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Neural PDEs

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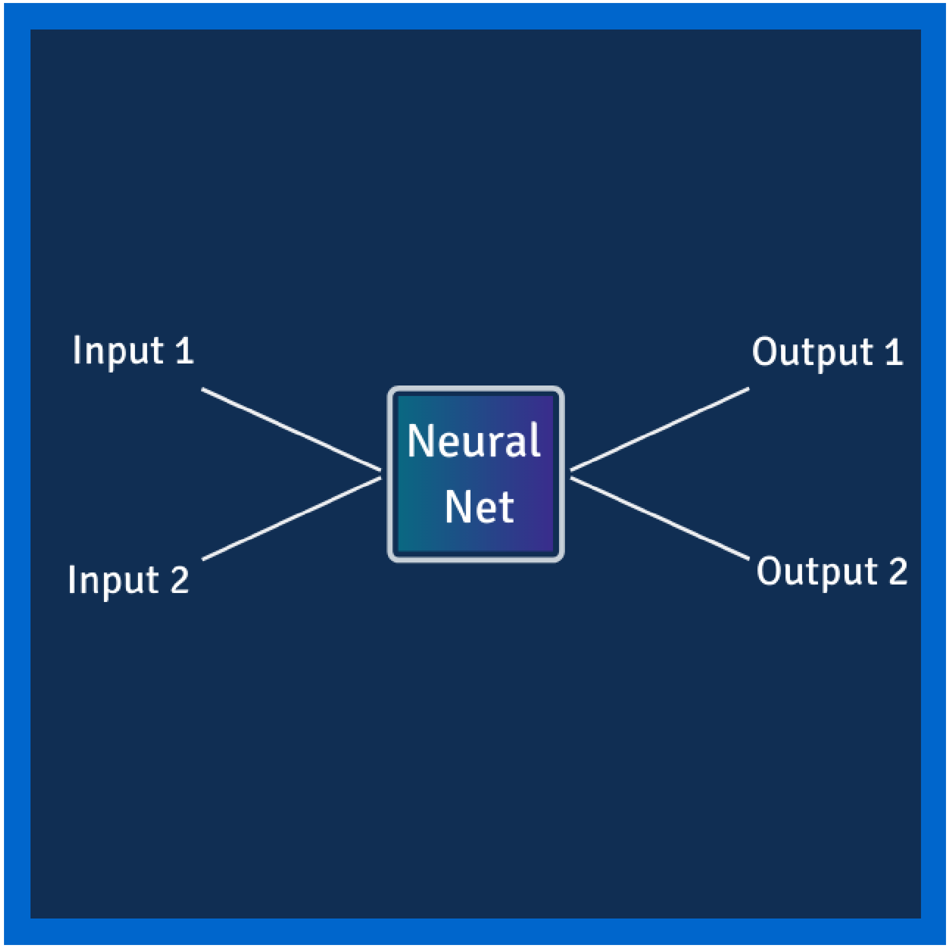
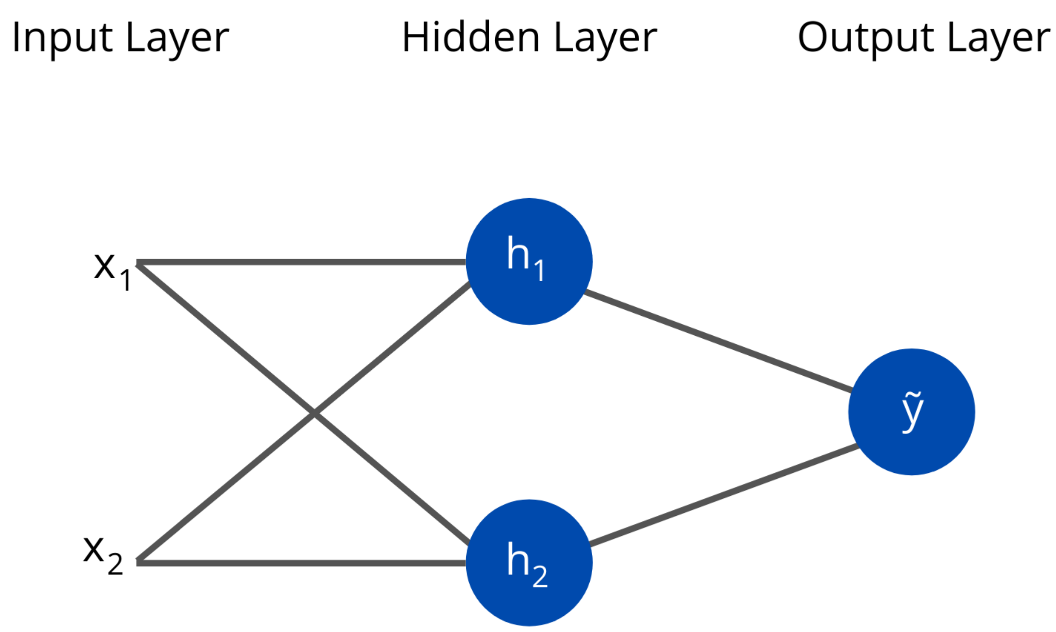
Fusion-EP Talks **28th May, 2020**

