

Physics Informed Neural Network!

Disclaimer: large parts of the lab are taken from [this github repository](#) and [this one](#) both based on the original work of [Raissi, Perdikaris and Karniadakis](#) (original paper).

The obstacle that they found to publish the article state in the fact that the idea is very simple, but produce good result.

- + Easy to code
- + Mesh free
- - Spectral problem with complicated problem

Definition

Physics Informed Neural Networks (PINN) relates deep learning and Partial Differential Equations (PDEs). The main idea is not to purely rely on data, but to exploit the physical model (i.e. the *residual* of the PDE) in the loss function.

Pro: the approach is totally mesh-free.

Cons: difficult to train for complicated problems.

The loss

Let us be more specific:

The loss function of a PINN is made by:

- boundary information
- residual information

Let us suppose that the physical system we are studying is described by a PDE of the form $\mathcal{R}(w(\mathbf{x})) = 0$

Namely, we want to find a surrogate Neural Network \tilde{w} that minimizes:

$$MSE \doteq MSE_b + MSE_p.$$

where

$$MSE_b \doteq \frac{1}{N_b} \sum_{k=1}^{N_b} |\tilde{w}(\mathbf{x}_k^b) - w(\mathbf{x}_k^b)|^2,$$

hence, it is defined in the boundary of the domain, for $\mathbf{x}_k^b \in \partial\Omega$.

Here, MSE_b is the *boundary* loss. While

$$MSE_p \doteq \frac{1}{N_p} \sum_{k=1}^{N_p} |\mathcal{R}(\tilde{w}(\mathbf{x}_k^p))|^2.$$

is the *physical* (or residual) loss for $\mathbf{x}_k^p \in \Omega$, the points in the domain are the collocation problem.

Indeed, the system is

$$\begin{cases} PDE(\Omega) = 0 \\ bcs \text{ Neumann condition on the boundary} \\ \omega(\partial\Omega) = 0 \text{ Dirichlet condition} \end{cases}$$

A first Example: the 1D heat equation

The physical model is given in the **space-time** domain $[0, 2] \times [0, 1]$:

$$\frac{du}{dx} = \frac{2du}{dt} + u$$

with the following boundary (initial) condition $u(x, 0) = 6e^{-3x}$

- Independent variables: x,t (input)
- Dependent variables: u (outputs)

We have to find out $u(x,t)$ for all x in range $[0,2]$ and t in range $[0,1]$

Analytically, the solution is $u(x, t) = 6e^{(-3x-2t)}$, that is our reference.

```
In [1]: ##### starting stuff #####

import torch
import torch.nn as nn
from torch.autograd import Variable

import numpy as np
```

Let us define the Neural Network!

