CS598: Physics-Informed Neural Networks: A deep learning framework for solving forward and inverse problems involving nonlinear PDEs

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DNNs: Universal Approximators

- Identify a nonlinear map from a few – potentially very high dimensional – input and output pairs of data

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PDEs

- Need both initial conditions and boundary conditions
- Point Collocation methods: Function Approximation + point evaluation, e.g. consider an approximation problem for a function $u(x)$ on $x \in (0, 1)$,

$$u(x) \sim \widetilde{u}(x) = a_0 + a_1 x + a_2 x^2; \quad \text{with} \quad \widetilde{u}\,(x_j) = \hat{u}_j,\ j = 1, 2$$

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Problem setup

- Parameterized, nonlinear PDE(s)

$$u_t + \mathcal{N}[u;\lambda] = 0, x \in \Omega \subset \mathbb{R}^D,\ t \in [0, T]; \quad (\cdot)_t = \frac{\partial\,(\cdot)}{\partial t}$$

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- The above setup covers a wide range of PDEs in math. physics, including conservation laws, diffusion, reac-diff-advec. PDE, kinetics etc. E.g., Burger's equation in 2D

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- Given λ what is $u(t,x)$ (Inference, filtering and smoothing or simply **data-driven solutions of PDEs**)
- Find λ that best describes observations $u(t_i, x_j)$ (Learning, system identification, or **data-driven discovery of PDEs**)

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Data-driven solutions

- Rewrite the PDE as $f(u; t, x) = 0$

$$f(u; t, x) \doteq u_t + \mathcal{N}[u], \quad \text{along with} \quad u = u_\theta(t, x)$$

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- Along with the above constraint (+ AD) this gives *Physics-informed neural network* **parameterized by θ**

$$\mathcal{L} = \mathcal{L}_u + \mathcal{L}_f$$

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- $\mathcal{L}_u$ helps to enforce initial and boundary data accurately, while $\mathcal{L}_f$ imposes the structure of the PDE into the total loss

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Data-driven solutions: Examples

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  - Optimizer: L-BFGS (quasi-second order)
  - Full-batch
- No theoretical guarantees, but as long as the PDE is well-posed $\Longrightarrow$ optimizer will find the solution

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Schrödinger equation

- Strong form of the PDE (note that $h(t,x) = u(t,x) + \mathrm{i}\, v(t,x)$)

$$
\begin{aligned}
f \doteq ih_t + 0.5h_{xx} + |h|^2 h = 0, \quad x \in [-5,5], \quad t \in [0,\pi/2] \\
h(0,x) = 2\,\mathrm{sech}(x) \\
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$$
\mathcal{L}_b = \frac{1}{N_b} \sum_{i=1}^{N_b} \left(\left| h^i\left(t_b^i, -5\right) - h^i\left(t_b^i, 5\right) \right|^2 + \left| h_x^i\left(t_b^i, -5\right) - h_x^i\left(t_b^i, 5\right) \right|^2 \right)
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Potential issues

- Continuous time NN models require a large number of collocation points through the domain N_f

Schrödinger equation

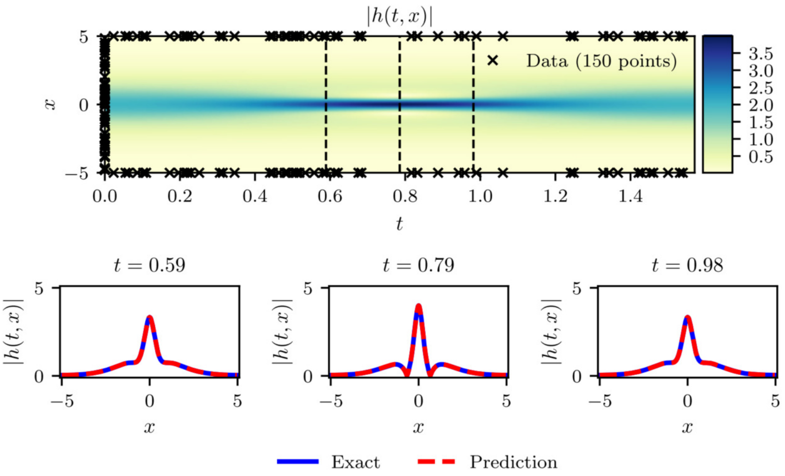

Figure: Top: Boundary and Initial data (150 points), Bottom: Snapshots of the solution of the Schrödinger equation using a PINN

Schrödinger equation

Flexible time-steppers:

Schrödinger equation

Flexible time-steppers:

- Use a generalized RK method with, say, q stages

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

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

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- The above update can be rewritten as

$$u^n = u_i^n, \quad i = 1, \ldots, q; \quad \text{and} \quad u^n = u_{q+1}^n$$

with

$$u_i^n \doteq u^{n+c_i} + \Delta t \sum_{j=1}^{q} a_{ij} \mathcal{N}\left[u^{n+c_j}\right], \quad i = 1, \ldots, q$$

$$u_{q+1}^n \doteq u^{n+1} + \Delta t \sum_{j=1}^{q} b_j \mathcal{N}\left[u^{n+c_j}\right]$$

