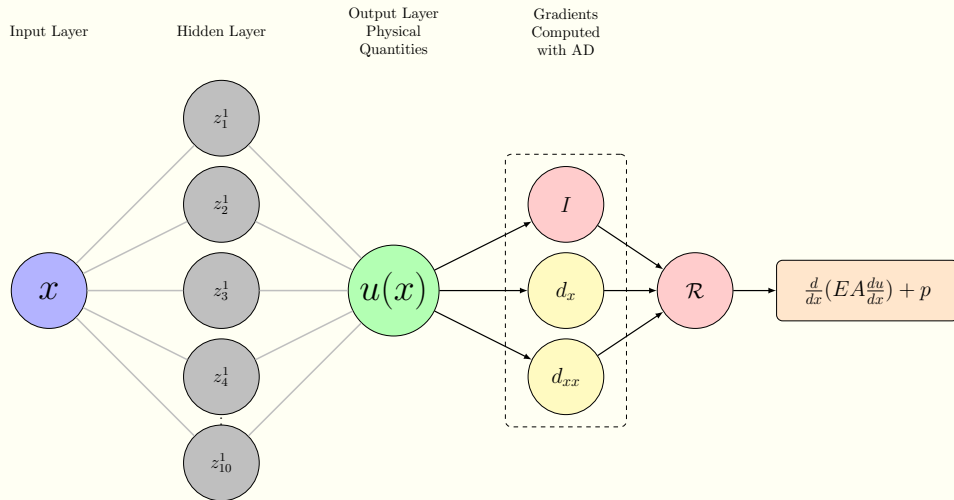
$$\tilde{v}(x, y) = g_v(y) + \mathcal{D}(x) \cdot \hat{v}_{NN}(x, y)$$

Where:

- $\mathcal{D}(x)$ : Distance function, zero at boundary
- $g_u(y), g_v(y)$ : Prescribed boundary values (from beam theory)
- $\hat{u}_{NN}, \hat{v}_{NN}$ : Network outputs

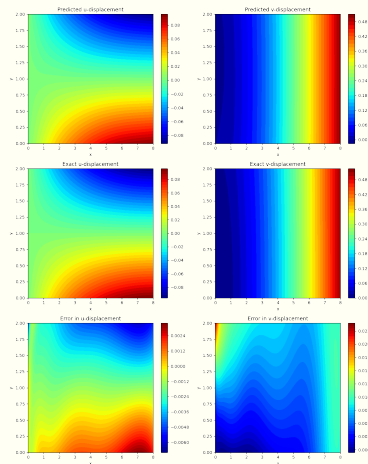
**Example:** For cantilever beam,  $\mathcal{D}(x) = x/L$  (simple linear function)

# PINN Architecture for Elasticity



Architecture for linear elasticity using energy minimization

# Results: 2D Cantilever Beam

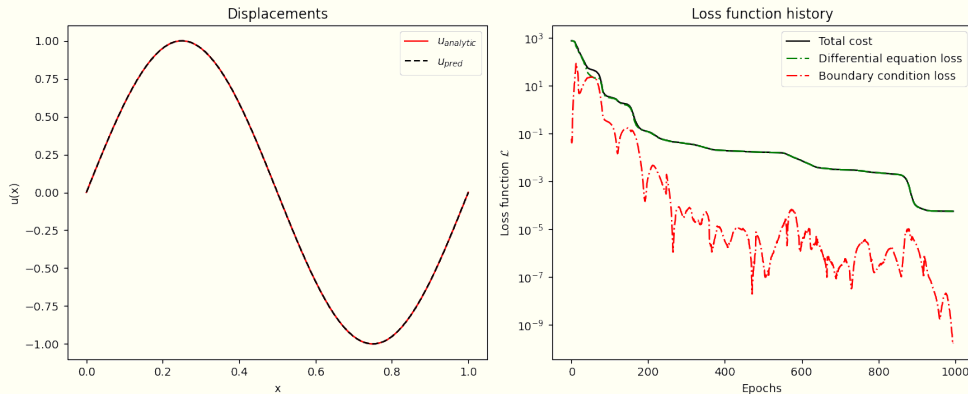


## Performance:

- Relative  $L^2$  error:  $2.4 \times 10^{-3}$
- Exact satisfaction of fixed-end BCs
- Slightly larger errors near loaded end (expected)
- No BC loss terms needed!

Error distribution using strong BC enforcement and energy minimization

# Static Beam: Complete Solution



Displacement and stress fields computed using energy minimization

## Observations:

- Smooth displacement fields

# Advantages of Energy Minimization

## Physical Meaning:

- Direct minimization of physical quantity
- Guaranteed energy conservation
- Natural handling of constraints

## Computational Benefits:

- Only first derivatives needed
- Better conditioned optimization
- No need for BC loss terms

## Improved Stability:

- Convex for linear problems
- Smoother loss landscape
- Faster convergence

## Applicability:

- Conservative systems
- Elasticity, electrostatics
- Not for dissipative systems

**When applicable, energy minimization often outperforms strong form**

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# Implementation Best Practices

## Architecture design:

- Start with 4-8 layers, 20-50 neurons
- Tanh or Swish for smooth problems
- Adaptive activation functions for shocks
- Skip connections for deep networks

## Training strategies:

- Adam optimizer with learning rate decay
- Start with  $\lambda = 1$ , then adapt
- Quasi-random collocation points
- Mini-batching for large problems

## Common pitfalls:

- Imbalanced loss terms
- Too few collocation points
- Wrong activation for problem type
- Ignoring boundary conditions

## Debugging tips:

- Visualize loss components separately
- Check gradient flow
- Start with manufactured solutions
- Verify BC/IC satisfaction

# When to Use PINNs

## **PINNs excel at:**

- Inverse problems
- Data assimilation
- High-dimensional PDEs
- Irregular geometries
- Parameter discovery
- Uncertainty quantification

## **Consider alternatives when:**

- Need guaranteed accuracy
- Have simple, regular geometry
- Require real-time solutions
- Conservation is critical
- Problem is well-suited to FEM/FDM

**PINNs complement, not replace, traditional methods**



Thank you!

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