Question time! what are the input and output dimension? Two dimension in input (`nn.Linear(2,5)`) and one dimension in output (`nn.Linear(5,1)`).

```
In [2]: # Implementation of the Net
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.input_layer = nn.Linear(2,5) # Input
        self.hidden_layer1 = nn.Linear(5,5) # Hidden Layer
        self.hidden_layer2 = nn.Linear(5,5)
        self.hidden_layer3 = nn.Linear(5,5)
        self.hidden_layer4 = nn.Linear(5,5)
        self.output_layer = nn.Linear(5,1) # Output

    def forward(self, x,t): # Activation function
        input = torch.cat([x,t],axis=1) # combines the column array just to have only one input
        layer1_out = torch.sigmoid(self.input_layer(input))
        layer2_out = torch.sigmoid(self.hidden_layer1(layer1_out))
        layer3_out = torch.sigmoid(self.hidden_layer2(layer2_out))
        layer4_out = torch.sigmoid(self.hidden_layer3(layer3_out))
        layer5_out = torch.sigmoid(self.hidden_layer4(layer4_out))
        output = self.output_layer(layer5_out)
        return output
```

```
In [3]: ### (2) Model
net = Net() # Call the function that we have just implemented
mse_cost_function = torch.nn.MSELoss() # Mean squared error
optimizer = torch.optim.Adam(net.parameters())
```

```
In [ ]: ## PDE as Loss function. Thus would use the network which we call as u_theta
def R(x,t, net): # PDE(w)=R(w) that is the residual
    u = net(x,t) # the dependent variable u is given by the network based on independent variables x,t
    ## Based on our  $R = du/dx - 2du/dt - u$ , we need  $du/dx$  and  $du/dt$  -- HOW TO PERFORM DERIVATIVES?
    u_x = torch.autograd.grad(u.sum(), x, create_graph=True)[0] #  $du/dx$ , taking the first element that is the derivative
    u_t = torch.autograd.grad(u.sum(), t, create_graph=True)[0] #  $du/dt$ 

    # We use  $u.sum()$  because when we have a tensor, we can transform it into a scalar
    # So that we can perform the backpropagation on this scalar

    # PAY ATTENTION - In this part we can give  $u.sum()$  or not in relation on what we have to do!
    # Hence, pay attention on the different case!

    pde = u_x - 2*u_t - u

    return pde
```

```
In [ ]: ## Data from Boundary Conditions
#  $u(x,0)=6e^{-3x}$ 
## BC just gives us datapoints for training

# BC tells us that for any  $x$  in range[0,2] and time=0, the value of  $u$  is given by  $6e^{-3x}$ 
# Take say 500 random numbers of  $x$ 
x_bc = np.random.uniform(low=0.0, high=2.0, size=(500,1)) # Define points in the boundary
t_bc = np.zeros((500,1)) # For every point in  $x$ , you have to associated a  $t$  point,
                        # for now we set 0 so that they are along the line of the boundary

# compute  $u$  based on BC
u_bc = 6*np.exp(-3*x_bc) # Using the solution
```

```
In [ ]: ### (3) Training / Fitting
iterations = 10000
for epoch in range(iterations): # Epoch == iteration, we're NOT working with mini-batch
    optimizer.zero_grad() # to make the gradients zero -- To not have accumulation (as always)

    # Loss based on boundary conditions
    # Variable() because we want to set that this is a variable, but ...
    # ... requires_grad=False, hence we do not want to compute the derivatives on this variable
    pt_x_bc = Variable(torch.from_numpy(x_bc).float(), requires_grad=False) # Take everything to  $x_{bc}$ , without computing the gradient
    pt_t_bc = Variable(torch.from_numpy(t_bc).float(), requires_grad=False)
    pt_u_bc = Variable(torch.from_numpy(u_bc).float(), requires_grad=False)

    net_bc_out = net(pt_x_bc, pt_t_bc) # output of  $u(x,t)$  -- Computing only in the boundary point
    mse_u = mse_cost_function(net_bc_out, pt_u_bc) # Compute the sum in the formula for the MSE := MSEb

    # Loss based on PDE
    x_collocation = np.random.uniform(low=0.0, high=2.0, size=(500,1)) # Compute some points inside the domain
    t_collocation = np.random.uniform(low=0.0, high=1.0, size=(500,1)) # As before, set all element of  $t$  related to  $x$ 
    all_zeros = np.zeros((500,1))

    # Definition of the variable
    # Here, we have requires_grad=True because we want to compute the gradient wrt
    # these variable when we call R function
    pt_x_collocation = Variable(torch.from_numpy(x_collocation).float(), requires_grad=True) # The points that we have just define  $x_{collocation}$ 
    pt_t_collocation = Variable(torch.from_numpy(t_collocation).float(), requires_grad=True)
    pt_all_zeros = Variable(torch.from_numpy(all_zeros).float(), requires_grad=False)

    f_out = R(pt_x_collocation, pt_t_collocation, net) # output of  $R(x,t)$  --> That we call here
    mse_f = mse_cost_function(f_out, pt_all_zeros)

    # Combining the Loss functions
    loss = mse_u + mse_f # We can add a coefficient to put the loss (mse_f & mse_u) at the same order of magnitude
```

```
loss.backward()  
optimizer.step()  
  
with torch.autograd.no_grad():  
    print(epoch, "Loss:", loss.item())
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9980 Loss: 0.002615078119561076
9981 Loss: 0.0028191618621349335
9982 Loss: 0.003163875313475728
9983 Loss: 0.005280236713588238
9984 Loss: 0.0033060433343052864
9985 Loss: 0.003710653632879257
9986 Loss: 0.0033798906952142715
9987 Loss: 0.004880223423242569
9988 Loss: 0.003036266192793846
9989 Loss: 0.004350394010543823
9990 Loss: 0.0032133536878973246
9991 Loss: 0.003102616174146533
9992 Loss: 0.002909323200583458
9993 Loss: 0.002726916689425707
9994 Loss: 0.0038629723712801933
9995 Loss: 0.0025391795206815004
9996 Loss: 0.0031294168438762426
9997 Loss: 0.003450652351602912
9998 Loss: 0.004076635465025902
9999 Loss: 0.003990635741502047

