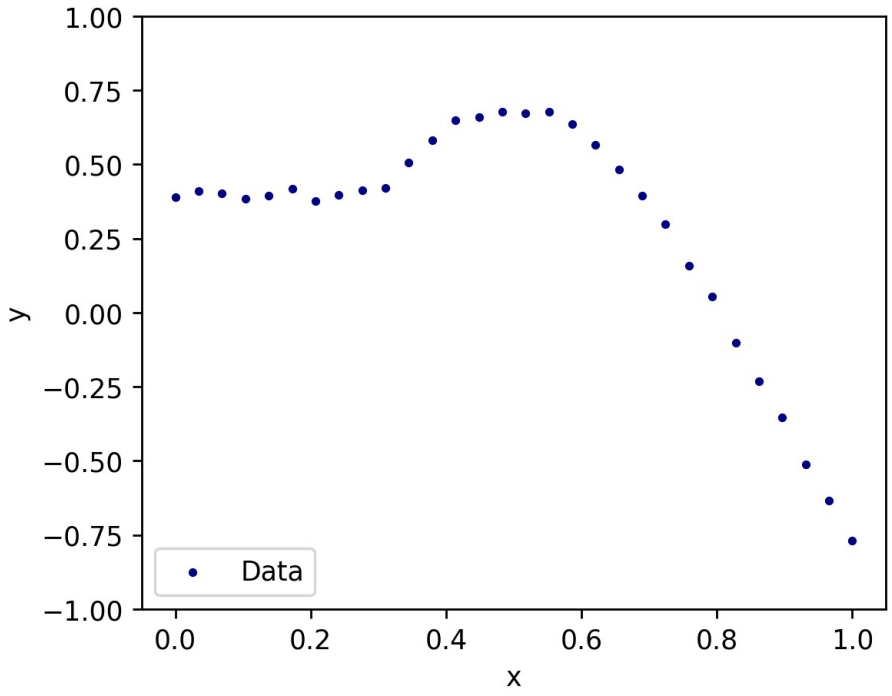
M7-L2 Problem 2

Here you will create a simple neural network for regression in PyTorch. PyTorch will give you a lot more control and flexibility for neural networks than SciKit-Learn, but there are some extra steps to learn.

Run the following cell to load our 1-D dataset:

```
import numpy as np
import matplotlib.pyplot as plt
import torch
from torch import optim, nn
import torch.nn.functional as F

x = np.array([0.        , 0.03448276, 0.06896552, 0.10344828,
0.13793103,0.17241379, 0.20689655, 0.24137931, 0.27586207,
0.31034483,0.34482759, 0.37931034, 0.4137931 , 0.44827586,
0.48275862,0.51724138, 0.55172414, 0.5862069 , 0.62068966,
0.65517241,0.68965517, 0.72413793, 0.75862069, 0.79310345,
0.82758621,0.86206897, 0.89655172, 0.93103448, 0.96551724,
1.        ]).reshape(-1,1)
y = np.array([ 0.38914369,  0.40997345,  0.40282978,  0.38493705,
0.394214  ,0.41651437,  0.37573321,  0.39571087,  0.41265936,
0.41953955,0.50596807,  0.58059196,  0.6481607 ,  0.66050901,
0.67741369,0.67348567,  0.67696078,  0.63537378,  0.56446933,
0.48265412,0.39540671,  0.29878237,  0.15893846,  0.05525194, -
0.10070259,-0.23055219, -0.35288448, -0.51317604, -0.63377544, -
0.76849408]).reshape(-1,1)


plt.figure(figsize=(5,4),dpi=250)
plt.scatter(x,y,s=5,c="navy",label="Data")
plt.legend(loc="lower left")
plt.ylim(-1,1)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```



PyTorch Tensors

PyTorch models only work with PyTorch Tensors, so we need to convert our dataset into a tensors.

To convert these back to numpy arrays we can use:

- `x.detach().numpy()`
- `y.detach().numpy()`

```
x = torch.Tensor(x)
y = torch.Tensor(y)
```

PyTorch Module

We create a subclass whose superclass is `nn.Module`, a basic predictive model, and we must define 2 methods.

`nn.Module` subclass:

- `__init__()`
  - runs when creating a new model instance
  - includes the line `super().__init__()` to inherit parent methods from `nn.Module`
  - sets up all necessary model components/parameters
- `forward()`
  - runs when calling a model instance

- performs a forward pass through the network given an input tensor.

This class `Net_2_layer` is an MLP for regression with 2 layers. At initialization, the user inputs the number of hidden neurons per layer, the number of inputs and outputs, and the activation function.

