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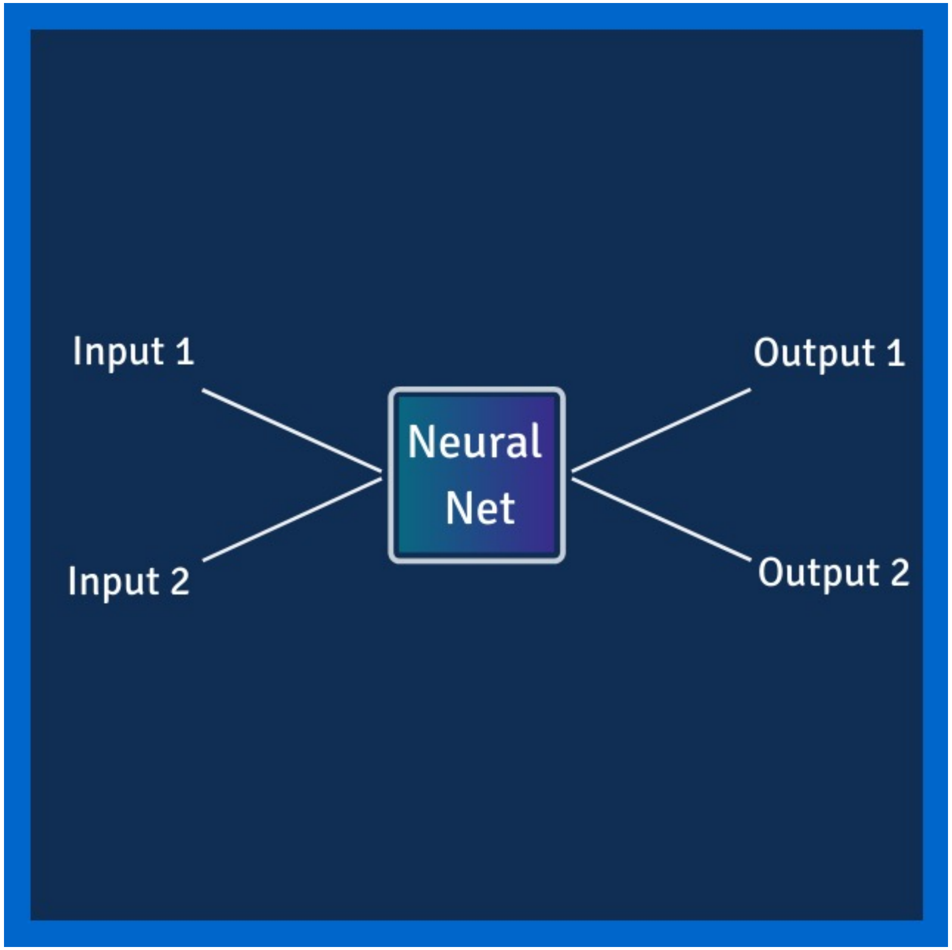
Fluid Surrogates using Neural PDEs

Vignesh Gopakumar

SciML Talks at RAL **1st October, 2020**

Regular NNs



Published: December 1989

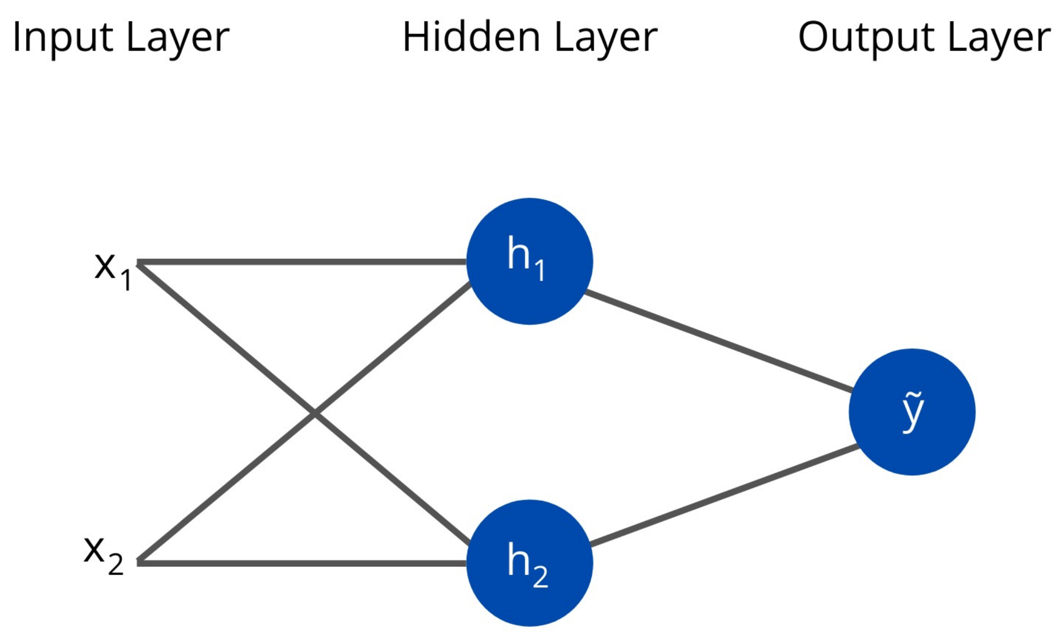
Approximation by superpositions of a sigmoidal function

G. Cybenko

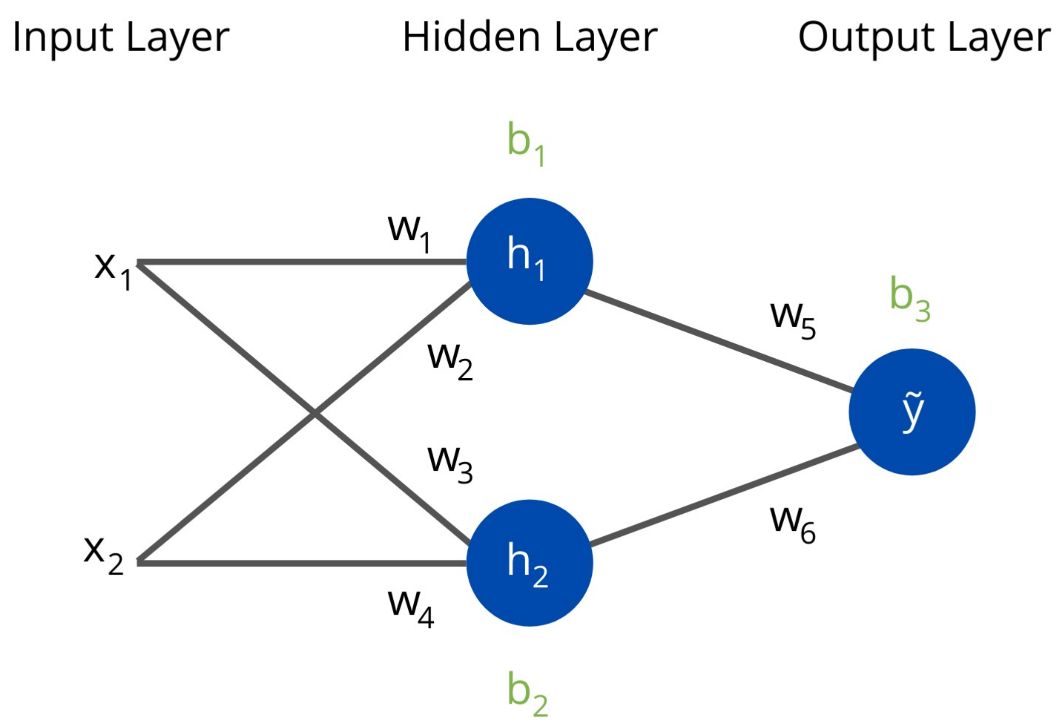
Mathematics of Control, Signals and Systems **2**, 303–314(1989) | Cite this article