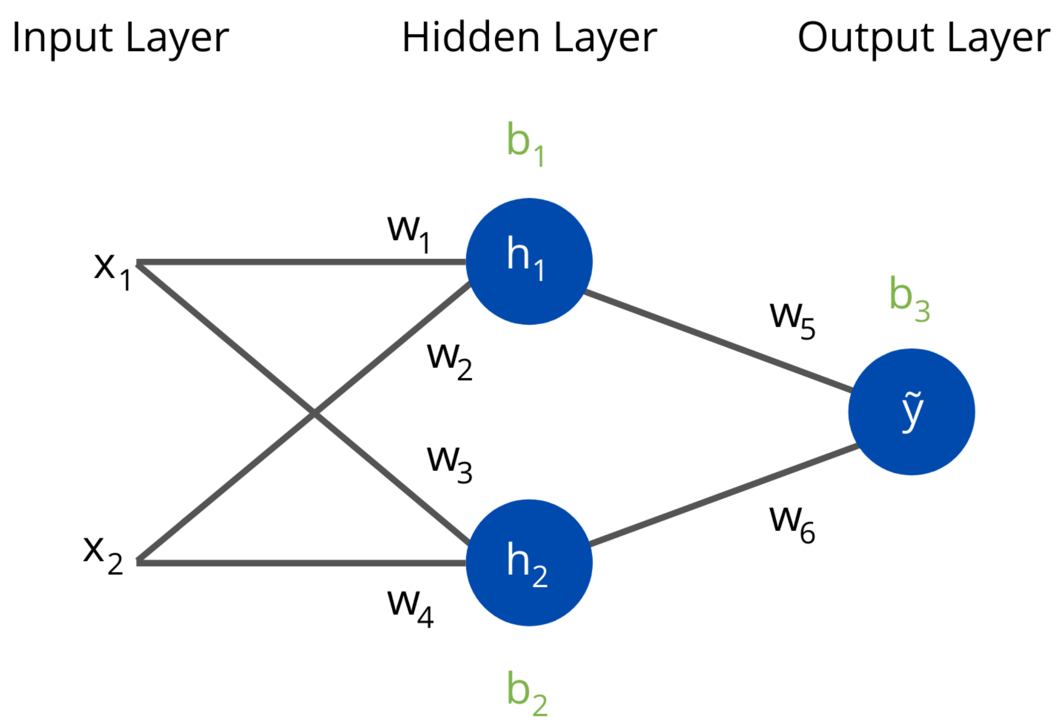
Regular NNs



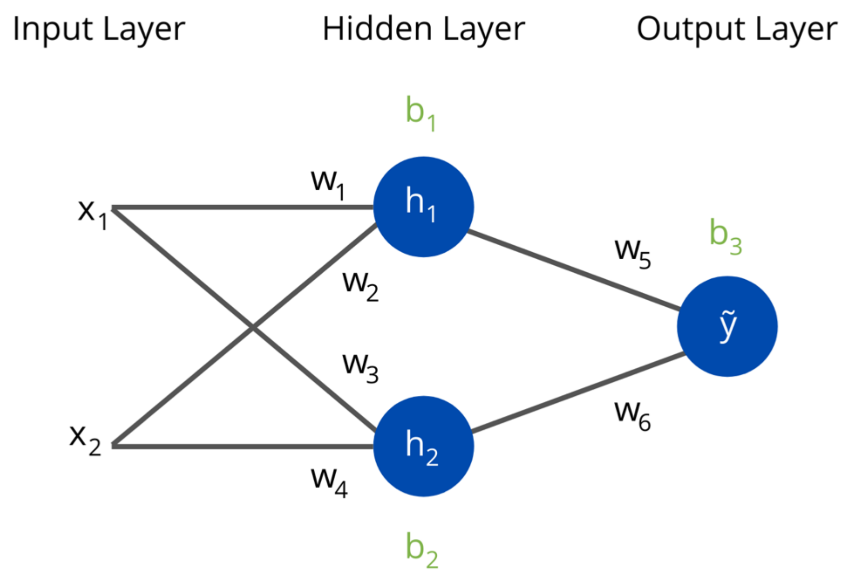
Feedforward Structure



Feedforward Structure



Feedforward Structure



$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

Backpropagation

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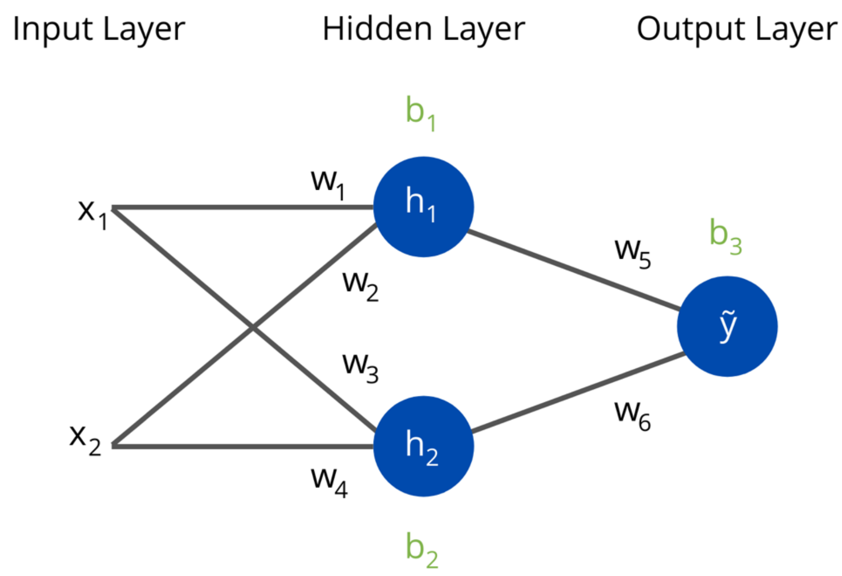


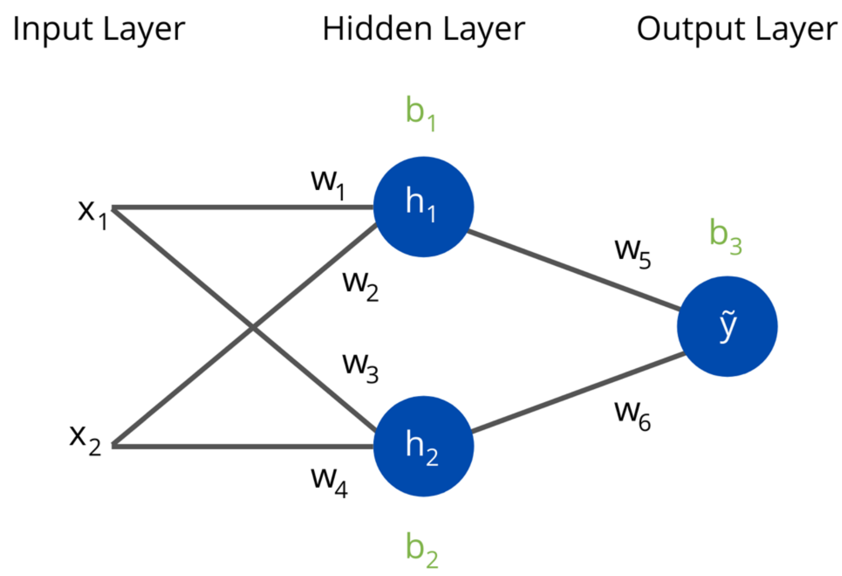
$$L = (y - \tilde{y})^2$$

$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

Backpropagation



$$L = (y - \tilde{y})^\wedge 2$$

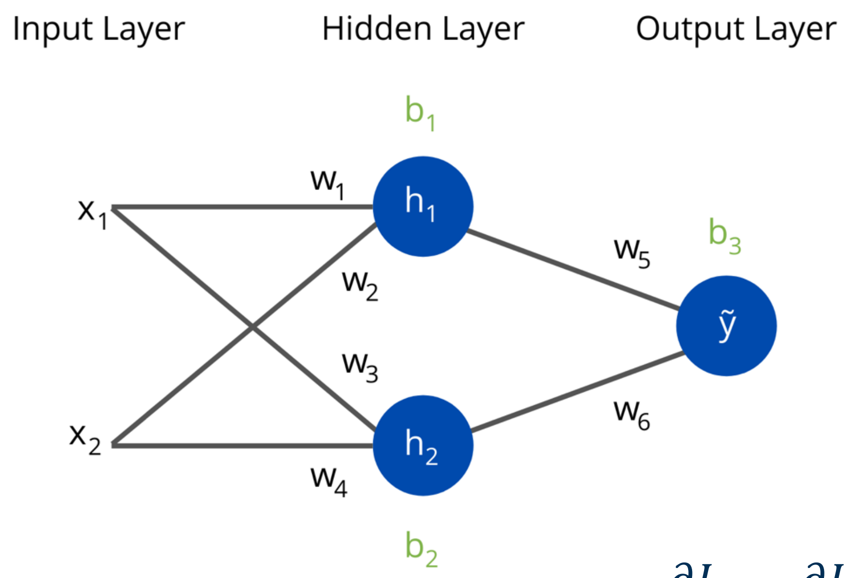
$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial L}{\partial w} = ?$$

Backpropagation



$$L = (y - \tilde{y})^2$$

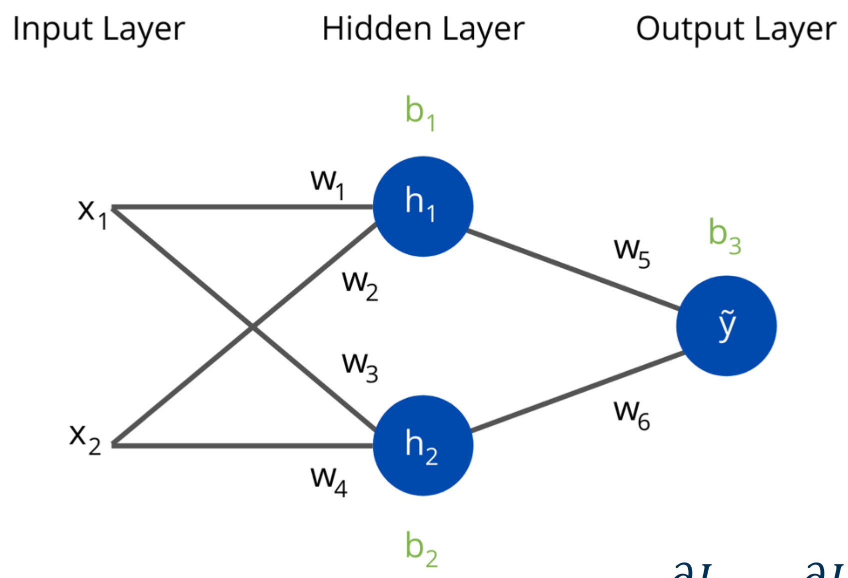
$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \tilde{y}} * \frac{\partial \tilde{y}}{\partial h_1} * \frac{\partial h_1}{\partial w_1}$$

$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

Backpropagation



$$L = (y - \tilde{y})^2$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \tilde{y}} * \frac{\partial \tilde{y}}{\partial h_1} * \frac{\partial h_1}{\partial w_1}$$

$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

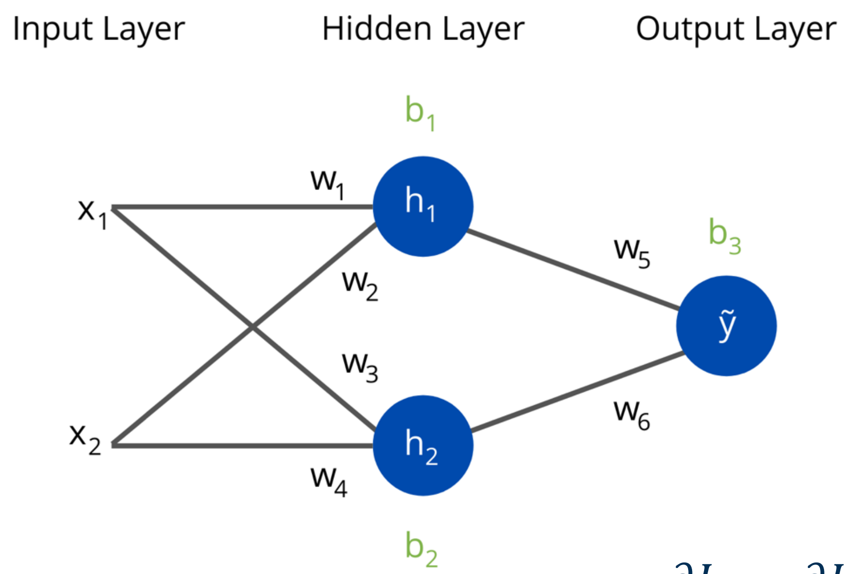
$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial L}{\partial \tilde{y}} = -2(y - \tilde{y})$$

$$\frac{\partial \tilde{y}}{\partial h_1} = w_5 * f'(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial h_1}{\partial w_1} = x_1 * f'(b_1 + w_1 * x_1 + w_2 * x_2)$$