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Allen-Cahn Equation

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- Make use of the above adaptive time-stepper

$$
\begin{aligned}
&u_t - 0.0001 u_{xx} + 5u^3 - 5u = 0, \quad x \in [-1, 1], \quad t \in [0, 1],\\
&u(0, x) = x^2 \cos(\pi x),\\
&u(t, -1) = u(t, 1),\\
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- The differential operator: $\mathcal{N}\left[u^{n+c_j}\right] = -0.0001 u_{xx}^{n+c_j} + 5\left(u^{n+c_j}\right)^3 - 5u^{n+c_j}$

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- The differential operator: $\mathcal{N}\left[u^{n+c_j}\right] = -0.0001 u_{xx}^{n+c_j} + 5\left(u^{n+c_j}\right)^3 - 5u^{n+c_j}$
- The loss function is the sum of squared losses

$$
SSE_n = \sum_{j=1}^{q+1} \sum_{i=1}^{N_n} \left| u_j^n\left(x^{n,i}\right) - u^{n,i} \right|^2
$$

$$
\begin{aligned}
SSE_b = &\sum_{i=1}^{q} \left| u^{n+c_i}(-1) - u^{n+c_i}(1) \right|^2 + \left| u^{n+1}(-1) - u^{n+1}(1) \right|^2\\
&+ \sum_{i=1}^{q} \left| u_x^{n+c_i}(-1) - u_x^{n+c_i}(1) \right|^2 + \left| u_x^{n+1}(-1) - u_x^{n+1}(1) \right|^2
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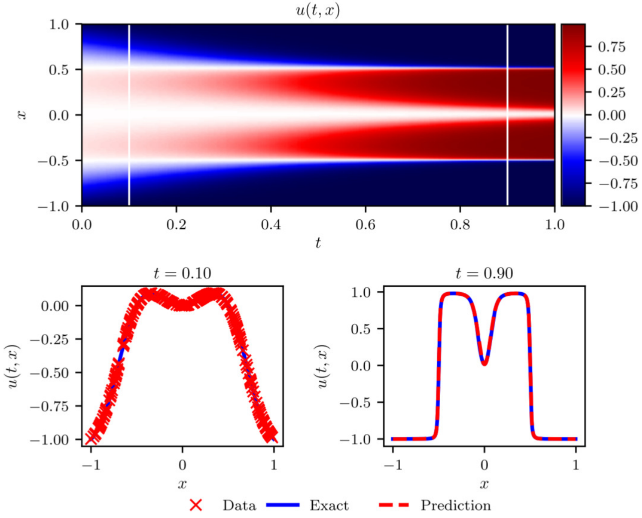

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Data-driven discovery of PDEs: Navier Stokes

Navier-Stokes Equations

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Navier-Stokes Equations

- Describe the physics of many phenomena, such as weather, ocean currents, water flow in a pipe and air flow around a wing.

$$\begin{aligned} u_t + \lambda_1 \left(u u_x + v u_y \right) &= -p_x + \lambda_2 \left(u_{xx} + u_{yy} \right) \\ v_t + \lambda_1 \left(u v_x + v v_y \right) &= -p_y + \lambda_2 \left(v_{xx} + v_{yy} \right) \end{aligned}; \quad \text{where} \quad (\cdot)_x = \frac{\partial (\cdot)}{\partial x}$$

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- $u(t, x, y)$ denotes the x-component of the velocity, $v(t, x, y)$ denotes the y component and $p(t, x, y)$ the pressure
- Conservation of mass: $u_x + v_y = 0 \implies u = \psi_y, \quad v = -\psi_x$

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Navier-Stokes Equations

- Describe the physics of many phenomena, such as weather, ocean currents, water flow in a pipe and air flow around a wing.

$$\begin{array}{l} u_t + \lambda_1 (u u_x + v u_y) = -p_x + \lambda_2 (u_{xx} + u_{yy}) \\ v_t + \lambda_1 (u v_x + v v_y) = -p_y + \lambda_2 (v_{xx} + v_{yy}) \end{array}; \quad \text{where} \quad (\cdot)_x = \frac{\partial (\cdot)}{\partial x}$$

- $u(t, x, y)$ denotes the x-component of the velocity, $v(t, x, y)$ denotes the y component and $p(t, x, y)$ the pressure
- Conservation of mass: $u_x + v_y = 0 \implies u = \psi_y, \quad v = -\psi_x$
- Given a set of observations: $\left\{t^i, x^i, y^i, u^i, v^i\right\}_{i=1}^N$

$$\begin{aligned} f &\doteq u_t + \lambda_1 (u u_x + v u_y) + p_x - \lambda_2 (u_{xx} + u_{yy}) \\ g &\doteq v_t + \lambda_1 (u v_x + v v_y) + p_y - \lambda_2 (v_{xx} + v_{yy}) \end{aligned}$$

Data-driven discovery of PDEs: Navier Stokes

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- Learn $\lambda = \{\lambda_1, \lambda_2\}$, and pressure field $p(t,x,y)$ by jointly approximating $[\psi(t,x,y) \quad p(t,x,y)]$ with a single NN with two outputs