7367 Accesses | **6133** Citations | **29** Altmetric | Metrics

Feedforward Structure



Feedforward Structure



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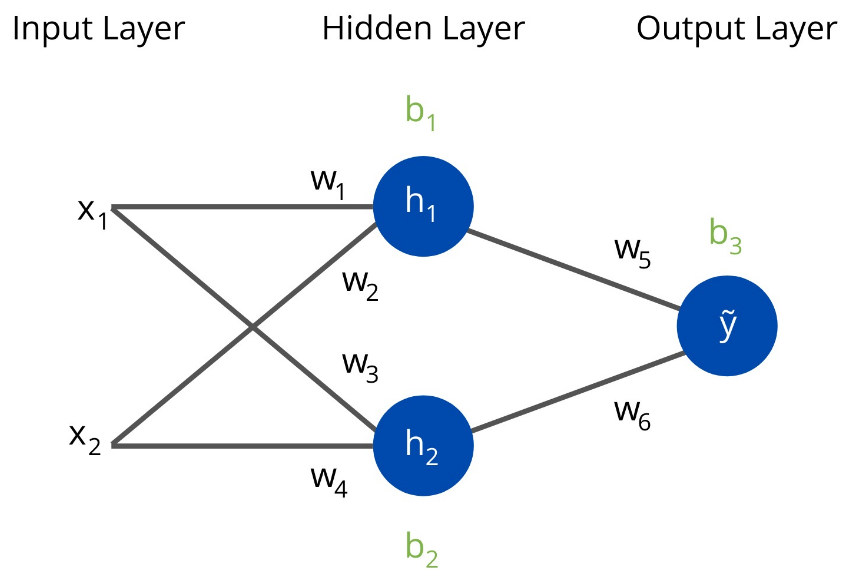
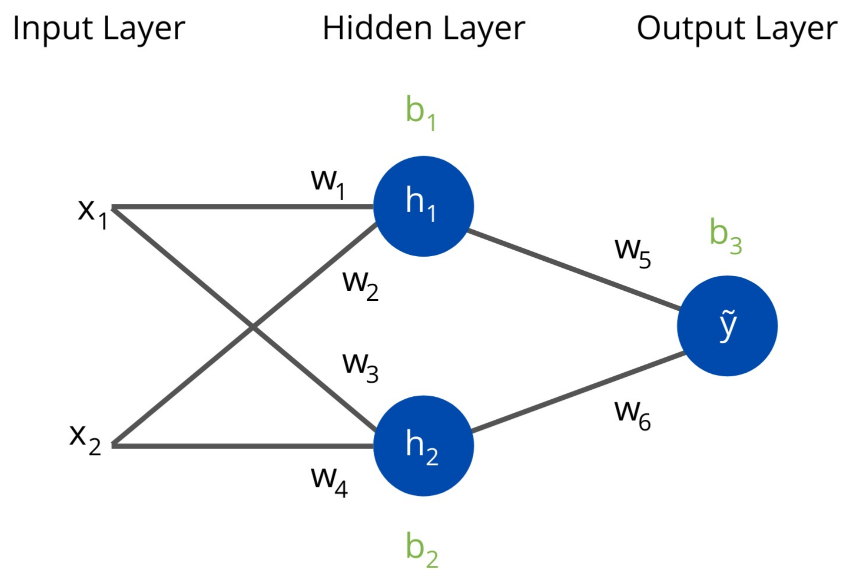


$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

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

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

Backpropagation



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

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

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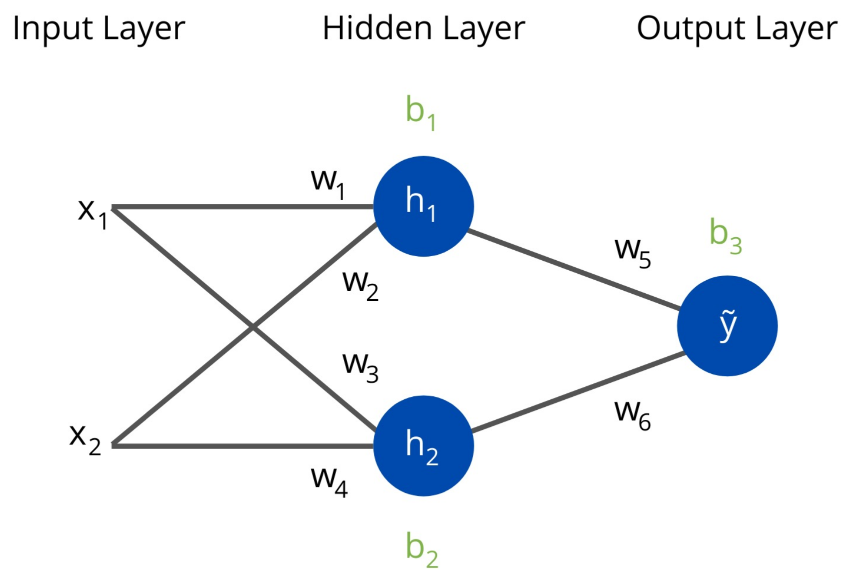
Backpropagation



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

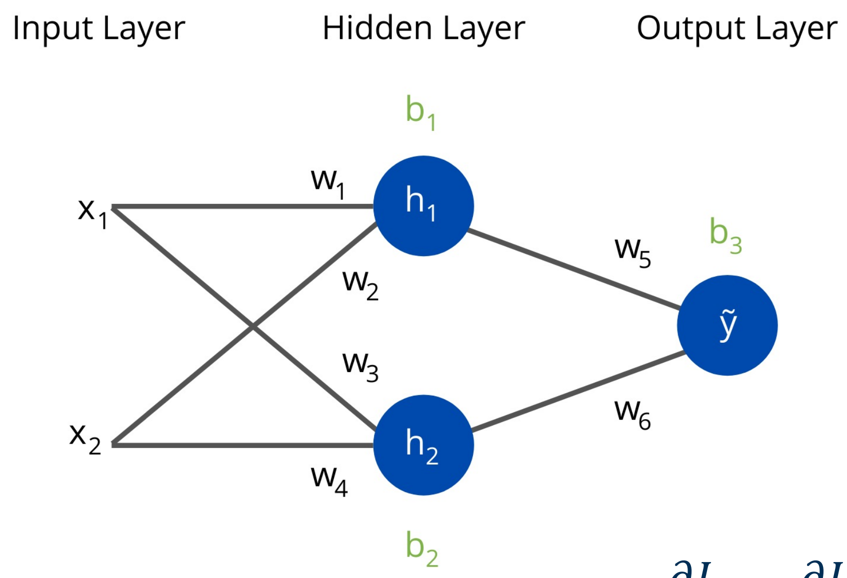
$$h_1 = f(b_1 + w_1 * x_1 + w_2 * x_2)$$