Backpropagation



$$L = (y - \tilde{y})^2$$

$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial \tilde{y}} * \frac{\partial \tilde{y}}{\partial h_1} * \frac{\partial h_1}{\partial w_1}$$

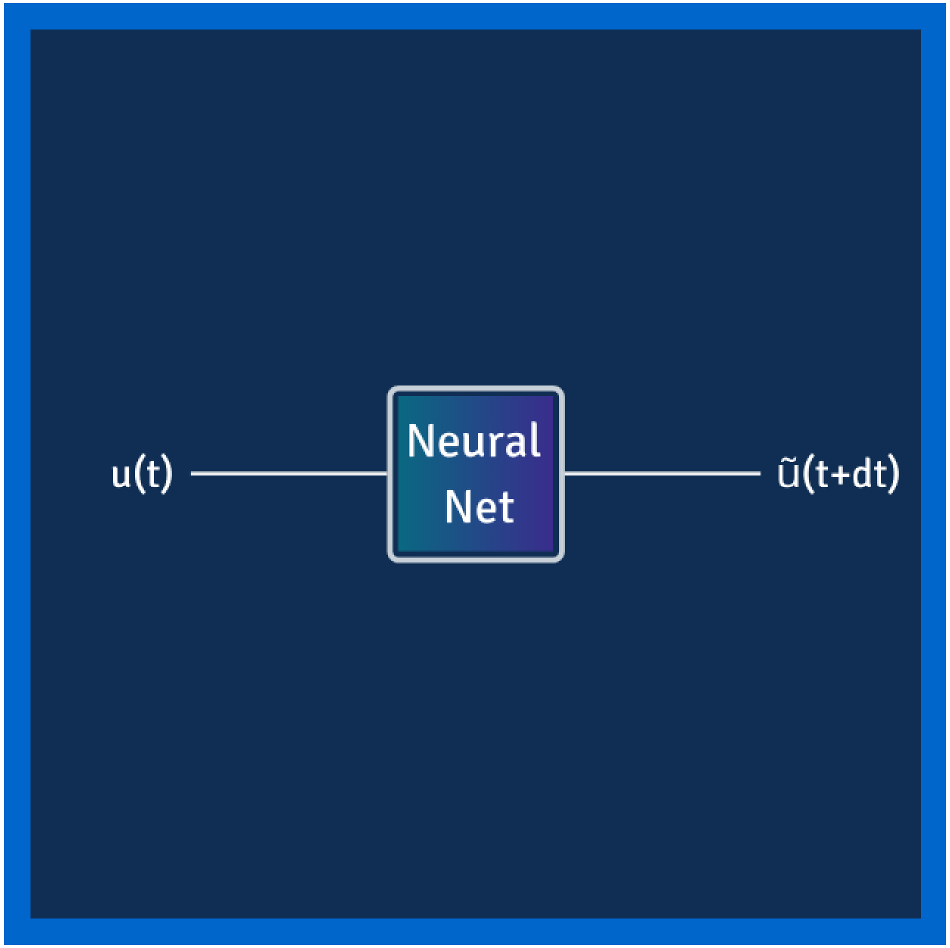
$$\frac{\partial L}{\partial \tilde{y}} = -2(y - \tilde{y})$$

$$\frac{\partial \tilde{y}}{\partial h_1} = w_5 * f'(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial h_1}{\partial w_1} = x_1 * f'(b_1 + w_1 * x_1 + w_2 * x_2)$$

$$w_1 = w_1 - \gamma \frac{\partial L}{\partial w_1}$$

Surrogate Model Layout

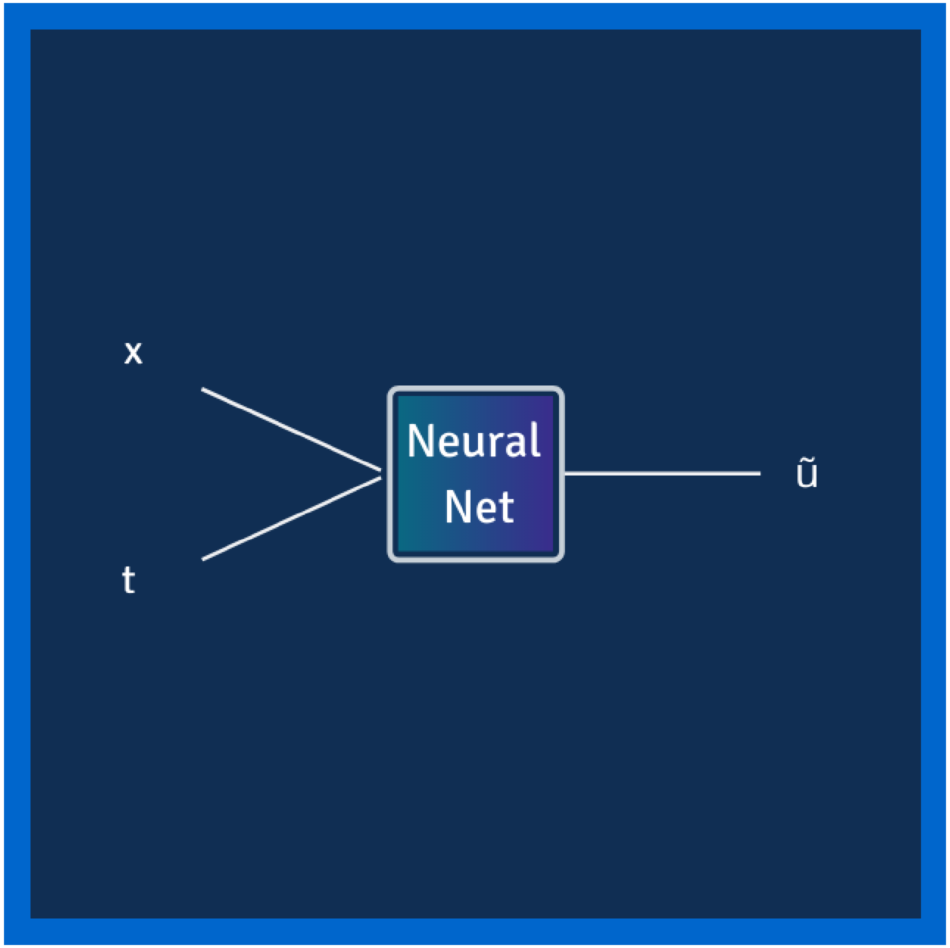


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u})$$

aka reconstruction error.

Surrogate Model Layout

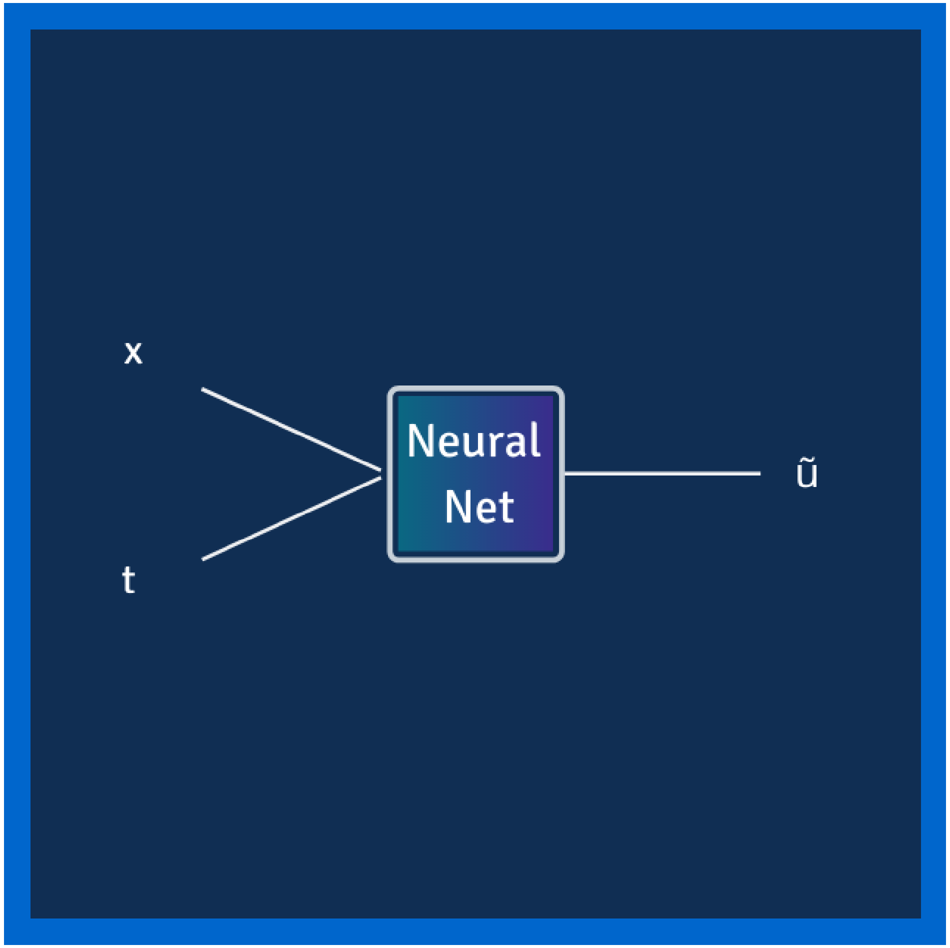


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u})$$

aka reconstruction error.

