Physics-informed neural networks

Pause and Ponder

3. What activation function should I choose when using 1 hidden layer NN to approximate functions?

    E.g. A pulse function → use tanh, sigmoid rather than sin, cos

4. Where should I place the collocation points?

    Nabian et al., 2021: Sampling the collocation points according to a distribution proportional to the loss function will improve the convergence behavior of the PINNs training.

Nabian, Mohammad Amin, Rini Jasmine Gladstone, and Hadi Meidani. "Efficient training of physics-informed neural networks via importance sampling." *Computer-Aided Civil and Infrastructure Engineering* (2021).

Empirical learning vs PINN

- Empirical learning

  Need training data of $u_i(x_i, t_i)$ to approximate $u(x, t)$

- PINN

  Only need training data (or knowledge) at IC, BC.
  $u(x, t)$ within the x, t domain can be predicted **without training data within the domain** (just like a PDE solver)

PINN

$$\frac{\partial u}{\partial t} + N(u, \lambda) = 0, \qquad x \in [-L, L], \qquad t \in [0\ T]$$

- Application 1: Prediction of solution for a well-posed problem (this is what a traditional numerical solver can do)

  Given an eqn + BC + IC and parameters λ, what's the model prediction?

- Application 2: Prediction of solution when data is available within the domain but not at the IC, BC (difficult for a traditional numerical solver!)

  Given an eqn and parameters λ, what's the model prediction best describes the data?

- Application 3: Data-driven discovery of unknown parameters (difficult for a traditional numerical solver!)

  What are the parameters λ that best describe the data and the eqn?

E.g., Nonlinear Schrodinger equation

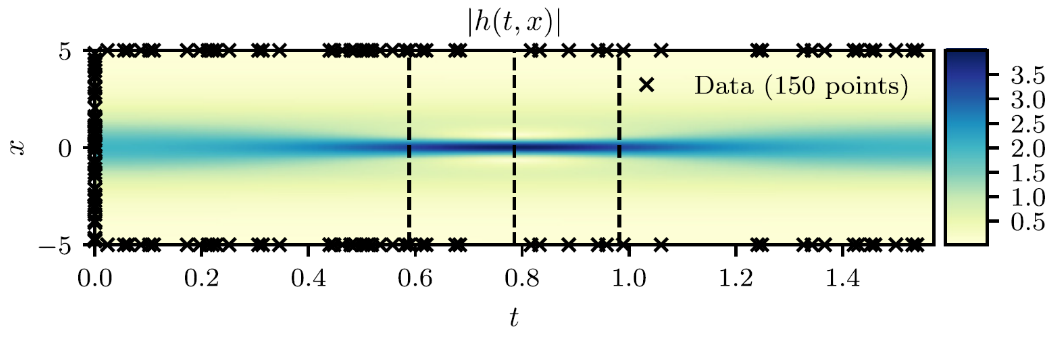
Problem statement

$$ih_t + 0.5h_{xx} + |h|^2 h = 0, \quad x \in [-5, 5], \quad t \in [0, \pi/2],$$

$$IC: \; h(0, x) = 2\,\text{sech}(x),$$

$$BC: \; h(t, -5) = h(t, 5),$$

$$h_x(t, -5) = h_x(t, 5),$$



Training data (from ground truth):

$$\{x_0^i, h_0^i\}_{i=1}^{N_0}$$

Collocation points:

$$\{t_b^i\}_{i=1}^{N_b} \qquad \{t_f^i, x_f^i\}_{i=1}^{N_f}$$

Physics equations:

$$f := ih_t + 0.5h_{xx} + |h|^2 h,$$

Loss function:

$$MSE_0 = \frac{1}{N_0} \sum_{i=1}^{N_0} |h(0, x_0^i) - h_0^i|^2,$$ (1) IC

$$MSE_b = \frac{1}{N_b} \sum_{i=1}^{N_b} \left(|h^i(t_b^i, -5) - h^i(t_b^i, 5)|^2 + |h_x^i(t_b^i, -5) - h_x^i(t_b^i, 5)|^2 \right)$$

(2) BC

$$MSE_f = \frac{1}{N_f} \sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2.$$ (3) Eqn