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

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

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

Backpropagation



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

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

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

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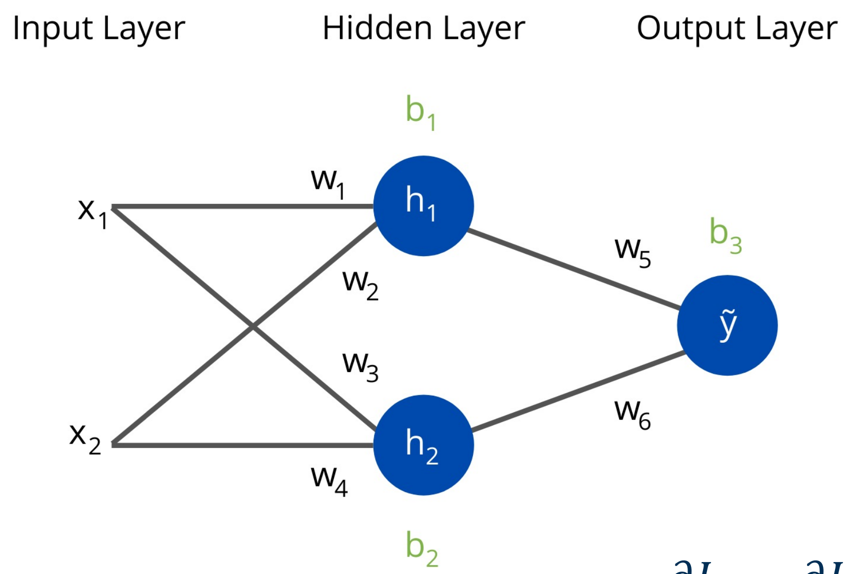
Backpropagation



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

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

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

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

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

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

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

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

Backpropagation

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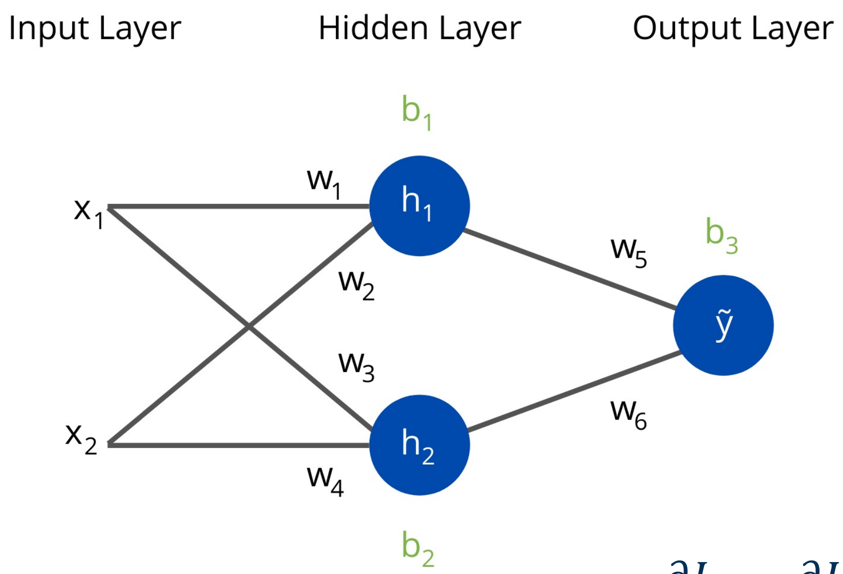

$$L = (y - \tilde{y})^2$$

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

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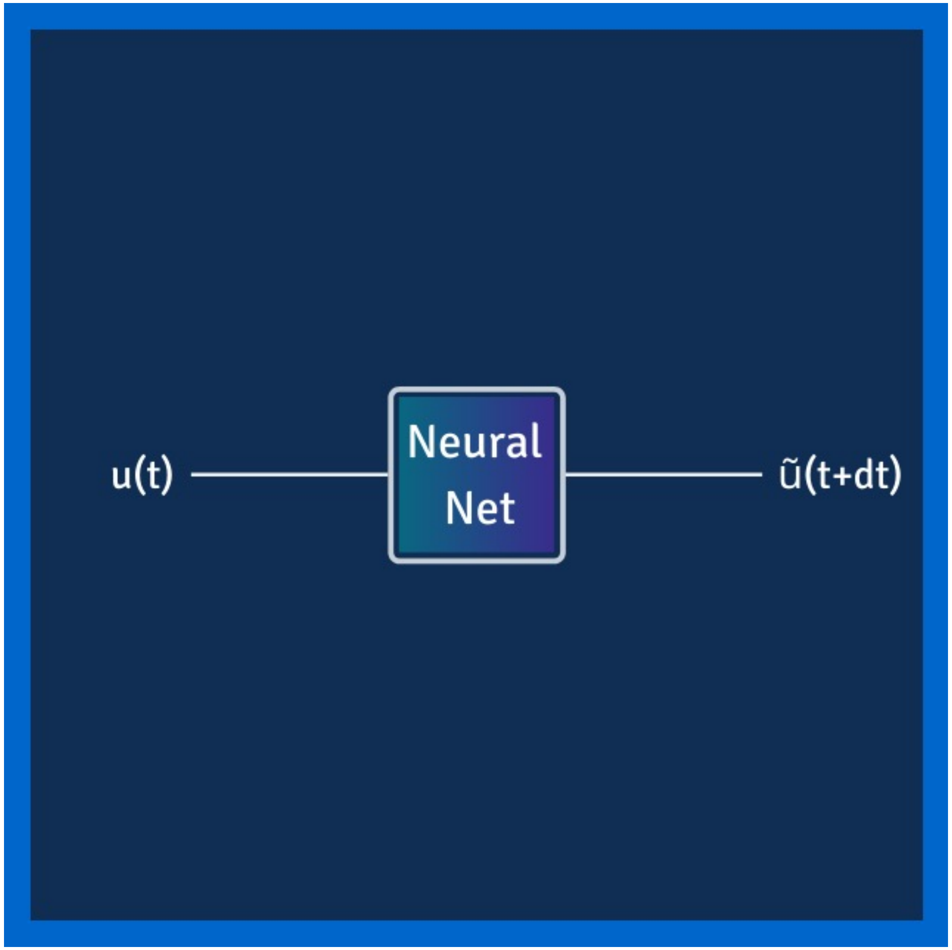
$$\frac{\partial \tilde{y}}{\partial h_1} = w_5 * f'(b_3 + w_5 * h_1 + w_6 * h_2)$$

