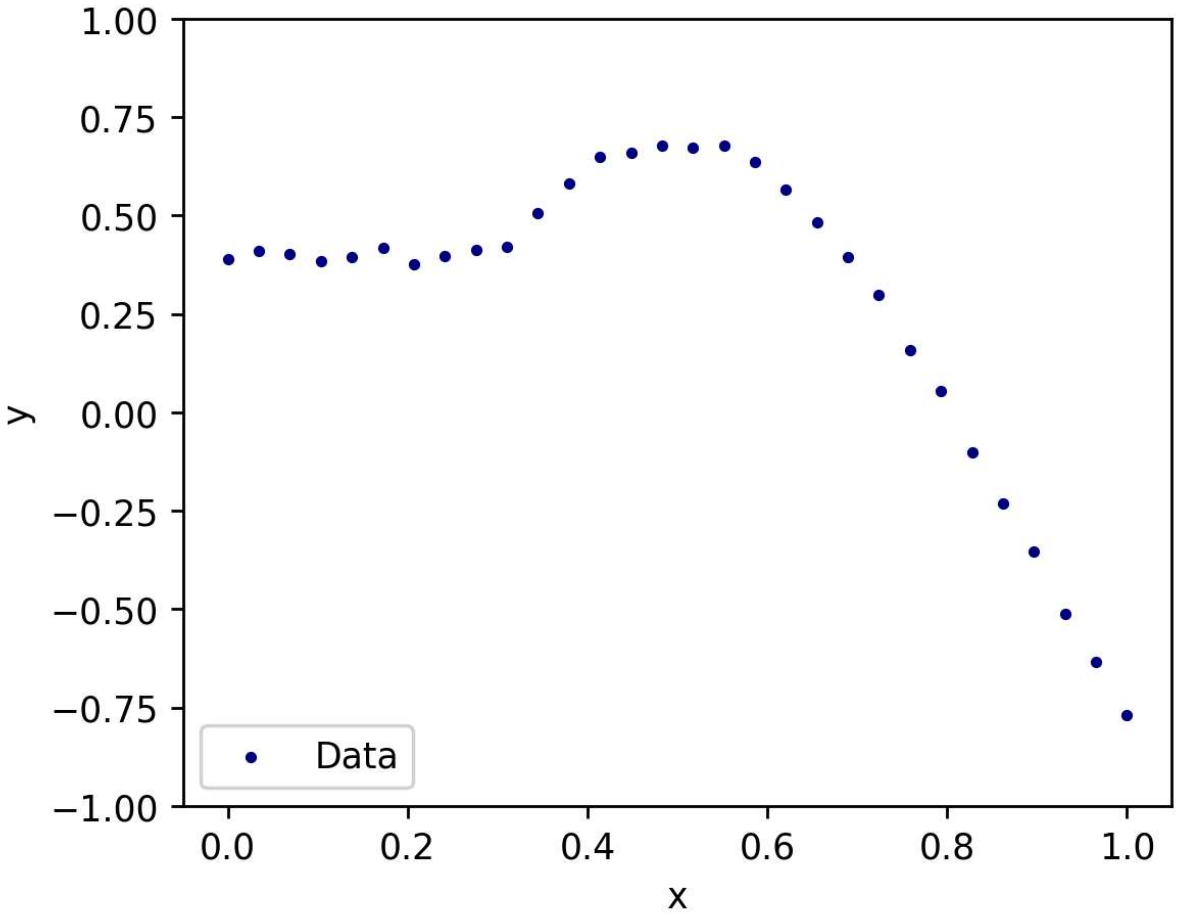
M7-L2 Problem 2

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:

In [82]:
```
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
y = np.array([ 0.38914369,  0.40997345,  0.40282978,  0.38493705,  0.394214  ,0.416


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()`

In [83]:
```
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.