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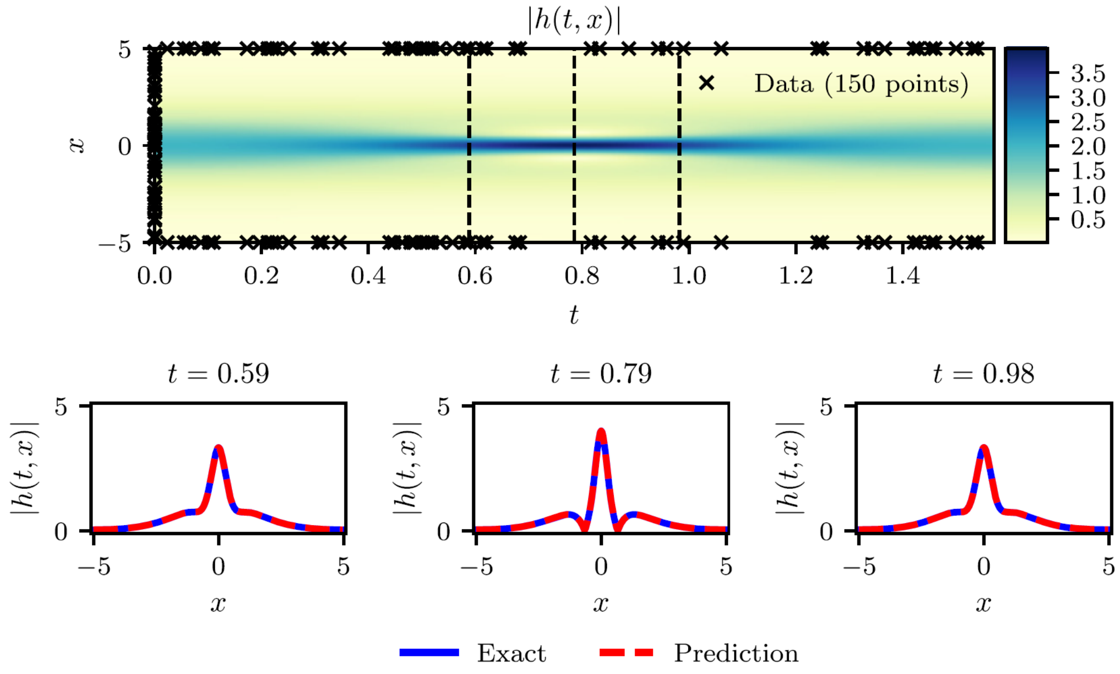


Trick

$h = u + iv$

eqn becomes

$i(u + iv)_t + 0.5(u_{xx} + iv_{xx}) + (u^2 + v^2)(u + iv) = 0$

IC: $u + iv\ (0, x) = 2\mathrm{sech}(x)$

BC: $u(t, -5) = u(t, -5),\ v(t, -5) = v(t, -5)$

$u_x(t, -5) = u_x(t, -5),\ v_x(t, -5) = v_x(t, -5)$

NN input: x,t

NN output: u,v

NN architecture: 5 layers 100 neurons per layer

Data points: 50 pts at t=0 (2sech(x))

Collocation points: 50 pts at x=5, x=-5,

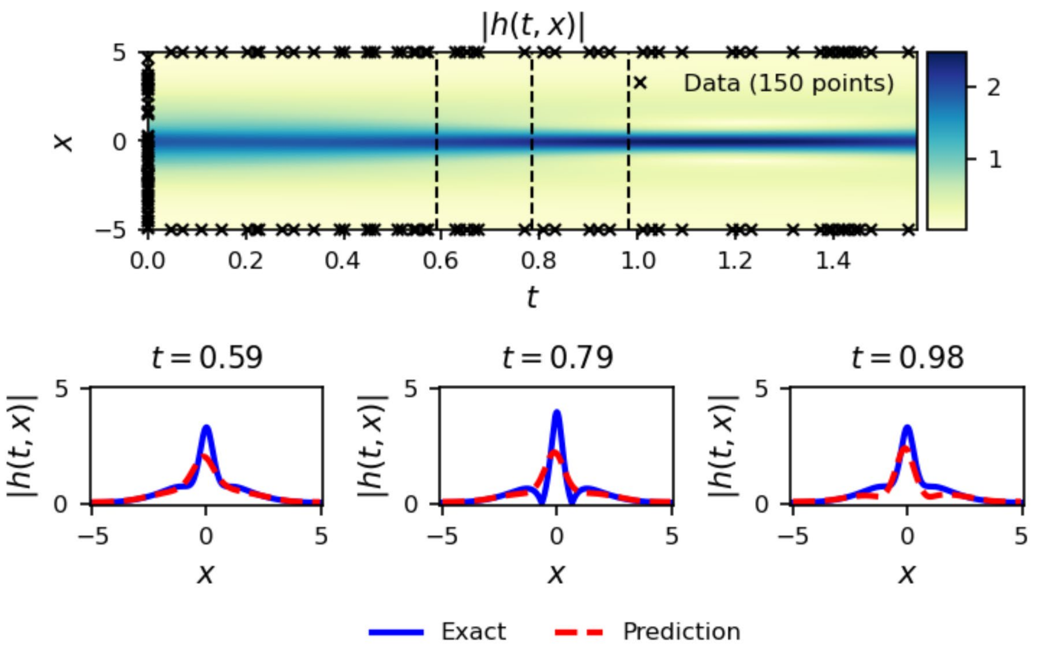
20000 pts within the domain

Schrodinger equation coding exercise

- TF1.14

layers = [2, 100, 100, 100, 100, 2]
Iterations: 2000

Tanh activation



Cos activation