```
class Net_2_layer(nn.Module):
    def __init__(self, N_hidden=6, N_in=1, N_out=1, activation =
F.relu):
        super().__init__()
        # Linear transformations -- these have weights and biases as
trainable parameters,
        # so we must create them here.
        self.lin1 = nn.Linear(N_in, N_hidden)
        self.lin2 = nn.Linear(N_hidden, N_hidden)
        self.lin3 = nn.Linear(N_hidden, N_out)
        self.act = activation

    def forward(self,x):
        x = self.lin1(x)
        x = self.act(x)  # Activation of first hidden layer
        x = self.lin2(x)
        x = self.act(x)  # Activation at second hidden layer
        x = self.lin3(x) # (No activation at last layer)

        return x
```

Instantiate a model

This model has 6 neurons at each hidden layer, and it uses ReLU activation.

```
model = Net_2_layer(N_hidden = 6, activation = F.relu)
loss_curve = []
```

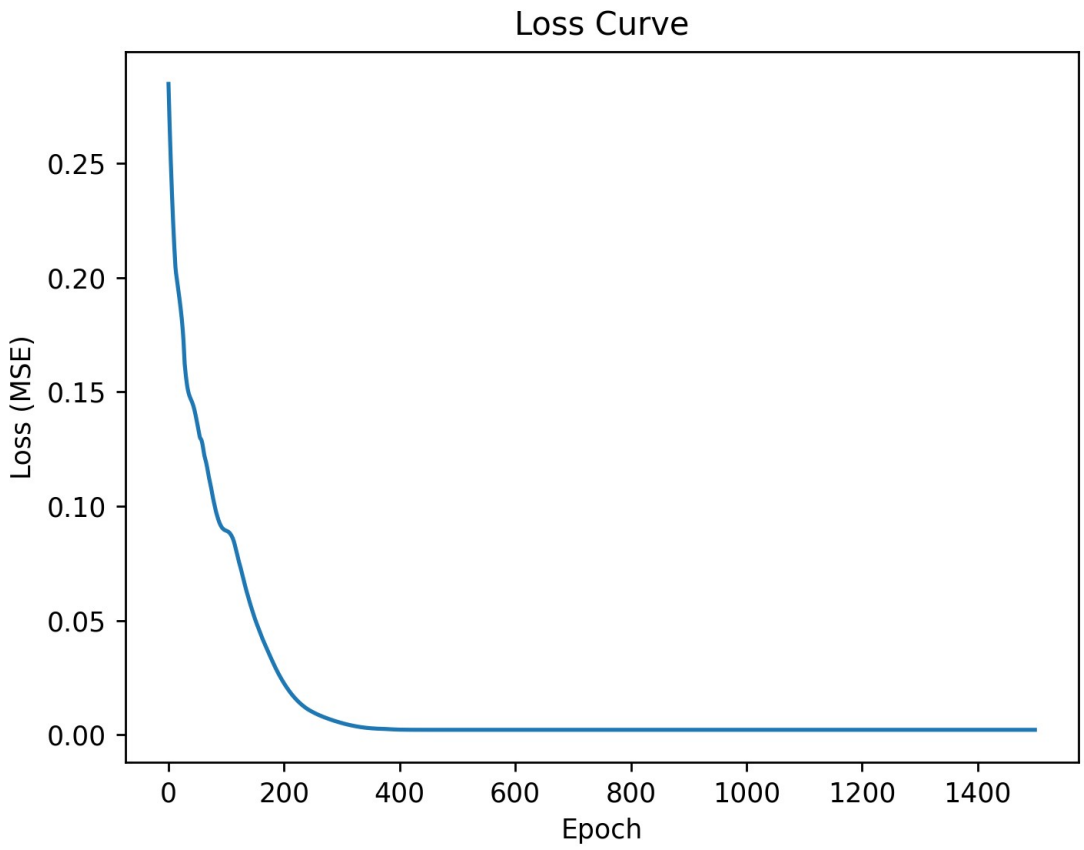
Training a model

```
# Training parameters: Learning rate, number of epochs, loss function
# (These can be tuned)
lr = 0.005
epochs = 1500
loss_fcn = F.mse_loss

# Set up optimizer to optimize the model's parameters using Adam with
the selected learning rate
opt = optim.Adam(params = model.parameters(), lr=lr)