In [84]:
```
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 para
        # 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.

In [85]:
```
model = Net_2_layer(N_hidden = 6, activation = F.relu)
loss_curve = []
```

Training a model

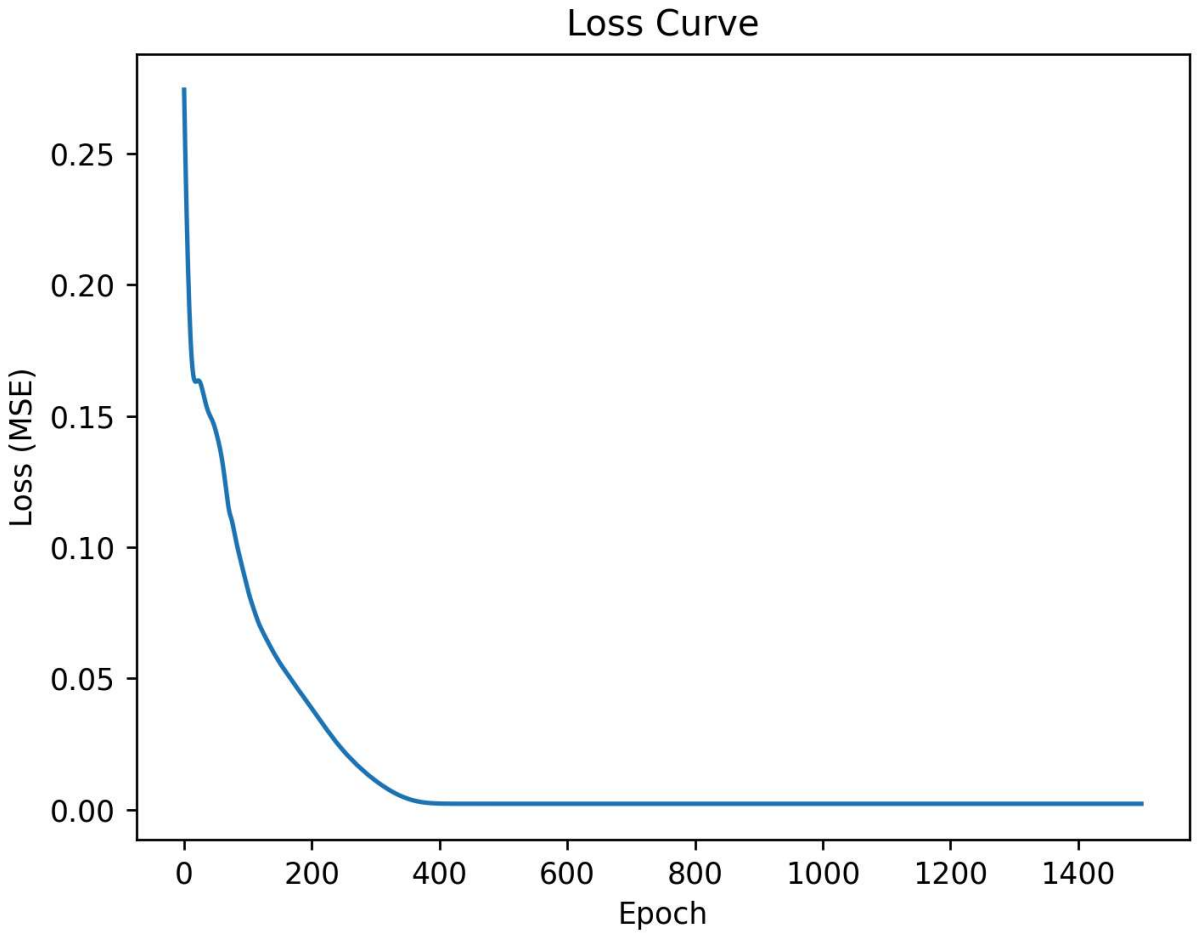
In [86]:
```
# Training parameters: Learning rate, number of epochs, loss function
# (These can be tuned)
lr = 0.005
epochs = 1500
loss_fcn = F.mse_loss

# Set up optimizer to optimize the model's parameters using Adam with the selected
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