Surrogate Model with Physical Penalty

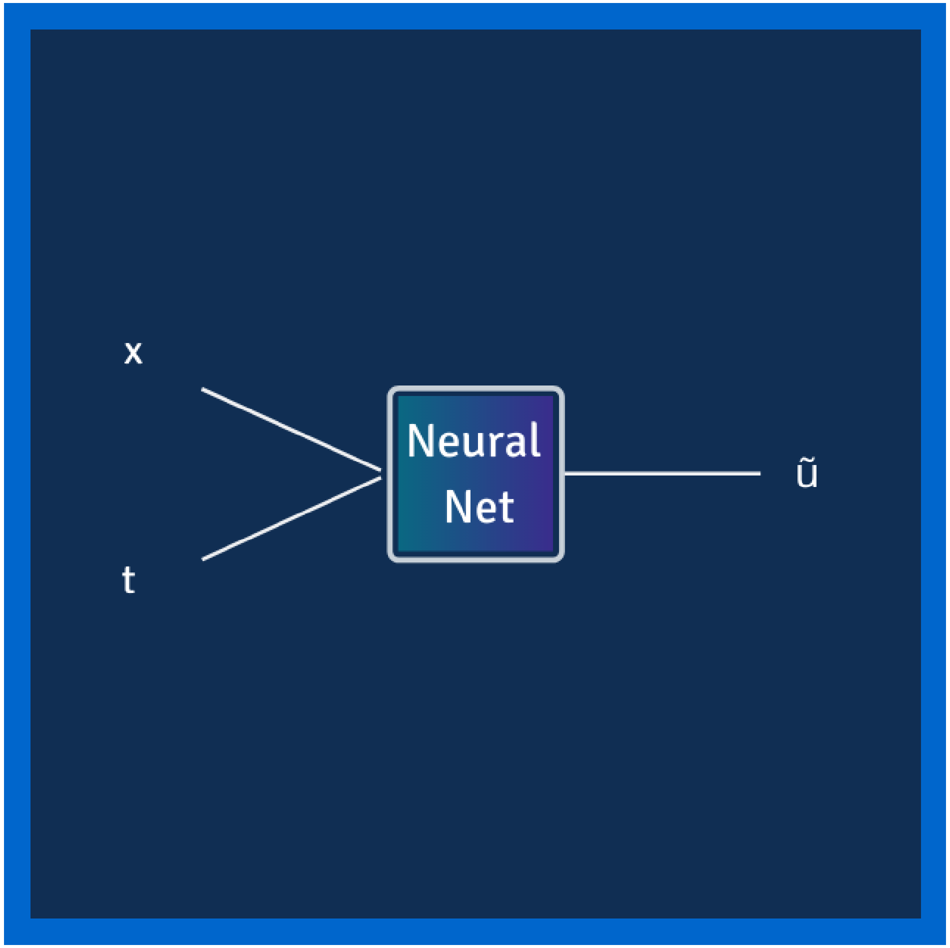


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u}) + \sum(m\tilde{u} - mu)$$

Momentum Conservation Equation playing an additional constraint (assuming $\tilde{u}$ is velocity in this case.)

Neural PDE Layout



Loss Function:

Initial Loss
\+ *Boundary Loss*
\+ *Domain Loss*

Consider a PDE written in the form:

$$f = u_t + \Lambda[u] = 0, \qquad x \in \Omega, \qquad t \in [0, T]$$

$$\mathrm{Initial\_Loss} = \mathrm{MSE} \sum \left(\mathrm{u}_{(\mathrm{x},\, \mathrm{t}=0)} - \tilde{u}_{(\mathrm{x},\, \mathrm{t}=0)} \right)$$

$$Boundary\_Loss = MSE \sum \left(BoundaryCondition\left(\tilde{u}_{(X\_lim,\, t)} \right) \right)$$

$$Domain\_Loss = MSE \sum \left(f(x, t) \right)$$

Consider the Korteweg-de Vries Equation :

$$f = u_t + u * u_x + \alpha * u_{xxx} = 0, \qquad x \epsilon [-1, 1], \qquad t \epsilon [0, 1]$$

with Periodic Boundary Conditions

$$u_{x=-1} = u_{x=1}$$

$$\frac{\partial u}{\partial x}_{x=-1} = \frac{\partial u}{\partial x}_{x=1}$$

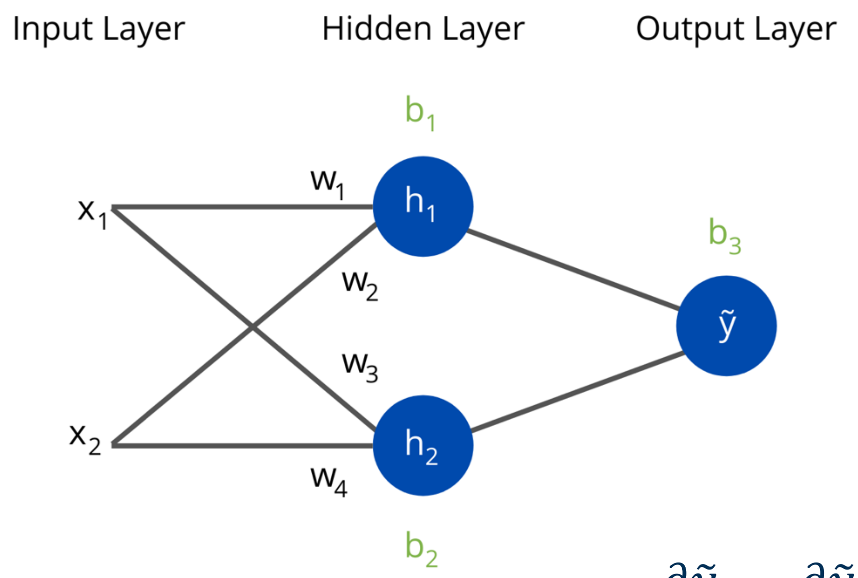
Loss Function Entities:

$$\text{Initial\_Loss} = \text{MSE} \sum \left(IC(x, 0) - \tilde{u}_{(\text{x, t=0})} \right)$$

$$Boundary\_Loss = MSE \sum \left(\frac{\partial u}{\partial x}_{x=-1,} - \frac{\partial u}{\partial x}_{x=1} + u_{x=-1} - u_{x=1} \right)$$

$$Domain\_Loss = MSE \sum \left(f(x, t) \right), \qquad x \epsilon (-1,1), \qquad t \epsilon (0,1)$$

Partial Derivatives via Backprop



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$$h_2 = f(b_2 + w_3 * x_1 + w_4 * x_2)$$

$$\tilde{y} = f(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial \tilde{y}}{\partial x_1} = \frac{\partial \tilde{y}}{\partial h_1} * \frac{\partial h_1}{\partial x_1}$$

$$\frac{\partial \tilde{y}}{\partial h_1} = w_5 * f'(b_3 + w_5 * h_1 + w_6 * h_2)$$

$$\frac{\partial h_1}{\partial x_1} = w_1 * f'(b_1 + w_1 * x_1 + w_2 * x_2)$$

NPDE Package – PDE_Kozhi

Neural PDE Parameters :

$$N_i : Number\ of\ Initial\ Points$$
$$N_b : Number\ of\ Boundary\ Points$$
$$N_f : Number\ of\ Domain\ Points$$

Each collocation point for each loss entity is obtained by calling upon a quasi-random sequence within the boundaries of each region.