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

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

Surrogate Model Layout

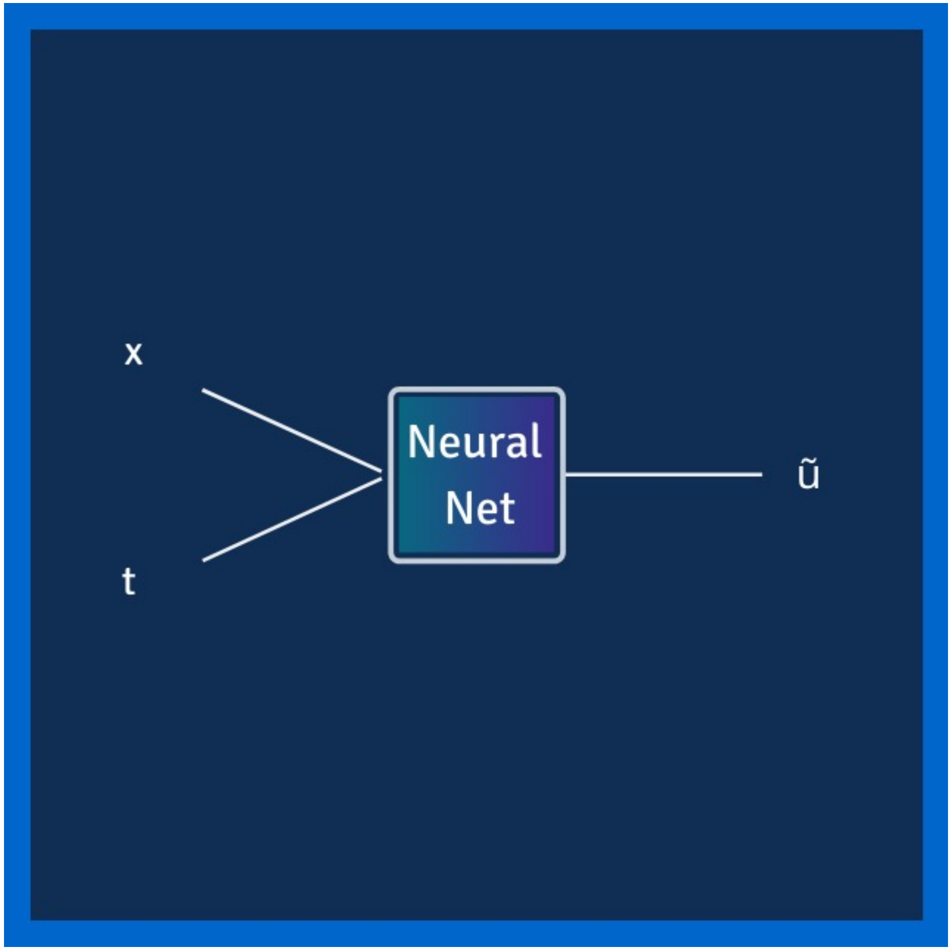


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u})^2$$

aka reconstruction error.

Surrogate Model Layout

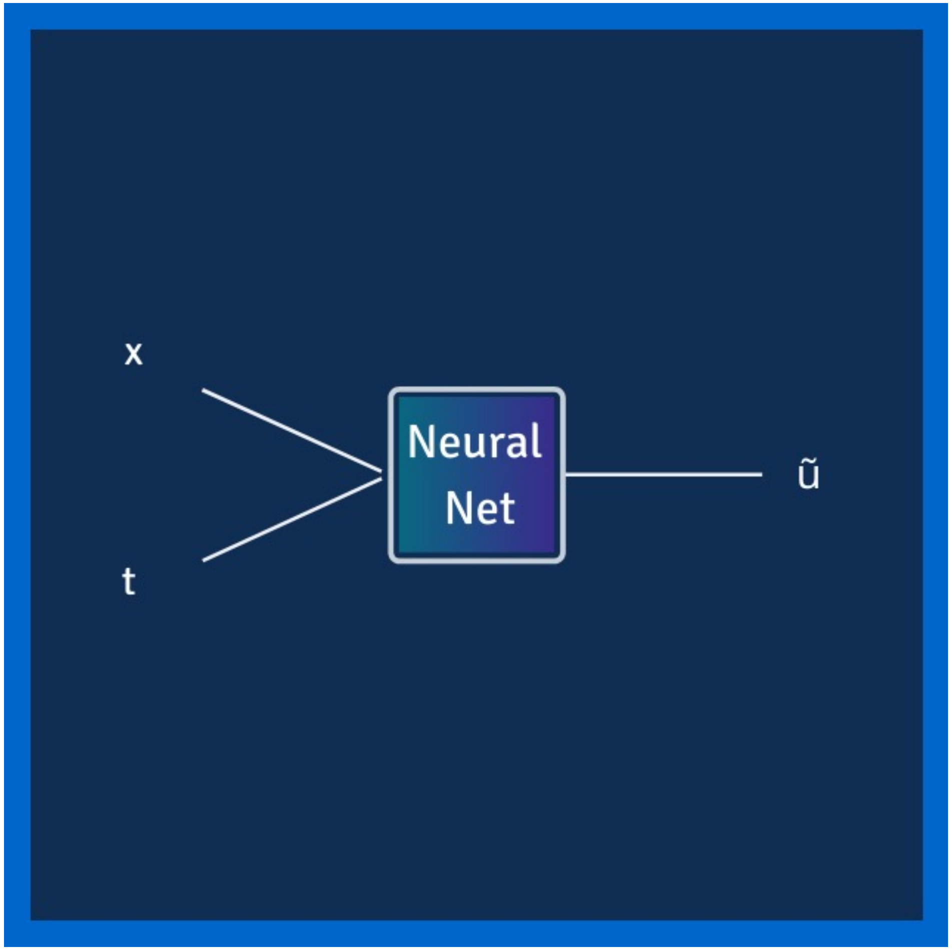


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u})^2$$

aka reconstruction error.

Surrogate Model with Physical Penalty

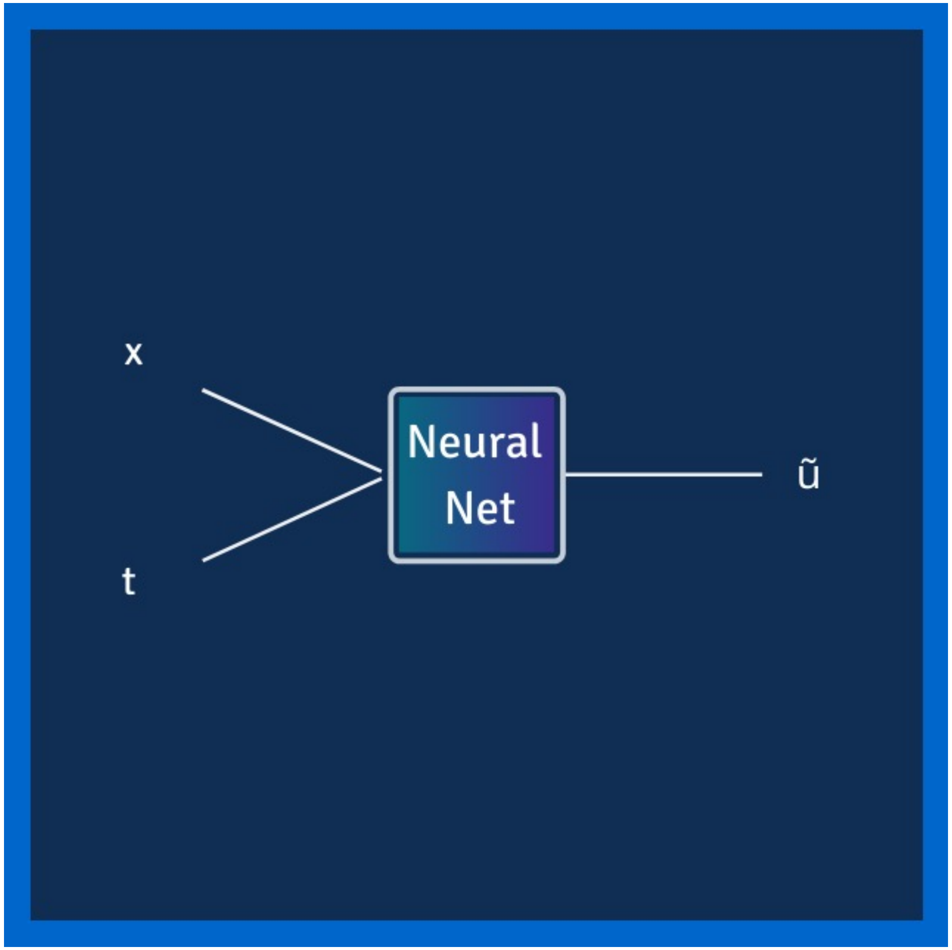


Loss Function:

$$\frac{1}{N}\sum(u - \tilde{u}^2) + \frac{1}{N}\sum(m\tilde{u} - mu)^2$$

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:

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

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

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

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

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

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

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

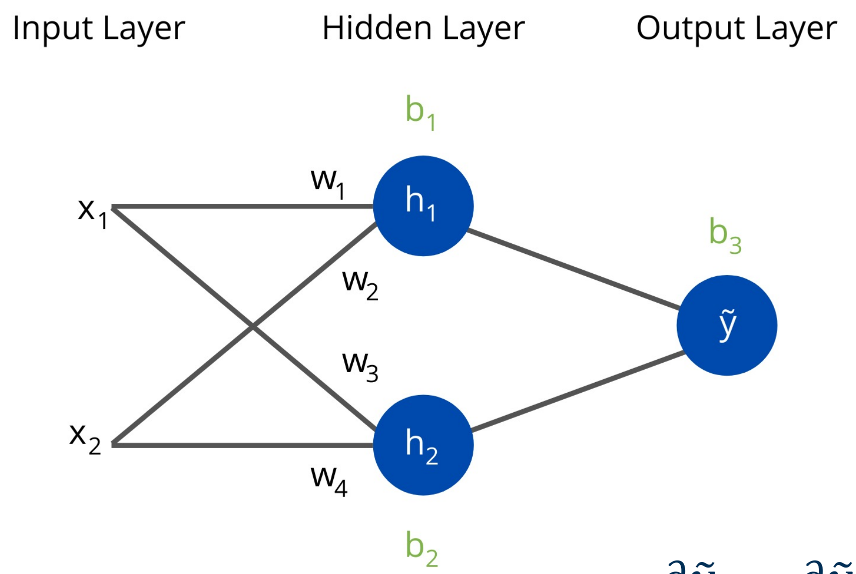
Loss Function Entities:

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

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

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

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 – ‘ tf-pde ’

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 :

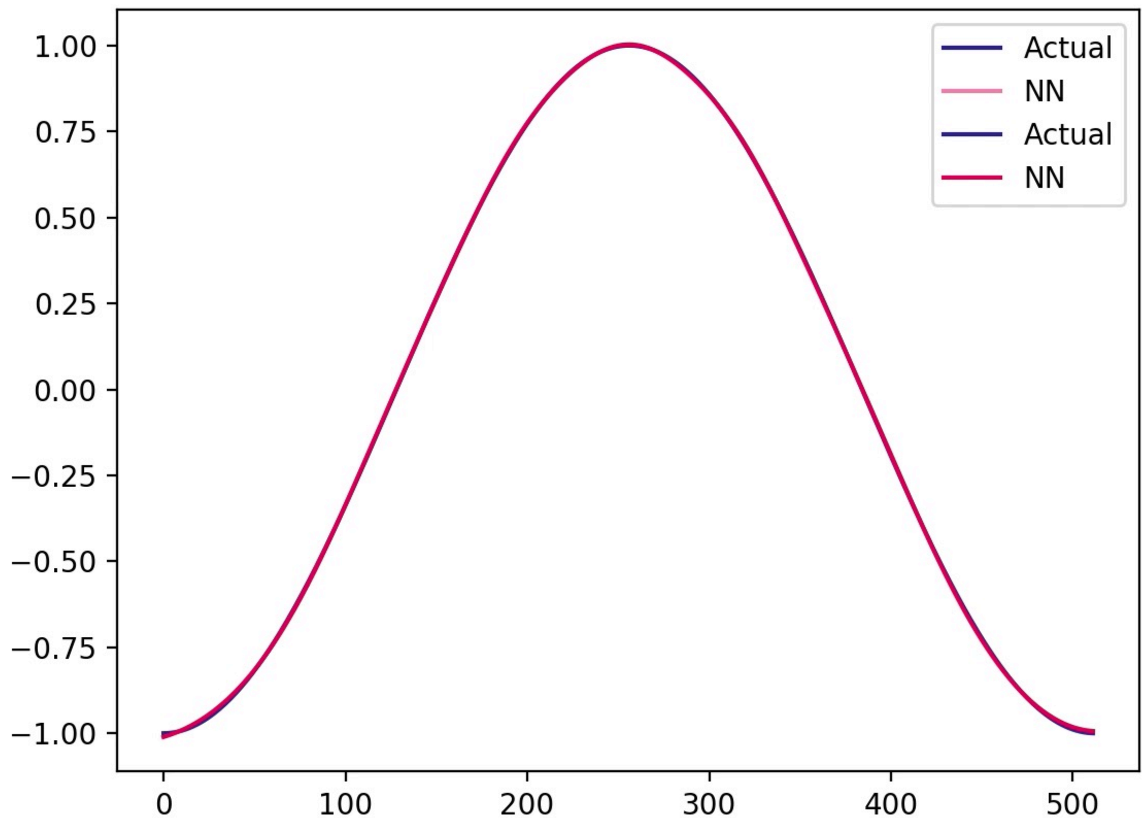
$$Number\ of\ layers\ and\ neurons$$

```
In [9]: #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)
                 }
```

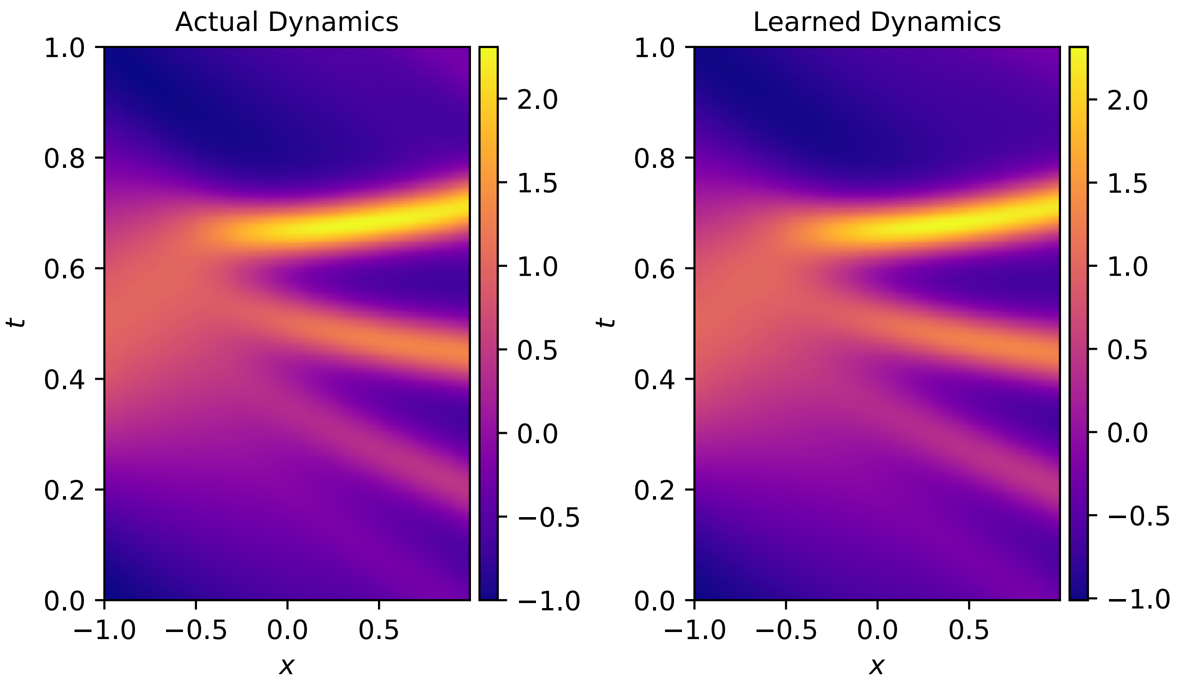
```
In [10]: #Obtaining the training data
soln_loc = '/Examples/Data/KdV.mat'
x, t, training_data, testing_input, testing_output  = npde.Main.solution_data(soln_loc, NN_parameters, PDE_parameters,

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

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