# Training loop
for epoch in range(epochs):
    out = model(x) # Evaluate the model
```

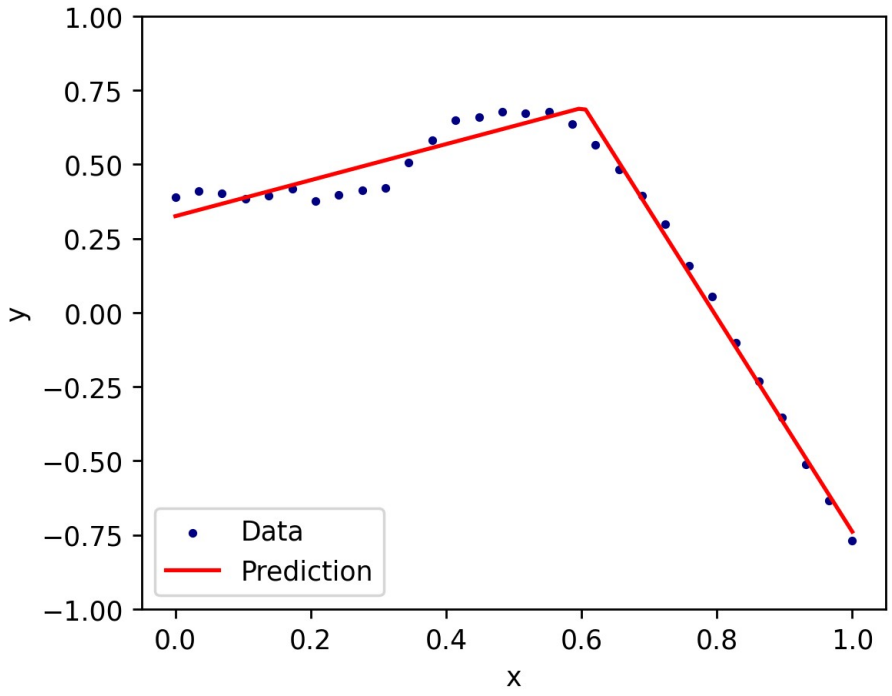
```
    loss = loss_fcn(out,y) # Calculate the loss -- error between
network prediction and y

    loss_curve.append(loss.item())

    # Print loss progress info 25 times during training
    if epoch % int(epochs / 25) == 0:
        print(f"Epoch {epoch} of {epochs}... \tAverage loss:
{loss.item()}")

    # Move the model parameters 1 step closer to their optima:
    opt.zero_grad()
    loss.backward()
    opt.step()
```

```
Epoch 0 of 1500...    Average loss: 0.2846282422542572
Epoch 60 of 1500...   Average loss: 0.12524329125881195
Epoch 120 of 1500...  Average loss: 0.07749786227941513
Epoch 180 of 1500...  Average loss: 0.03207949176430702
Epoch 240 of 1500...  Average loss: 0.011363743804395199
Epoch 300 of 1500...  Average loss: 0.0051547870971262455
Epoch 360 of 1500...  Average loss: 0.0027225306257605553
Epoch 420 of 1500...  Average loss: 0.0022241221740841866
Epoch 480 of 1500...  Average loss: 0.0022069227416068316
Epoch 540 of 1500...  Average loss: 0.0022069131955504417
Epoch 600 of 1500...  Average loss: 0.002206912962719798
Epoch 660 of 1500...  Average loss: 0.00220691086724400 5
Epoch 720 of 1500...  Average loss: 0.0022069106344133615
Epoch 780 of 1500...  Average loss: 0.0022069106344133615
Epoch 840 of 1500...  Average loss: 0.0022069106344133615
Epoch 900 of 1500...  Average loss: 0.0022069106344133615
Epoch 960 of 1500...  Average loss: 0.0022069106344133615
Epoch 1020 of 1500...      Average loss: 0.002206911100074649
Epoch 1080 of 1500...      Average loss: 0.002206911100074649
Epoch 1140 of 1500...      Average loss: 0.002206911100074649
Epoch 1200 of 1500...      Average loss: 0.002206911565735936
Epoch 1260 of 1500...      Average loss: 0.002206911565735936
Epoch 1320 of 1500...      Average loss: 0.002206911565735936
Epoch 1380 of 1500...      Average loss: 0.002206911565735936
Epoch 1440 of 1500...      Average loss: 0.002206911565735936
```

```
plt.figure(dpi=250)
plt.plot(loss_curve)
plt.xlabel('Epoch')
plt.ylabel('Loss (MSE)')
plt.title('Loss Curve')
plt.show()
```