Data-driven discovery of PDEs: Navier Stokes

Navier-Stokes Equations

Navier-Stokes Equations

- Train by minimizing the total loss

$$\mathcal{L} \doteq \frac{1}{N}\sum_{i=1}^{N}\left(\left|u\left(t^i,x^i,y^i\right)-u^i\right|^2+\left|v\left(t^i,x^i,y^i\right)-v^i\right|^2\right)$$
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- Consider the prototypical problem of an incompressible flow past a (rigid) cylinder, with various values of the Reynolds number $Re = u_\infty D/\nu$

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- Higher order piecewise approximation in space (tenth-order jacobi polynomials), third-order approximation in time (stable for stiff problems)
- Given stream-wise $u(t,x,y)$ and transverse $v(t,x,y)$ velocity data, identify unknown $\lambda = \{\lambda_1, \lambda_2\}$ as well as reconstruct $p(t,x,y)$

Navier-Stokes PDE

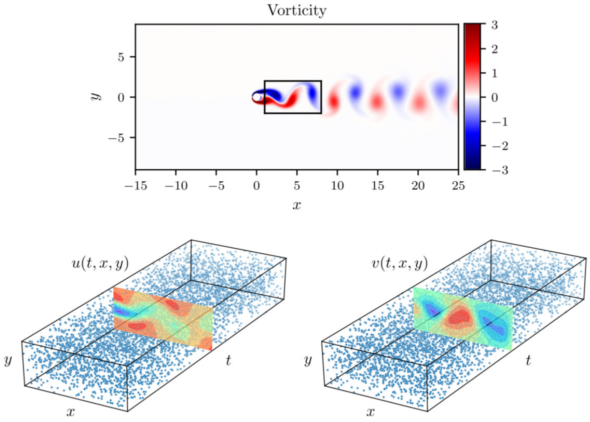

Figure: Navier-Stokes equation: **Top**: Incompressible flow and dynamic vortex shedding past a circular cylinder at Re $= 100$. The spatio-temporal training data correspond to the depicted rectangular region in the cylinder wake. **Bottom**: Locations of training data-points for the stream-wise and transverse velocity components, $u(t, x, y)$ and $v(t, x, t)$, respectively.

Navier-Stokes PDE: Observations

- Set $N = 5000 \sim 1\%$ of the total available data

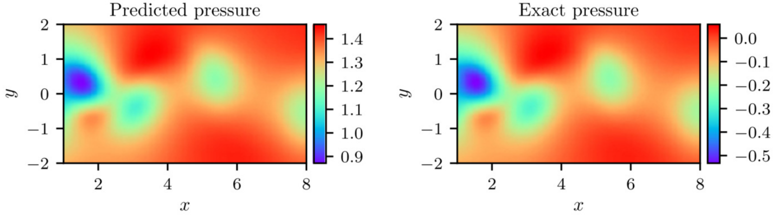

Figure: Results for predicted pressure field

Correct PDE	$u_t + (uu_x + vu_y) = -p_x + 0.01\,(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01\,(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.999\,(uu_x + vu_y) = -p_x + 0.01047\,(u_{xx} + u_{yy})$ $v_t + 0.999\,(uv_x + vv_y) = -p_y + 0.01047\,(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.998\,(uu_x + vu_y) = -p_x + 0.01057\,(u_{xx} + u_{yy})$ $v_t + 0.998\,(uv_x + vv_y) = -p_y + 0.01057\,(v_{xx} + v_{yy})$

Table: Correct partial differential equation along with the identified one obtained by learning λ_1, λ_2 and $p(t, x, y)$.

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Korteweg-de Vries equation

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- KdV equation has higher order derivatives (models shallow water waves)

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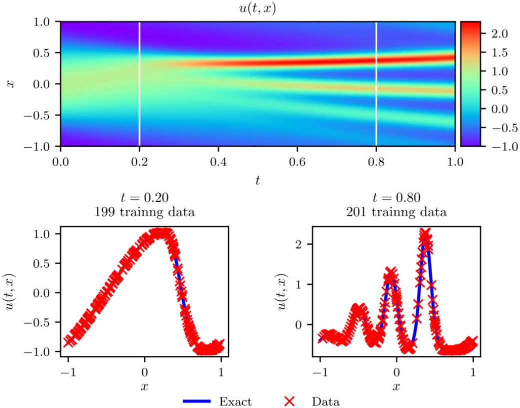
- Learn a set of parameters (similar to NS)

$$\mathcal{N}\left[u^{n+c_j}\right] = \lambda_1 u^{n+c_j} u_x^{n+c_j} - \lambda_2 u_{xxx}^{n+c_j}$$



Korteweg-de Vries equation

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- Even for large temporal variations in the solution, the model is able to resolve the dynamics accurately

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- Can we improve on initializing the network weights or normalizing the data? Loss function choices (MSE, SSE)? Robustness?

Code

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- IDRLNet: https://github.com/idrl-lab/idrlnet (PyTorch)

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