PDE Parameters :

$$Equation\ (as\ a\ string)$$
$$Lower\ and\ Upper\ bounds$$
$$Initial\ Condition$$
$$Boundary\ Condition\ and\ Value$$

NN Parameters :

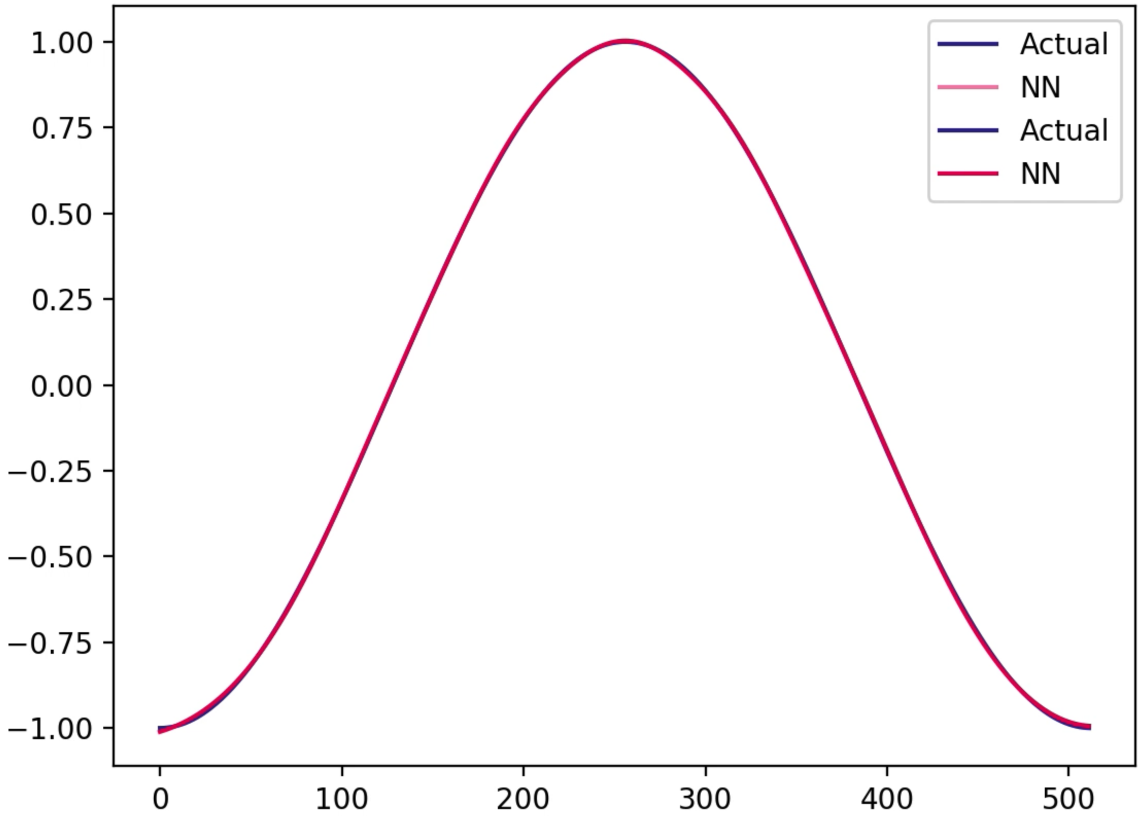
$$Number\ of\ layers\ and\ neurons$$

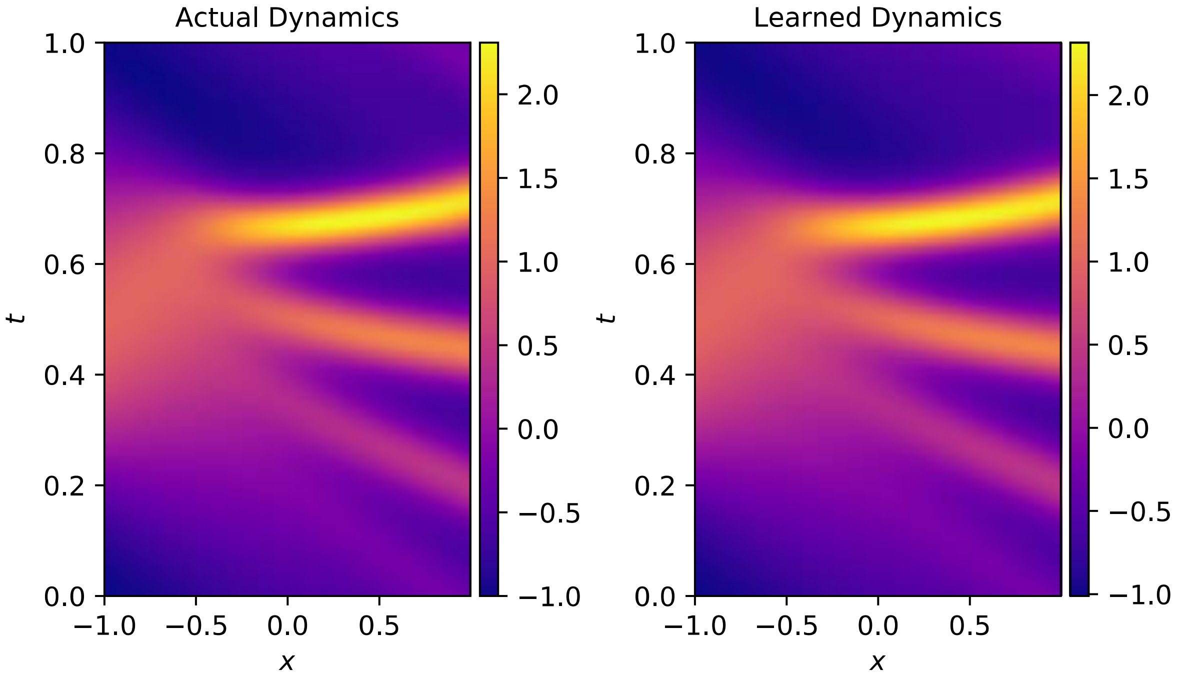
In [9]:
```python
#Neural Network Hyperparameters
NN_parameters = {
                'input_neurons' : 2,
                'output_neurons' : 1,
                'num_layers' : 4,
                'num_neurons' : 100,
                }


#Neural PDE Hyperparameters
NPDE_parameters = {'Sampling_Method': 'Random',
                   'N_initial' : 300, #Number of Randomly sampled Data points from the IC vector
                   'N_boundary' : 300, #Number of Boundary Points
                   'N_domain' : 20000 #Number of Domain points generated
                  }


#PDE
PDE_parameters = {'Equation': ' u_t + u*u_x + 0.0025*u_xxx',
                  'order': 3,
                  'lower_range': [-1., 0.],
                  'upper_range': [1., 1.],
                  'Boundary_Condition': "Periodic",
                  'Boundary_Vals' : None,
                  'Initial_Condition': lambda x: np.cos(np.pi*x)
                 }
```

In [10]:
```python
#Obtaining the training data
soln_loc = '/Examples/Data/KdV.mat'
x, t, training_data, testing_input, testing_output  = npde.Main.solution_data(soln_loc, NN_parameters, PDE_parameters,

params = npde.Parameters.parameters(PDE_parameters, NN_parameters, NPDE_parameters, Model_Name, Equation_Name)
```

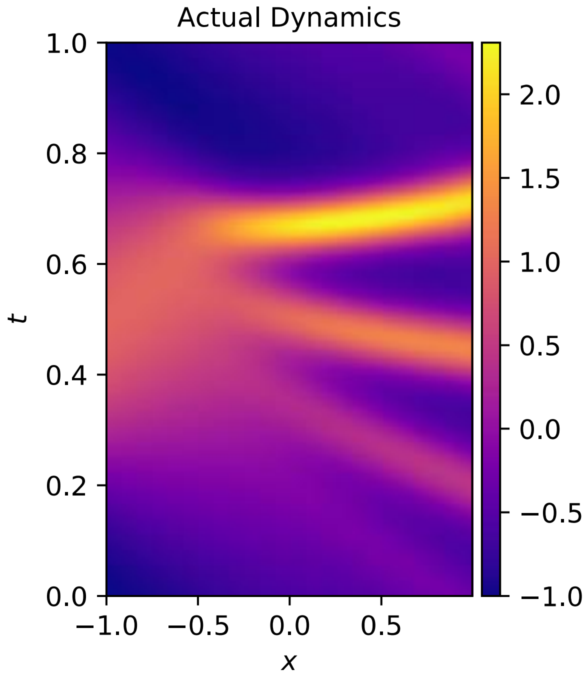
In [ ]:
```python
#Initialising the Model
model = npde.Main.setup(params, training_data)
```

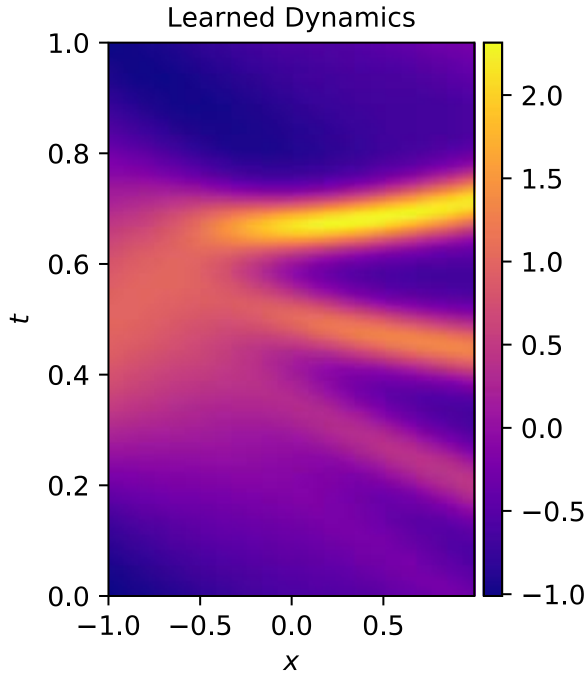
In [ ]:
```python
#Training Conditions -----------------------------------------------------
optimiser = {
            'opt_type' : "GD",
            'optimizer' : "adam",
            'learning_rate' : 0.001,
            'nIter' : 2000,
            'qn_source' : None
            }

start_time = time.time()
loss_GD = model.train(optimiser, Model_Name)
time_GD = time.time() - start_time


optimiser = {
            'opt_type' : "QN",
            'optimizer' : "L-BFGS-B",
            'learning_rate' : None,
            'nIter' : None,
            'qn_source' : "Scipy"
            }

start_time = time.time()
loss_Scipy = model.train(optimiser, Model_Name)
time_Scipy = time.time() - start_time
```