    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()
```

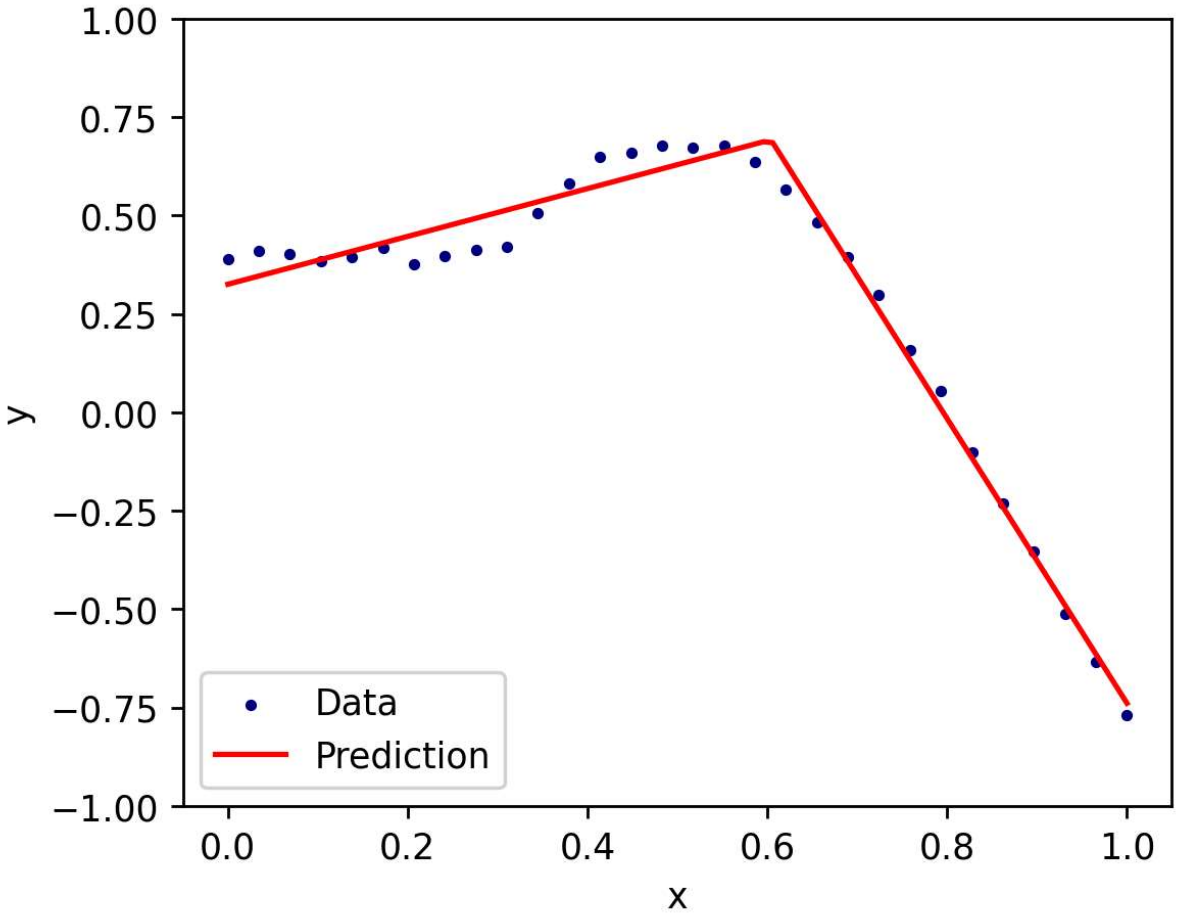
```
Epoch 0 of 1500...      Average loss: 0.2743450999259949
Epoch 60 of 1500...     Average loss: 0.132395401597023
Epoch 120 of 1500...    Average loss: 0.0693087950348854
Epoch 180 of 1500...    Average loss: 0.04530538618564606
Epoch 240 of 1500...    Average loss: 0.02516205795109272
Epoch 300 of 1500...    Average loss: 0.010957315564155579
Epoch 360 of 1500...    Average loss: 0.0034239196684211493
Epoch 420 of 1500...    Average loss: 0.0022208059672266245
Epoch 480 of 1500...    Average loss: 0.0022069222759455442
Epoch 540 of 1500...    Average loss: 0.0022069131955504417