```

```

In [ ]: # Plot some results
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
import numpy as np

fig = plt.figure()
ax = fig.add_subplot(projection='3d')

x=np.arange(0,2,0.02)
t=np.arange(0,1,0.02)
ms_x, ms_t = np.meshgrid(x, t)

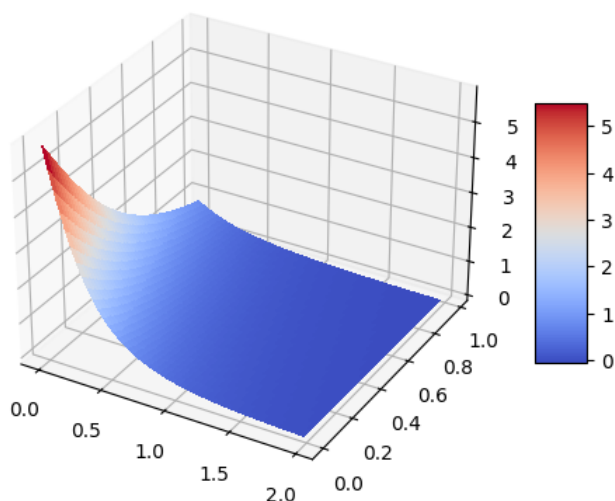
## Just because meshgrid is used, we need to do the following adjustment
x = np.ravel(ms_x).reshape(-1,1)
t = np.ravel(ms_t).reshape(-1,1)

pt_x = Variable(torch.from_numpy(x).float(), requires_grad=True)
pt_t = Variable(torch.from_numpy(t).float(), requires_grad=True)
pt_u = net(pt_x,pt_t)
u=pt_u.data.cpu().numpy()
ms_u = u.reshape(ms_x.shape)

surf = ax.plot_surface(ms_x,ms_t,ms_u, cmap=cm.coolwarm,linewidth=0, antialiased=False)
fig.colorbar(surf, shrink=0.5, aspect=5)

plt.show()

```



```

In [8]: fig = plt.figure()
ax = fig.add_subplot(projection='3d')

pt_x = Variable(torch.from_numpy(x).float(), requires_grad=True).detach().numpy()

```

```

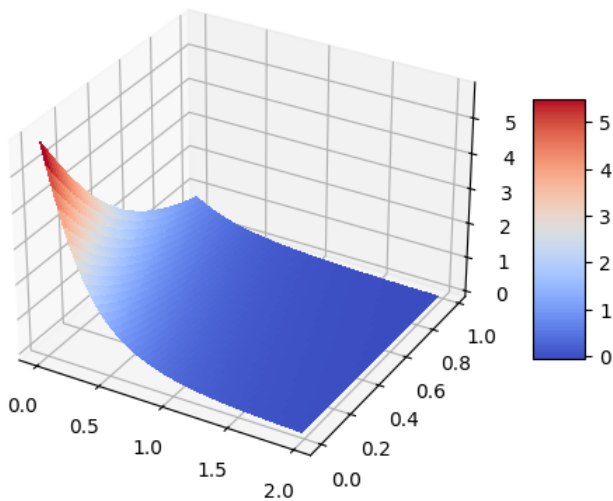
pt_t = Variable(torch.from_numpy(t).float(), requires_grad=True).detach().numpy()
R_u = 6*np.exp(-3*pt_x - 2*pt_t)
u=pt_u.data.cpu().numpy()
ms_u = u.reshape(ms_x.shape)

surf = ax.plot_surface(ms_x,ms_t,ms_u, cmap=cm.coolwarm,linewidth=0, antialiased=False)

fig.colorbar(surf, shrink=0.5, aspect=5)

plt.show()

```



Your Turn: let's change the equation

Take a look to [this github repository](#). The proposed tutorial is a bit more involved.

We suggest to study it and to try to understand it line-by-line. Try to solve this equations that is a little bit more complicated.

It tries to represent the solution of the Burgers equation

$$u_t + \lambda_1 u u_x - \lambda_2 u_{xx}$$

for some fixed parameters λ_1 and λ_2 .