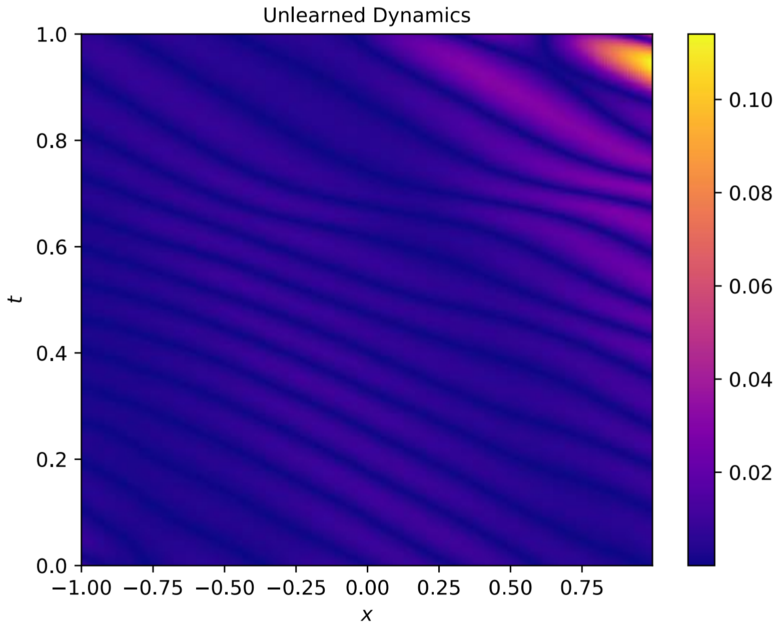

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
100
200
300
400
500
Actual
NN
Actual
NN



Actual Dynamics
Learned Dynamics
1.0
0.8
0.6
0.4
0.2
0.0
t
−1.0
−0.5
0.0
0.5
x
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0

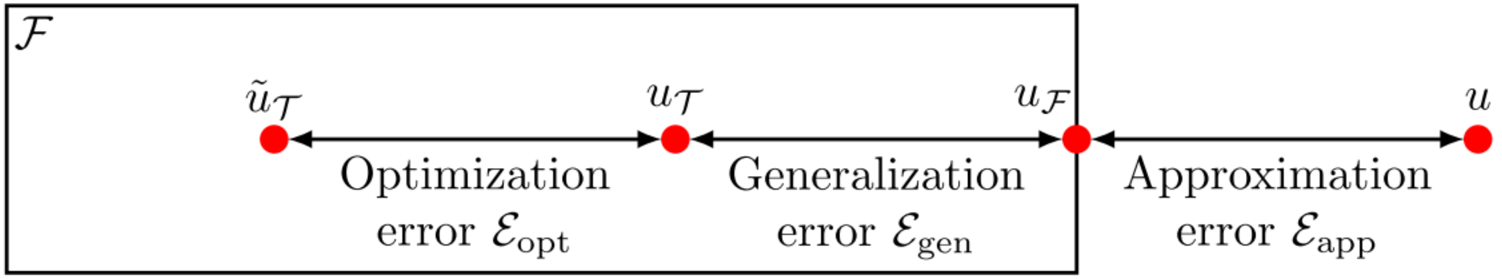

Actual Dynamics
t
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.0
−0.5
0.0
0.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0


Learned Dynamics
t
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.0
−0.5
0.0
0.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0


Unlearned Dynamics
t
x
1.0
0.8
0.6
0.4
0.2
0.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
0.10
0.08
0.06
0.04
0.02

Approx. Theory and Error Analysis for Neural PDEs

- Approximation Error (Best function close to u in the Function Space F – Global Minimum)
- Generalisation Error (Governed by the number of Points)
- Optimisation Error (Network stuck at local minimum)
- Networks with larger size have smaller approximation errors but could lead to higher generalization errors (Bias-Variance Tradeoff).



Source: DeepXdE

Numerical Solvers Compared with Neural PDEs

- Traditional Solvers have high round-off and truncation errors.
- Expensive at Higher Dimensions (Curse of Dimensionality)
- Confined to a Mesh
- Neural PDEs can be be accelerated on GPUs and TPUs

Still this isn't extremely cheap to run.

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Took approximately two hours to get to the final solution on a single CPU.

But accelerated by a single GPU, converges within 10 minutes.

Throwing away 'learned general dynamics' being thrown away with this case-specific approach.

Deep Hidden Physics Models

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Learn the general behavior of the PDE by mapping inputs to outputs of an already known solution.

Two different Neural Networks are used to attain this characterized by :

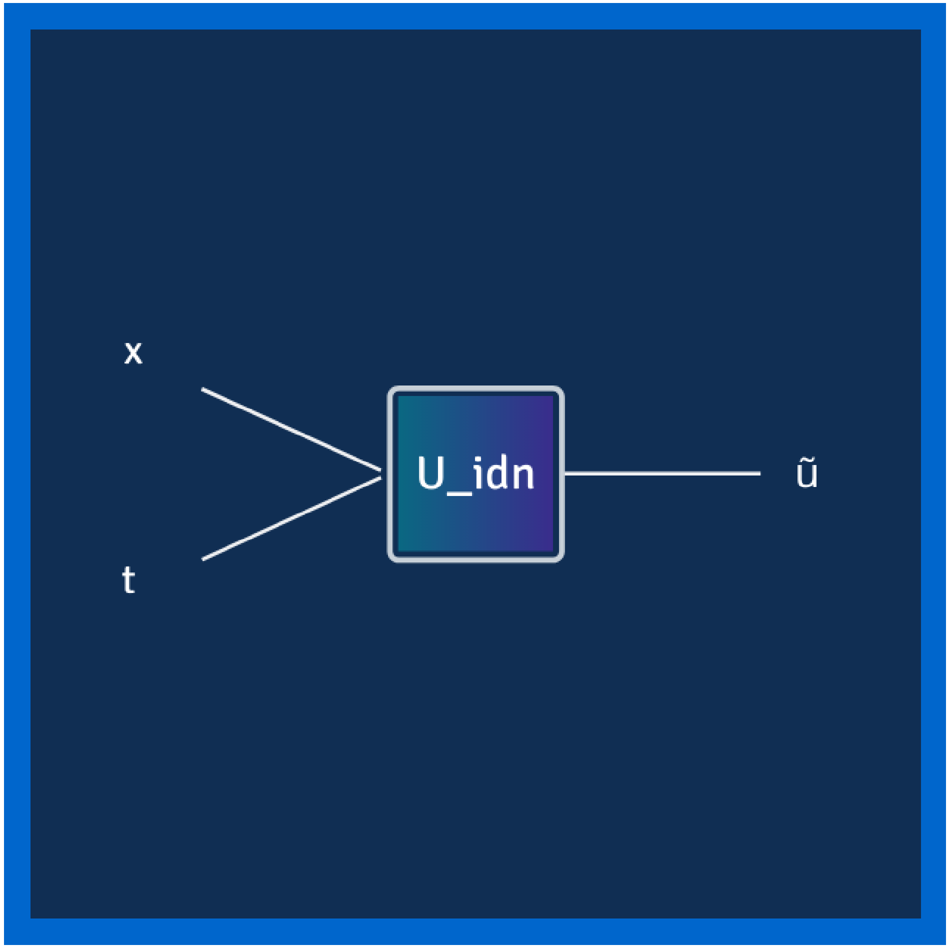
$$\boldsymbol{u_{idn}} \;\&\; \boldsymbol{\Lambda}$$

Where, u_{idn} learns the mapping of the input coordinates to the known solution, while Λ learns the general behaviour of the PDE using u_{idn}.

The final solution is attained by using another neural network $\boldsymbol{u_{soln}}$ by using the function Λ.