```
In [ ]: #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



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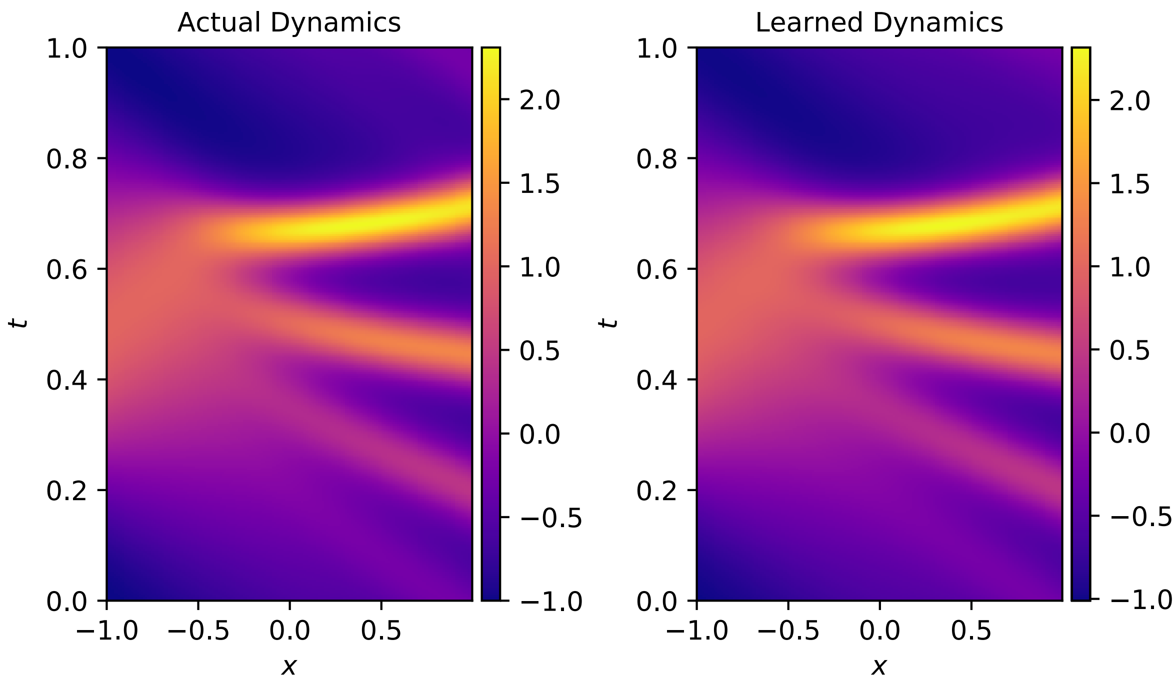
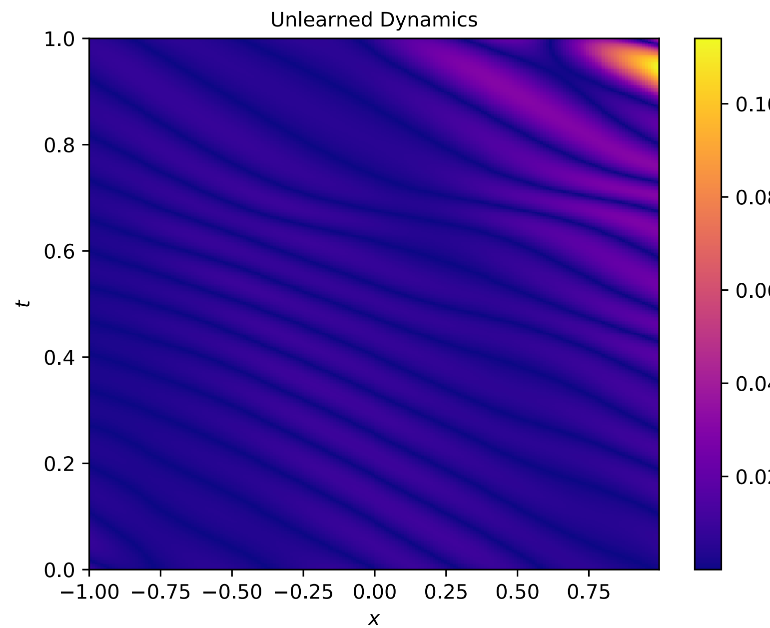
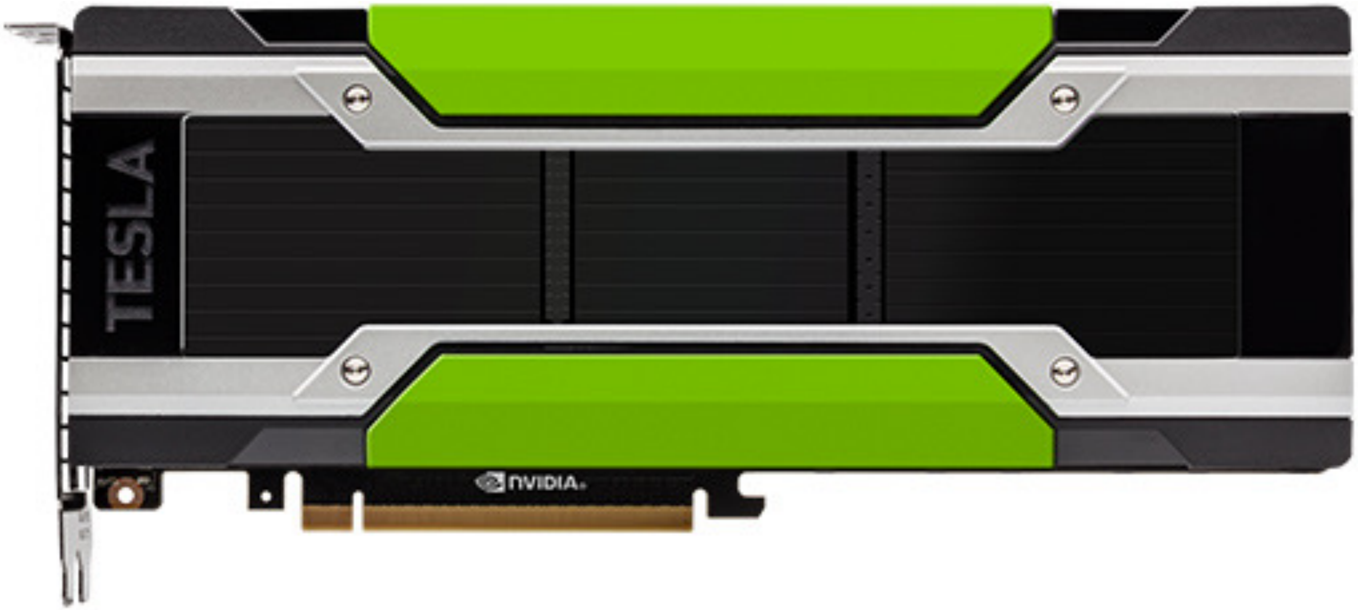
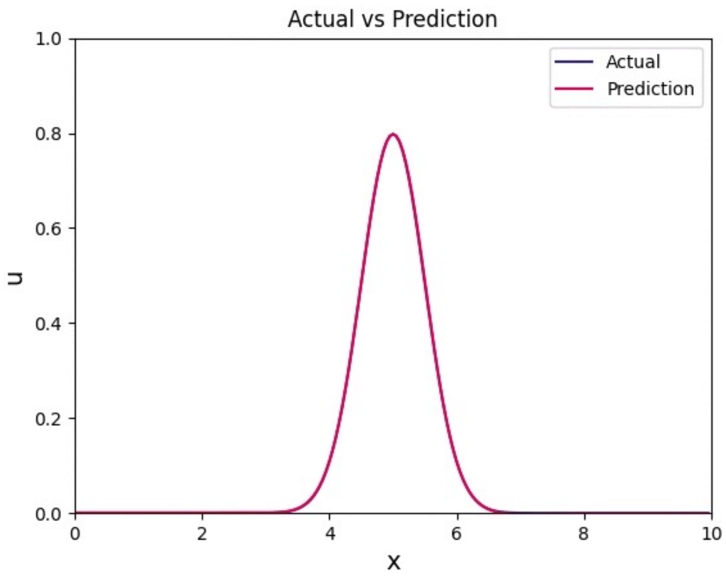
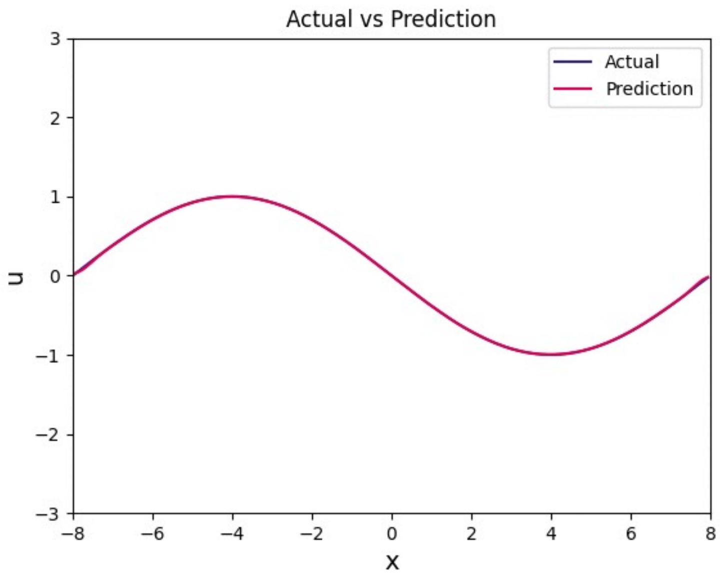




NVIDIA TESLA P100







Convection-Diffusion :

$$\frac{\partial u}{\partial t} = \frac{\partial \left(D \frac{\partial u}{\partial x} \right)}{\partial x} - c \frac{\partial u}{\partial x}$$

Net: 4x64 (Tanh)
MSE: 0.0001103
Time: 110 seconds

Burgers' :

$$\frac{\partial u}{\partial t} = 0.1 \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x}$$

Net: 4x64 (Tanh)
MSE: 0.0001059
Time: 95 seconds

Wave Equation

$$f = \ u_{tt} - \ 1.0 * \left(u_{xx} + \ u_{yy}\right) = \ 0, \qquad x \,\epsilon\, [-1, 1], \qquad y \,\epsilon\, [-1, 1], \qquad t \,\epsilon\, [0, 1]$$

with No Flux Boundary Conditions

$$u_{boundary} = 0$$

and Initial Velocity Conditions:

$$\frac{\partial u}{\partial t}(x, y, t = 0) \ = 0$$

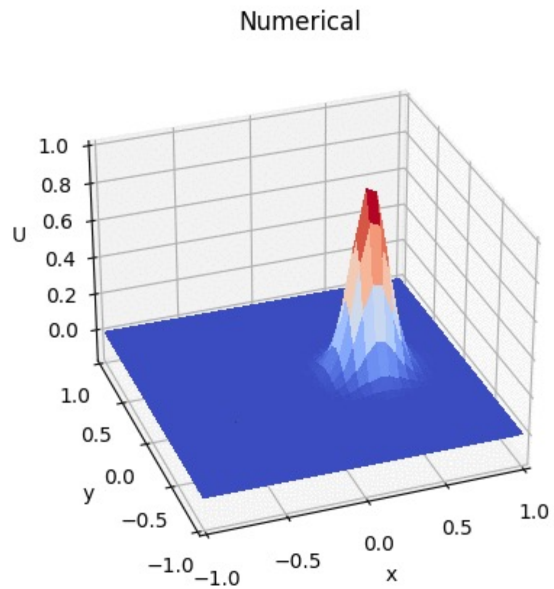
Loss Function Entities:

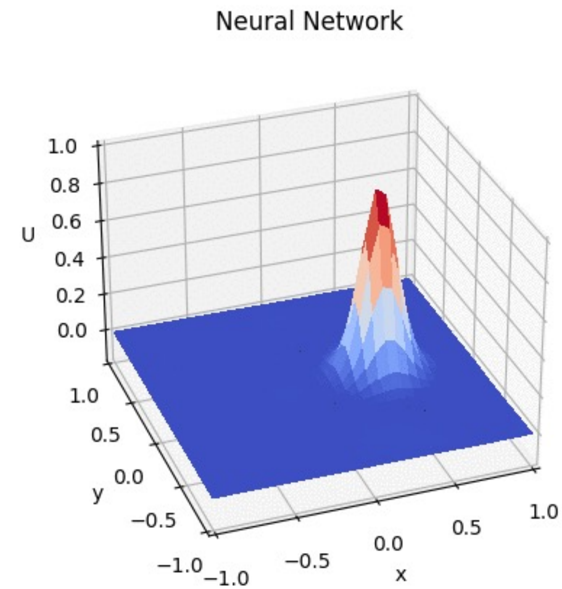
$$\text{Initial\_Loss} \ = \ \text{MSE}\big(IC(x, 0) - \ \tilde{u}_{(\text{x, t=0})}\big) + \text{MSE}\left(\frac{\partial u}{\partial t}(x, y, t = 0) \ = 0 \ \right)$$