Since no analytical solution is present, the code uses data provided by numerical simulations (that you can find in the folder data). Notice, that the solution changing varying the parameters, and we can consider them fixed or variable.

```

In [9]: import sys
sys.path.insert(0, '../Utilities/')

import torch
from collections import OrderedDict

import numpy as np
import matplotlib.pyplot as plt
import scipy.io
from scipy.interpolate import griddata
from mpl_toolkits.axes_grid1 import make_axes_locatable
import matplotlib.gridspec as gridspec
import warnings

warnings.filterwarnings('ignore')

np.random.seed(1234)

```

```

In [10]: # the deep neural network

# Build the construction of the net, just in a contract for with some for Loop
class DNN(torch.nn.Module):
    def __init__(self, layers):
        super(DNN, self).__init__()

        # parameters
        self.depth = len(layers) - 1

        # set up layer order dict
        self.activation = torch.nn.Tanh

        layer_list = list()
        for i in range(self.depth - 1):
            layer_list.append(
                ('layer_%d' % i, torch.nn.Linear(layers[i], layers[i+1]))
            )
            layer_list.append(('activation_%d' % i, self.activation()))

        layer_list.append(
            ('layer_%d' % (self.depth - 1), torch.nn.Linear(layers[-2], layers[-1]))

```

```

    )
    layerDict = OrderedDict(layer_list)

    # deploy layers
    self.layers = torch.nn.Sequential(layerDict) ## layer, activation, layer, activation

def forward(self, x):
    out = self.layers(x) # self.layers := are the sequential of all the layer --> Just done in a compact way
    return out

```

In []: # the physics-guided neural network

```

# PNN definition
class PhysicsInformedNN():
    def __init__(self, X, u, layers, lb, ub):

        # boundary conditions
        self.lb = torch.tensor(lb).float()
        self.ub = torch.tensor(ub).float()

        # data
        self.x = torch.tensor(X[:, 0:1], requires_grad=True).float()
        self.t = torch.tensor(X[:, 1:2], requires_grad=True).float()
        self.u = torch.tensor(u).float()

        # settings -- If you want to fix
        self.lambda_1 = torch.tensor([0.0], requires_grad=True)
        self.lambda_2 = torch.tensor([-6.0], requires_grad=True)

        # settings -- If you want to find the value of lambda, you have just to set them as parameters
        self.lambda_1 = torch.nn.Parameter(self.lambda_1)
        self.lambda_2 = torch.nn.Parameter(self.lambda_2)

        # deep neural networks
        self.dnn = DNN(layers) # We call the net define before
        self.dnn.register_parameter('lambda_1', self.lambda_1)
        self.dnn.register_parameter('lambda_2', self.lambda_2)

        # optimizers: using the same settings
        self.optimizer = torch.optim.LBFGS(
            self.dnn.parameters(),
            lr=1.0,
            max_iter=50000,
            max_eval=50000,
            history_size=50,
            tolerance_grad=1e-5,
            tolerance_change=1.0 * np.finfo(float).eps,
            line_search_fn="strong_wolfe" # can be "strong_wolfe"
        )

        self.optimizer_Adam = torch.optim.Adam(self.dnn.parameters())
        self.iter = 0

    def net_u(self, x, t):
        u = self.dnn(torch.cat([x, t], dim=1))
        return u

    def net_f(self, x, t):
        """ The pytorch autograd version of calculating residual """
        lambda_1 = self.lambda_1
        lambda_2 = torch.exp(self.lambda_2)
        u = self.net_u(x, t)

        # Definition of first derivative wrt to t
        u_t = torch.autograd.grad(
            u, t,
            grad_outputs=torch.ones_like(u),
            retain_graph=True,
            create_graph=True
        )[0]

        # Definition of first derivative wrt to x
        u_x = torch.autograd.grad(
            u, x, # Here I do NOT put the sum, so I'm working with all the tensor and not just a scalar ...
            grad_outputs=torch.ones_like(u), # ... hence we have to tell that dT/dT=1 with T a variable that we define
            # Indeed, here we have just write that du/du=1 because we're working with the tensor,
            # and no more with the scalar how we did before writing u.sum()
            retain_graph=True,
            create_graph=True
        )[0]

        # Definition of second derivatives wrt x
        u_xx = torch.autograd.grad(
            u_x, x,
            grad_outputs=torch.ones_like(u_x),
            retain_graph=True,
            create_graph=True
        )[0]

        f = u_t + lambda_1 * u * u_x - lambda_2 * u_xx
        return f

    def loss_func(self):
        u_pred = self.net_u(self.x, self.t)