Epoch 600 of 1500...    Average loss: 0.0022069134283810854
Epoch 660 of 1500...    Average loss: 0.00220691435970366
Epoch 720 of 1500...    Average loss: 0.00220691435970366
Epoch 780 of 1500...    Average loss: 0.00220691435970366
Epoch 840 of 1500...    Average loss: 0.00220691435970366
Epoch 900 of 1500...    Average loss: 0.0022069131955504417
Epoch 960 of 1500...    Average loss: 0.0022069131955504417
Epoch 1020 of 1500...   Average loss: 0.0022069131955504417
Epoch 1080 of 1500...   Average loss: 0.0022069131955504417
Epoch 1140 of 1500...   Average loss: 0.0022069131955504417
Epoch 1200 of 1500...   Average loss: 0.0022069131955504417
Epoch 1260 of 1500...   Average loss: 0.0022069131955504417
Epoch 1320 of 1500...   Average loss: 0.0022069131955504417
Epoch 1380 of 1500...   Average loss: 0.0022069131955504417
Epoch 1440 of 1500...   Average loss: 0.0022069131955504417
```

In [87]:

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



In [88]:
```
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()
```



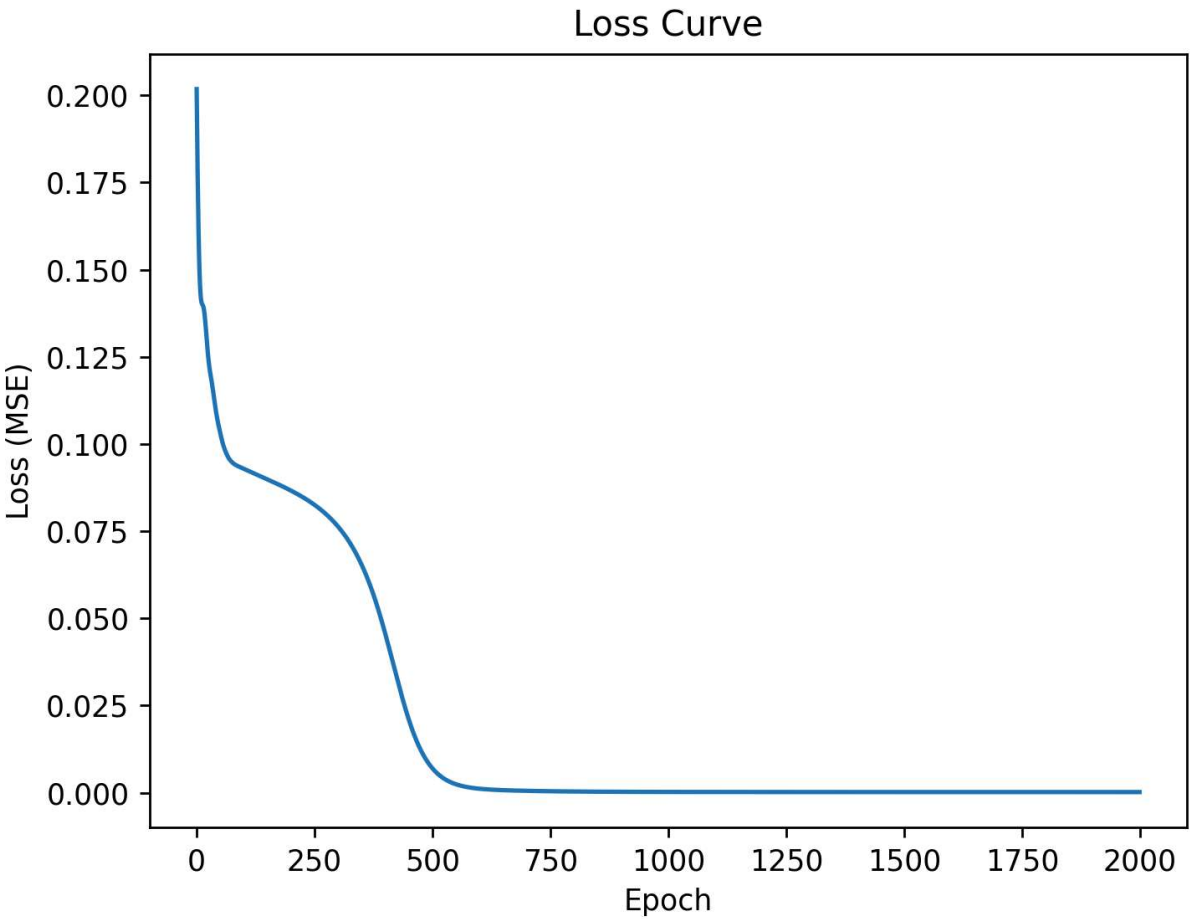
Your Turn

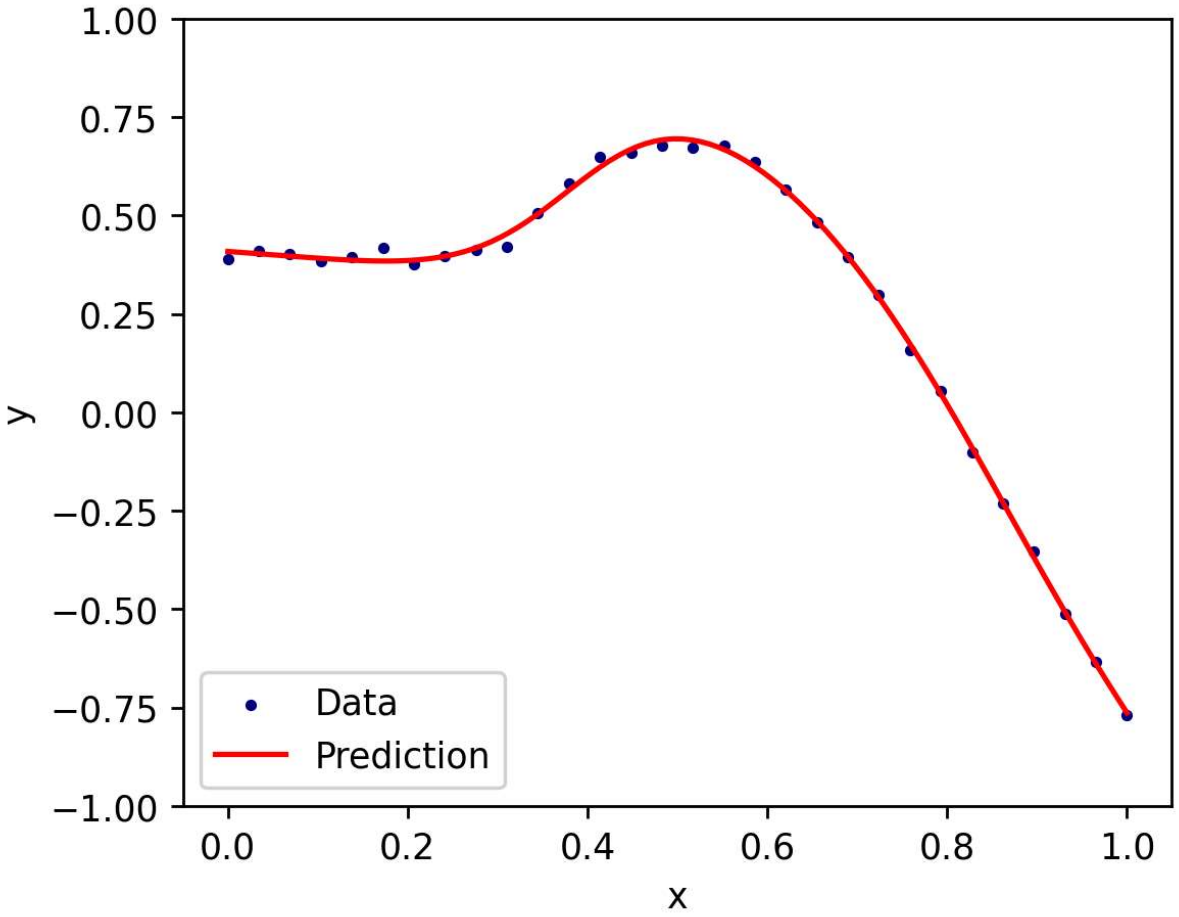
In the cells below, create a new instance of `Net_2_layer`. This time, use 20 neurons per hidden layer, and an activation of `F.tanh`. Plot the loss curve and a visualization of the prediction with the data.

In [94]:
```
# YOUR CODE GOES HERE
model1 = Net_2_layer(N_hidden = 20, activation = F.tanh)
loss_curve1 = []