```
xs = torch.linspace(0,1,100).reshape(-1,1)
ys = model(xs)

plt.figure(figsize=(5,4),dpi=250)
plt.scatter(x,y,s=5,c="navy",label="Data")
plt.plot(xs.detach().numpy(),
ys.detach().numpy(),"r-",label="Prediction")
plt.legend(loc="lower left")
plt.ylim(-1,1)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```



Your Turn

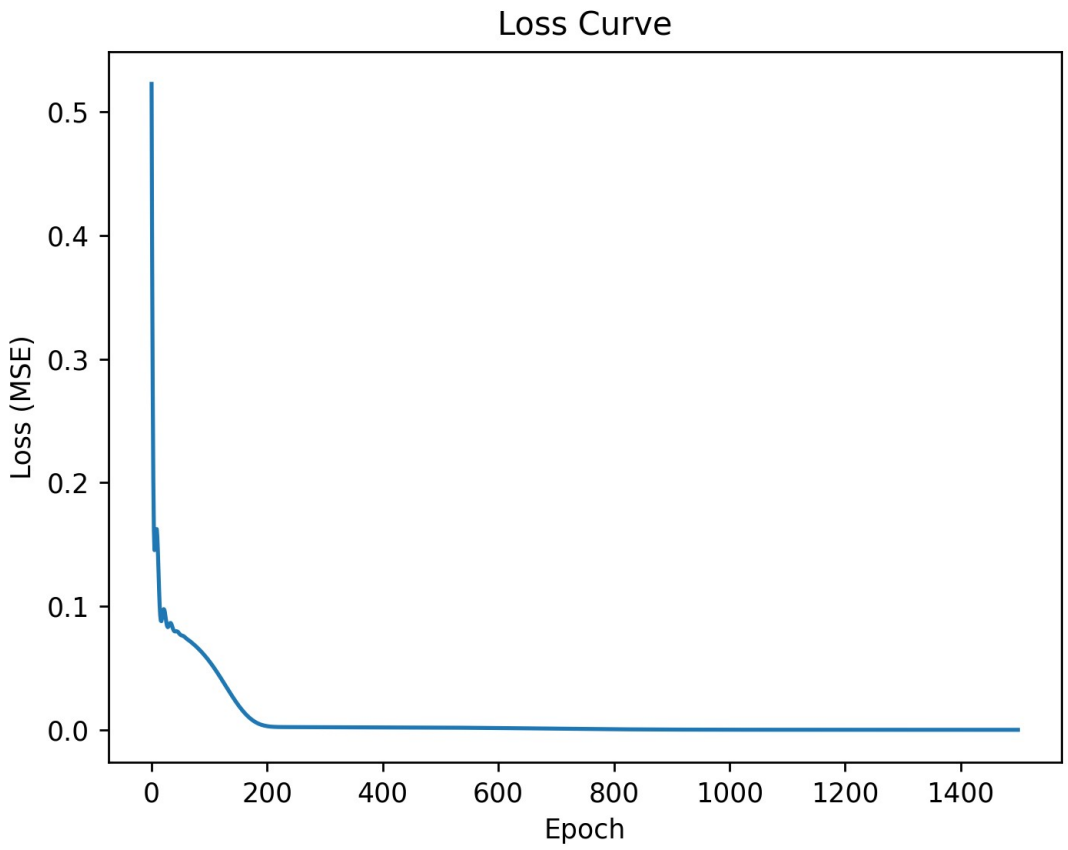
In the cells below, create a new instance of `Net_2_layer`. This time, use 20 neurons per hidden layer, and an activation of `F.tanh`. Plot the loss curve and a visualization of the prediction with the data.

```
# YOUR CODE GOES HERE
# 20 neruons per hidden layer, and an activation function of F.tanh
model1 = Net_2_layer(N_hidden = 20, activation = F.tanh)
loss_curve = []

# Training parameters: Learning rate, number of epochs, loss function
lr = 0.005
epochs = 1500
loss_fcn = F.mse_loss

# Set up optimizer to optimize the model's parameters using Adam with
the selected learning rate
opt = optim.Adam(params = model1.parameters(), lr=lr)

# Training loop
for epoch in range(epochs):
    out = model1(x) # Evaluate the model
    loss = loss_fcn(out,y) # Calculate the loss -- error between
network prediction and y

    loss_curve.append(loss.item())
```