Source: Deep hidden physics models: Deep learning of nonlinear partial differential equations – M. Raissi

Identifier

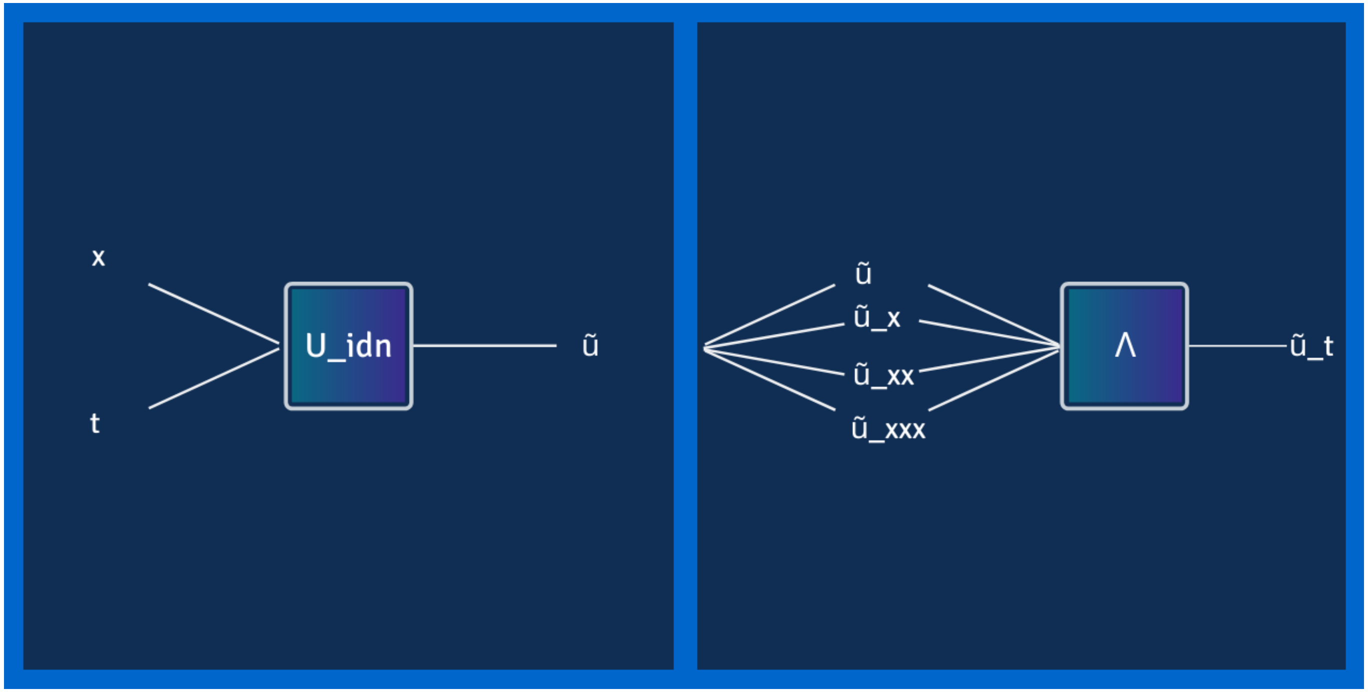


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u})$$

aka reconstruction error.

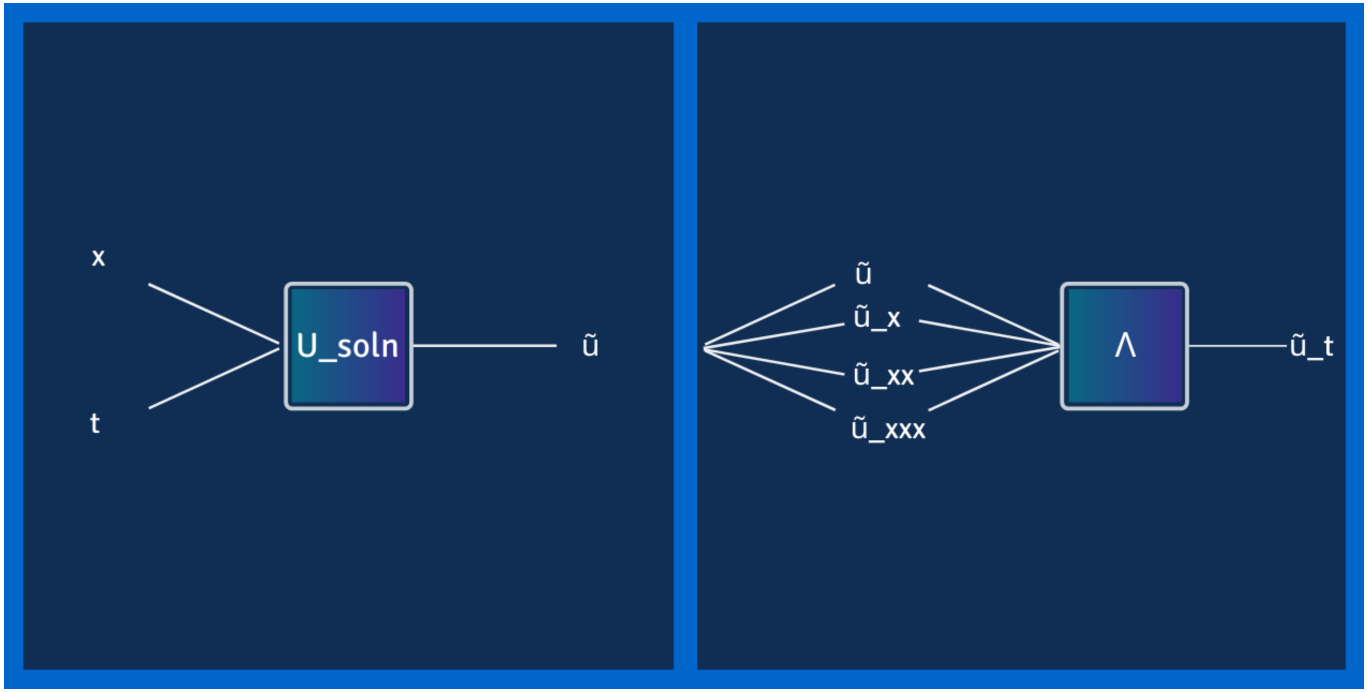
Lambda



Loss Function:

$$MSE((\tilde{u}_t - tf.concat(\tilde{u}, \tilde{u}_x, \tilde{u}_{xx}, \tilde{u}_{xxx})))$$

Solution



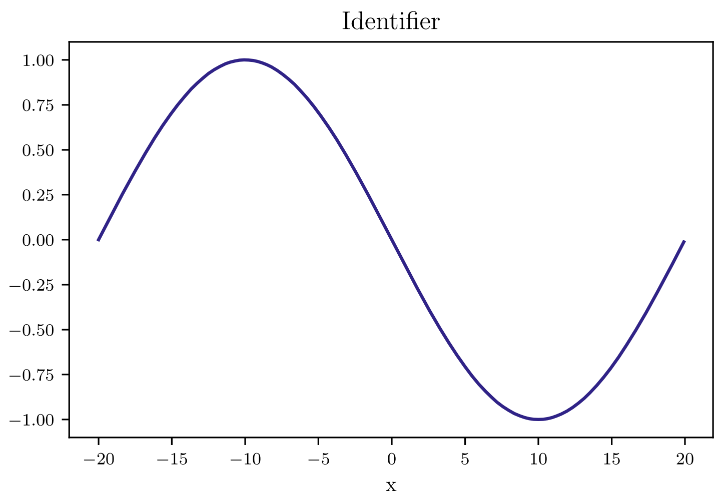
Loss Function:

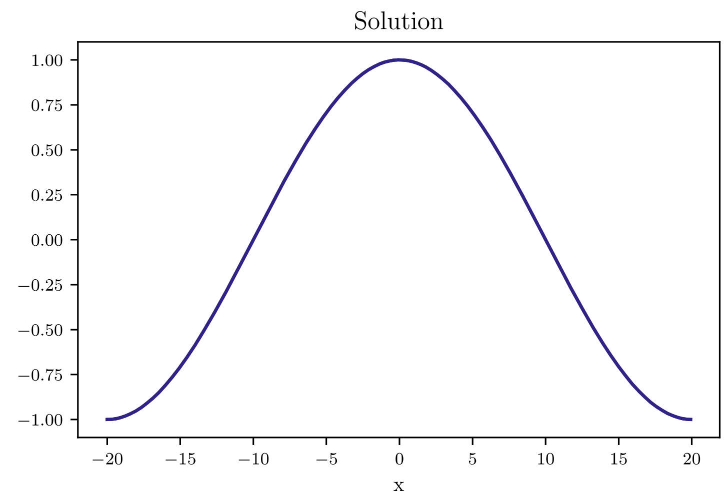
$$MSE(u_{ic} - \tilde{u}_{ic})$$

$$MSE(u_{bc} - \tilde{u}_{bc})$$

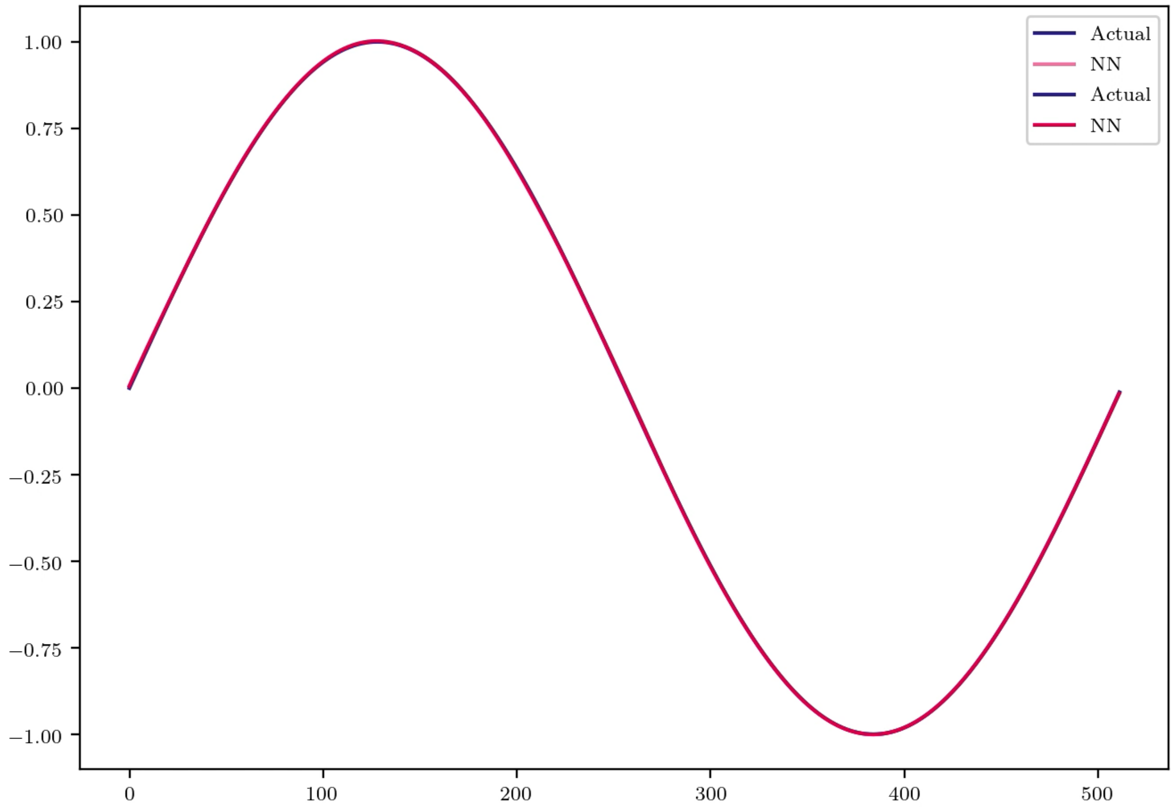
$$MSE((\tilde{u}_t \ - tf.concat(\tilde{u}, \tilde{u}_x \ , \tilde{u}_{xx}, \tilde{u}_{xxx})))$$

Identifier and Solution – Initial Condition

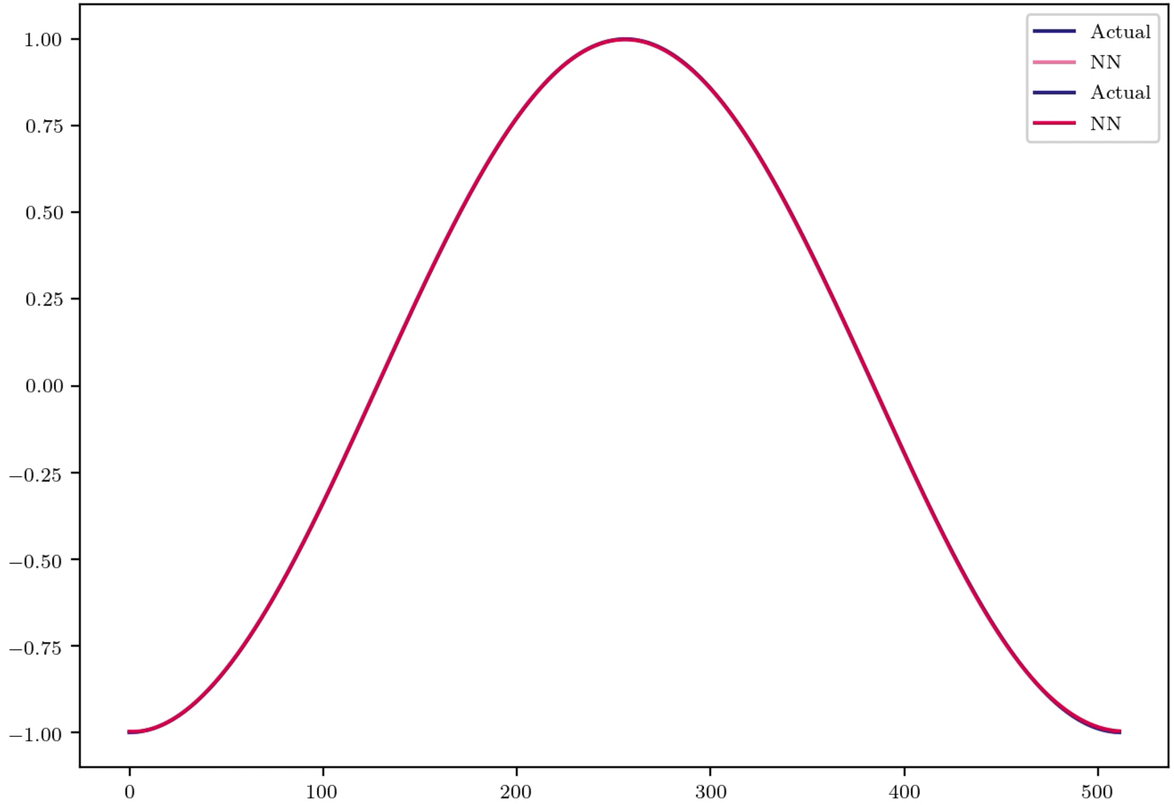


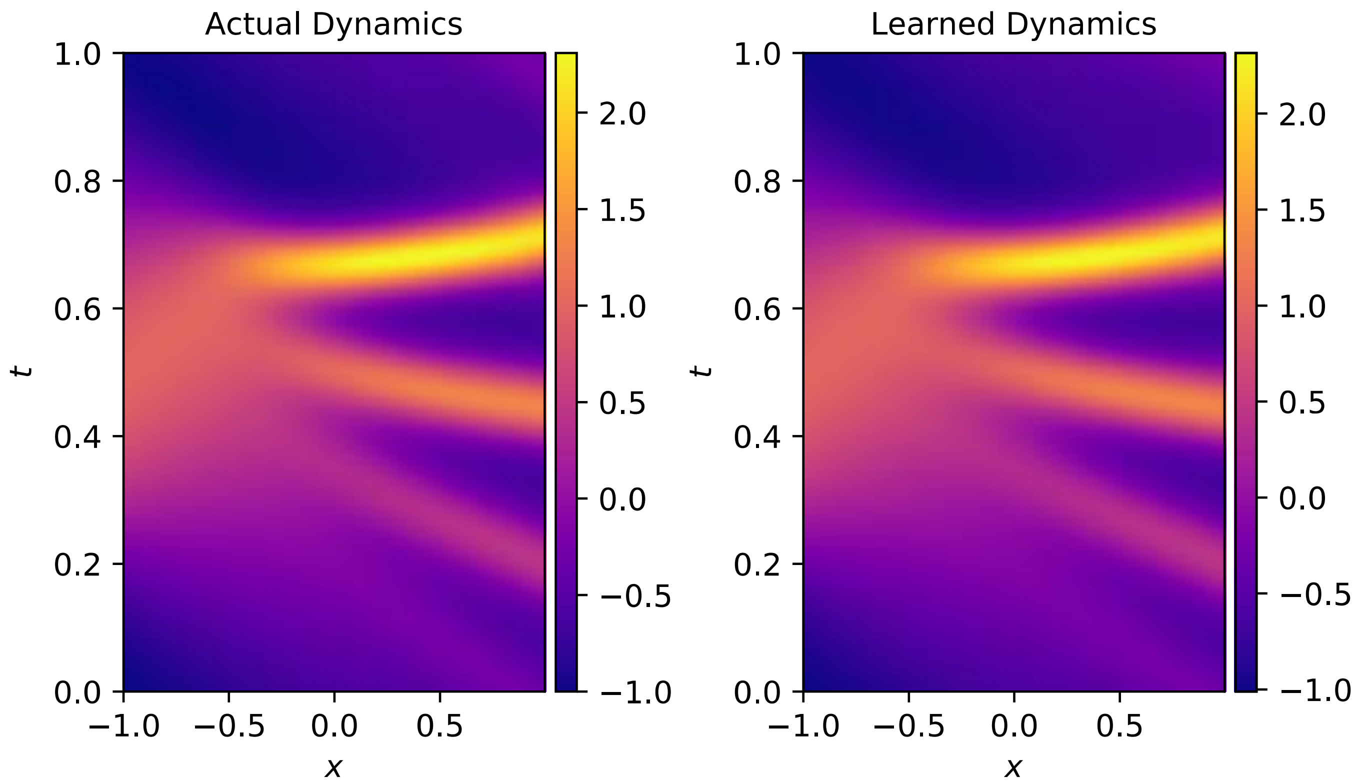


Identifier - U_{idn}



Solution - U_{soln}




Actual Dynamics
Learned Dynamics
1.0
0.8
0.6
0.4
0.2
0.0
t
−1.0
−0.5
0.0
0.5
x
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0

Additional Functionality:

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- Better Sampling Strategies : Spatio-Temporal Residual Based
- Higher Order Approximations represented by perturbations – Deep Galerkin Methods
- More complex Network Elements – Batch Normalisation, Sparse Nets, Resnets
- Case-agnostic modelling

References :

Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, *378*, 686–707. https://doi.org/10.1016/j.jcp.2018.10.045

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