```



```

f_pred = self.net_f(self.x, self.t)
loss = torch.mean((self.u - u_pred) ** 2) + torch.mean(f_pred ** 2)
self.optimizer.zero_grad()
loss.backward()

self.iter += 1
if self.iter % 100 == 0:
    print(
        'Loss: %e, l1: %.5f, l2: %.5f' %
        (
            loss.item(),
            self.lambda_1.item(),
            torch.exp(self.lambda_2.detach()).item()
        )
    )
return loss

def train(self, nIter):
    self.dnn.train()
    for epoch in range(nIter):
        u_pred = self.net_u(self.x, self.t)
        f_pred = self.net_f(self.x, self.t)
        loss = torch.mean((self.u - u_pred) ** 2) + torch.mean(f_pred ** 2)

        # Backward and optimize
        self.optimizer_Adam.zero_grad()
        loss.backward()
        self.optimizer_Adam.step()

        if epoch % 100 == 0:
            print(
                'It: %d, Loss: %.3e, Lambda_1: %.3f, Lambda_2: %.6f' %
                (
                    epoch,
                    loss.item(),
                    self.lambda_1.item(), # The prediction is also for lambda -- we need some data
                    torch.exp(self.lambda_2).item()
                )
            )

        # Backward and optimize
        self.optimizer.step(self.loss_func)

def predict(self, X):
    x = torch.tensor(X[:, 0:1], requires_grad=True).float()
    t = torch.tensor(X[:, 1:2], requires_grad=True).float()

    self.dnn.eval()
    u = self.net_u(x, t)
    f = self.net_f(x, t)
    u = u.detach().cpu().numpy()
    f = f.detach().cpu().numpy()
    return u, f

```

```

In [12]: nu = 0.01/np.pi

N_u = 2000
layers = [2, 20, 20, 20, 20, 20, 20, 20, 20, 1]

data = scipy.io.loadmat('data/burgers_shock.mat') # Import the data

t = data['t'].flatten()[:,None]
x = data['x'].flatten()[:,None]
Exact = np.real(data['usol']).T

X, T = np.meshgrid(x,t)

X_star = np.hstack((X.flatten()[:,None], T.flatten()[:,None]))
u_star = Exact.flatten()[:,None]

# Domain bounds
lb = X_star.min(0)
ub = X_star.max(0)

```

```

In [13]: noise = 0.0

# create training set
idx = np.random.choice(X_star.shape[0], N_u, replace=False)
X_u_train = X_star[idx,:]
u_train = u_star[idx,:]

# training
model = PhysicsInformedNN(X_u_train, u_train, layers, lb, ub)
model.train(0)

# At the end we reach a good approximation