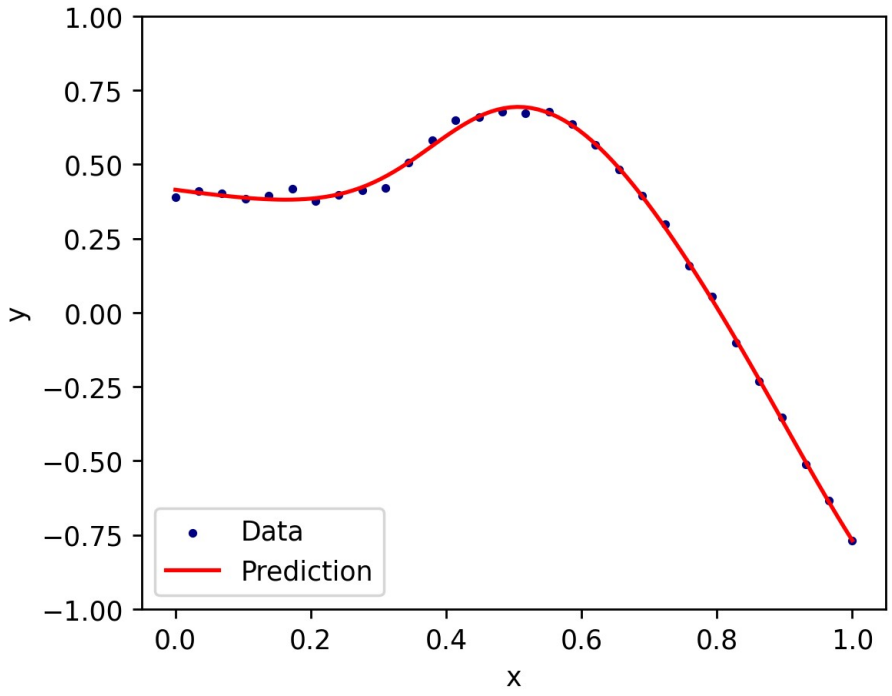
```
    # Print loss progress info 25 times during training
    if epoch % int(epochs / 25) == 0:
        print(f"Epoch {epoch} of {epochs}... \tAverage loss:
{loss.item()}")

    # Move the model parameters 1 step closer to their optima:
    opt.zero_grad()
    loss.backward()
    opt.step()
```

```
Epoch 0 of 1500...    Average loss: 0.5223419666290283
Epoch 60 of 1500...   Average loss: 0.07408086210489273
Epoch 120 of 1500...  Average loss: 0.04191172122955322
Epoch 180 of 1500...  Average loss: 0.006381927989423275
Epoch 240 of 1500...  Average loss: 0.002428209176287055
Epoch 300 of 1500...  Average loss: 0.002365131163969636
Epoch 360 of 1500...  Average loss: 0.0022913666907697916
Epoch 420 of 1500...  Average loss: 0.002200573915615678
Epoch 480 of 1500...  Average loss: 0.0020795234013348818
Epoch 540 of 1500...  Average loss: 0.0019061658531427383
Epoch 600 of 1500...  Average loss: 0.0016590988961979747
Epoch 660 of 1500...  Average loss: 0.001347280340269208
Epoch 720 of 1500...  Average loss: 0.0010233799694105983
Epoch 780 of 1500...  Average loss: 0.0007491824799217284
Epoch 840 of 1500...  Average loss: 0.0005512729403562844
Epoch 900 of 1500...  Average loss: 0.0004194226348772645
Epoch 960 of 1500...  Average loss: 0.0003373590006958693
Epoch 1020 of 1500...      Average loss: 0.00029409301350824535
Epoch 1080 of 1500...      Average loss: 0.00027269343263469636
Epoch 1140 of 1500...      Average loss: 0.00026076758513227105
Epoch 1200 of 1500...      Average loss: 0.00025270588230341673
Epoch 1260 of 1500...      Average loss: 0.0002462092961650342
Epoch 1320 of 1500...      Average loss: 0.0002403251564828679
Epoch 1380 of 1500...      Average loss: 0.0002346175751881674
Epoch 1440 of 1500...      Average loss: 0.0002288554678671062
```

```
plt.figure(dpi=250)
plt.plot(loss_curve)
plt.xlabel('Epoch')
plt.ylabel('Loss (MSE)')
plt.title('Loss Curve')
plt.show()
```




```
xs = torch.linspace(0,1,100).reshape(-1,1)
ys = model1(xs)

plt.figure(figsize=(5,4),dpi=250)
plt.scatter(x,y,s=5,c="navy",label="Data")
plt.plot(xs.detach().numpy(),
ys.detach().numpy(),"r-",label="Prediction")
plt.legend(loc="lower left")
plt.ylim(-1,1)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
y
0.0
0.2
0.4
0.6
0.8
1.0
x
Data
Prediction