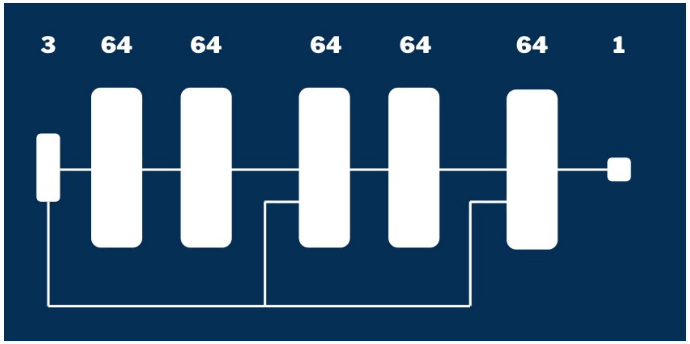
$$Boundary\_Loss \ = \ MSE\left(\frac{\partial u}{\partial t}(x = 1, y, t) + \frac{\partial u}{\partial t}(x = -1, y, t) + u(x, y = 1, t) + u(x, y = -1, t)\right)$$

$$Domain\_Loss \ = \ MSE\big(f(x, y, t)\big) \quad x \,\epsilon\, (-1,1), \qquad y \,\epsilon\, (-1,1), \qquad t \,\epsilon\, (0,1)$$

Wave Equation







MSE: 0.0000135
Time: 1 hr 55 mins

Navier Stokes for Incompressible Flow

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$$f_u = u_t + \left(u * u_x + v * u_y\right) + p_x - 0.01 * (u_{xx} + u_{yy}) = 0$$
$$f_v = v_t + \left(u * v_x + v * v_y\right) + p_y - 0.01 * \left(v_{xx} + v_{yy}\right) = 0$$
$$f_{continutiy} = u_x + v_y$$

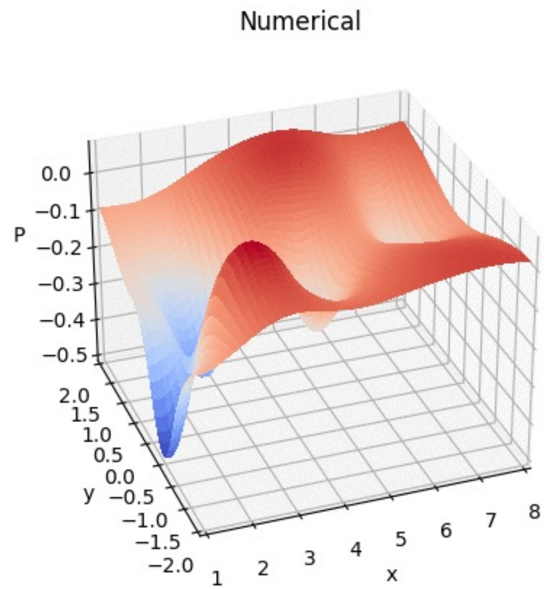
$$x \epsilon [1, 8], \qquad y \epsilon [-2, 2], \qquad t \epsilon [0, 20]$$

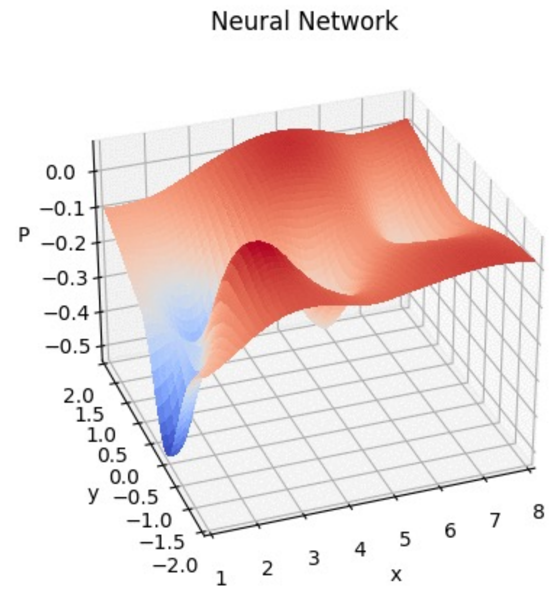
Loss Function Entities:

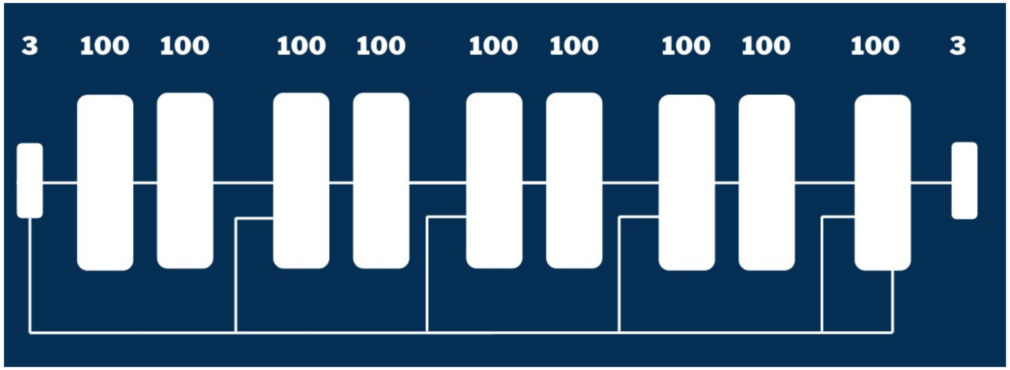
$$\text{Reconstruction\_Loss} = \text{MSE}(u - \tilde{u}) + \text{MSE}(v - \tilde{v}) + \text{MSE}(p - \tilde{p})$$

$$Domain\_Loss = MSE\left(f_u(x, y, t) + f_v(x, y, t) + f_{continuity}\right) \quad x \epsilon (1, 8), \qquad y \epsilon (-2, 2), \qquad t \epsilon (0, 20)$$

Wave Equation





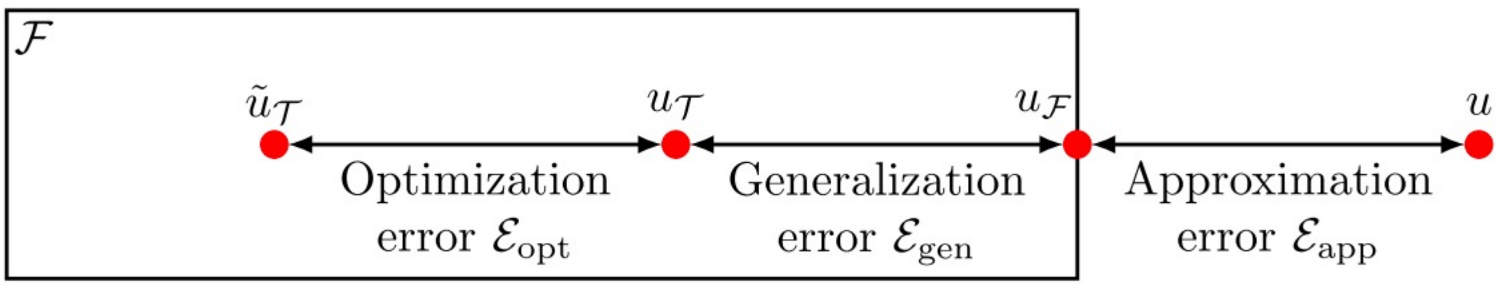


MSE: 0.0000095
Time: 1 hr 20 mins

Hybrid Net : PDE Loss + Recon Loss
(with only 0.5 percent of simulation data)

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
- Hybrid Solvers can be created combining it with the data.

Still this isn't extremely cheap to run.

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.

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