```

```

Loss: 2.379245e-02, l1: 0.18653, l2: 0.00230
Loss: 1.510439e-02, l1: 0.53338, l2: 0.00260
Loss: 1.136508e-02, l1: 0.58937, l2: 0.00322
Loss: 7.742971e-03, l1: 0.70138, l2: 0.00377
Loss: 5.504389e-03, l1: 0.75810, l2: 0.00399
Loss: 4.173984e-03, l1: 0.80020, l2: 0.00479
Loss: 3.057414e-03, l1: 0.85740, l2: 0.00573
Loss: 1.870770e-03, l1: 0.91171, l2: 0.00614
Loss: 1.104523e-03, l1: 0.94429, l2: 0.00595
Loss: 6.797987e-04, l1: 0.96606, l2: 0.00546
Loss: 4.730221e-04, l1: 0.97706, l2: 0.00504
Loss: 3.102128e-04, l1: 0.97665, l2: 0.00454
Loss: 2.329755e-04, l1: 0.98243, l2: 0.00416
Loss: 1.885898e-04, l1: 0.98526, l2: 0.00384
Loss: 1.491945e-04, l1: 0.98392, l2: 0.00347
Loss: 1.337306e-04, l1: 0.98290, l2: 0.00332
Loss: 1.136881e-04, l1: 0.98878, l2: 0.00339
Loss: 8.821491e-05, l1: 0.98976, l2: 0.00324
Loss: 7.781447e-05, l1: 0.98876, l2: 0.00328
Loss: 6.914230e-05, l1: 0.98658, l2: 0.00325
Loss: 5.792868e-05, l1: 0.99498, l2: 0.00329
Loss: 5.094261e-05, l1: 0.99577, l2: 0.00325
Loss: 4.715933e-05, l1: 0.99587, l2: 0.00323
Loss: 4.308285e-05, l1: 0.99407, l2: 0.00323
Loss: 3.923191e-05, l1: 0.99645, l2: 0.00325
Loss: 3.632144e-05, l1: 0.99563, l2: 0.00326
Loss: 3.335014e-05, l1: 0.99453, l2: 0.00328
Loss: 3.036366e-05, l1: 0.99730, l2: 0.00333
Loss: 2.859140e-05, l1: 0.99810, l2: 0.00334
Loss: 2.707079e-05, l1: 0.99648, l2: 0.00334
Loss: 2.496797e-05, l1: 0.99625, l2: 0.00333
Loss: 2.288576e-05, l1: 0.99695, l2: 0.00332
Loss: 2.108958e-05, l1: 0.99812, l2: 0.00330
Loss: 1.974920e-05, l1: 0.99783, l2: 0.00329
Loss: 1.837065e-05, l1: 0.99751, l2: 0.00329
Loss: 1.706044e-05, l1: 0.99787, l2: 0.00326
Loss: 1.594443e-05, l1: 0.99880, l2: 0.00325
Loss: 1.509693e-05, l1: 0.99860, l2: 0.00323
Loss: 1.452912e-05, l1: 0.99852, l2: 0.00323
Loss: 1.388160e-05, l1: 0.99782, l2: 0.00322
Loss: 1.314326e-05, l1: 0.99835, l2: 0.00321
Loss: 1.261405e-05, l1: 0.99876, l2: 0.00320
Loss: 1.215868e-05, l1: 0.99843, l2: 0.00320
Loss: 1.141523e-05, l1: 0.99895, l2: 0.00319
Loss: 1.057932e-05, l1: 0.99880, l2: 0.00318
Loss: 9.982006e-06, l1: 0.99879, l2: 0.00317
Loss: 9.204959e-06, l1: 0.99888, l2: 0.00315
Loss: 8.633679e-06, l1: 0.99892, l2: 0.00315
Loss: 8.033985e-06, l1: 0.99944, l2: 0.00316
Loss: 7.348279e-06, l1: 0.99957, l2: 0.00316
Loss: 6.853191e-06, l1: 0.99935, l2: 0.00316
Loss: 6.467846e-06, l1: 0.99928, l2: 0.00317
Loss: 6.223004e-06, l1: 0.99905, l2: 0.00317
Loss: 5.909767e-06, l1: 0.99806, l2: 0.00317
Loss: 5.534403e-06, l1: 0.99861, l2: 0.00317
Loss: 5.255200e-06, l1: 0.99928, l2: 0.00318
Loss: 5.015365e-06, l1: 0.99949, l2: 0.00319
Loss: 4.844318e-06, l1: 0.99994, l2: 0.00319
Loss: 4.622019e-06, l1: 0.99892, l2: 0.00319
Loss: 4.388066e-06, l1: 0.99873, l2: 0.00319
Loss: 4.258453e-06, l1: 0.99893, l2: 0.00320
Loss: 4.064746e-06, l1: 0.99918, l2: 0.00320
Loss: 3.914304e-06, l1: 0.99964, l2: 0.00321
Loss: 3.780486e-06, l1: 0.99966, l2: 0.00321
Loss: 3.646520e-06, l1: 0.99938, l2: 0.00321
Loss: 3.507149e-06, l1: 0.99979, l2: 0.00322

```

```

In [14]: # evaluations
u_pred, f_pred = model.predict(X_star)

error_u = np.linalg.norm(u_star-u_pred,2)/np.linalg.norm(u_star,2)

U_pred = griddata(X_star, u_pred.flatten(), (X, T), method='cubic')

lambda_1_value = model.lambda_1.detach().cpu().numpy()
lambda_2_value = model.lambda_2.detach().cpu().numpy()
lambda_2_value = np.exp(lambda_2_value)

error_lambda_1 = np.abs(lambda_1_value - 1.0) * 100
error_lambda_2 = np.abs(lambda_2_value - nu) / nu * 100

print('Error u: %e' % (error_u))
print('Error l1: %.5f%%' % (error_lambda_1))
print('Error l2: %.5f%%' % (error_lambda_2))

```

```

Error u: 1.394462e-03
Error l1: 0.04777%
Error l2: 1.05141%

```