lr = 0.001
epochs1 = 2000
loss_fcn = F.mse_loss

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

# Training loop
for epoch1 in range(epochs1):
    out = model1(x) # Evaluate the model
    loss = loss_fcn(out,y) # Calculate the loss -- error between network prediction

    loss_curve1.append(loss.item())
```

```
    # Print loss progress info 25 times during training
    if epoch1 % int(epochs1 / 25) == 0:
        print(f"Epoch {epoch1} of {epochs1}... \tAverage loss: {loss.item()}")

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


plt.figure(dpi=250)
plt.plot(loss_curve1)
plt.xlabel('Epoch')
plt.ylabel('Loss (MSE)')
plt.title('Loss Curve')
plt.show()

xs1 = torch.linspace(0,1,100).reshape(-1,1)
ys1 = model1(xs1)

plt.figure(figsize=(5,4),dpi=250)
plt.scatter(x,y,s=5,c="navy",label="Data")
plt.plot(xs1.detach().numpy(), ys1.detach().numpy(),"r-",label="Prediction")
plt.legend(loc="lower left")
plt.ylim(-1,1)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

```
Epoch 0 of 2000...      Average loss: 0.20178550481796265
Epoch 80 of 2000...     Average loss: 0.0942194014787674
Epoch 160 of 2000...    Average loss: 0.08923618495464325
Epoch 240 of 2000...    Average loss: 0.0834728479385376
Epoch 320 of 2000...    Average loss: 0.07267088443040848
Epoch 400 of 2000...    Average loss: 0.045521676540374756
Epoch 480 of 2000...    Average loss: 0.010963868349790573
Epoch 560 of 2000...    Average loss: 0.00200986722484231
Epoch 640 of 2000...    Average loss: 0.000779082125518471
Epoch 720 of 2000...    Average loss: 0.0004827996017411351
Epoch 800 of 2000...    Average loss: 0.00034238473745062947
Epoch 880 of 2000...    Average loss: 0.00026838452322408557
Epoch 960 of 2000...    Average loss: 0.0002306915557710454
Epoch 1040 of 2000...   Average loss: 0.00021219441259745508
Epoch 1120 of 2000...   Average loss: 0.00020320624753367156
Epoch 1200 of 2000...   Average loss: 0.00019859996973536909
Epoch 1280 of 2000...   Average loss: 0.0001958789798663929
Epoch 1360 of 2000...   Average loss: 0.0001939320791279897
Epoch 1440 of 2000...   Average loss: 0.00019230498583056033
Epoch 1520 of 2000...   Average loss: 0.0001908357662614435
Epoch 1600 of 2000...   Average loss: 0.00018947015632875264
Epoch 1680 of 2000...   Average loss: 0.00018819657270796597
Epoch 1760 of 2000...   Average loss: 0.00018701274530030787
Epoch 1840 of 2000...   Average loss: 0.00018592110427562147
Epoch 1920 of 2000...   Average loss: 0.00018492127128411084
```


Loss Curve
Loss (MSE)
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
0
250
500
750
1000
1250
1500
1750
2000
Epoch


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

In [ ]:

In [ ]: