pdf_1

February 28, 2024

[ ]:
```python
import torch
import numpy as np
import matplotlib.pyplot as plt
import torch.nn as nn
import torch.optim as optim
import numpy as np
from torch.utils.data import TensorDataset, DataLoader
from sklearn.model_selection import train_test_split
import torch.nn.functional as F
from torcheval.metrics import R2Score
import sympy as sp
import torch_optimizer
import scipy
from torch.nn.utils import parameters_to_vector as Params2Vec,␣
↪vector_to_parameters as Vec2Params
```

[ ]:
```python
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
```

[ ]:
```python
num_samples = 1000
```

[ ]:
```python
class Net_general(nn.Module):
    def __init__(self, input_size, hidden_size, num_layers, activation_function␣
↪= torch.relu):
        super(Net_general, self).__init__()
        self.layers = nn.ModuleList()
        self.layers.append(nn.Linear(input_size, hidden_size))
        for _ in range(num_layers - 1):
            self.layers.append(nn.Linear(hidden_size, hidden_size))
        self.layers.append(nn.Linear(hidden_size, 1))
        self.activation_function = activation_function

    def forward(self, x, activations=False):
        for layer in self.layers[:-1]:
            x = self.activation_function(layer(x))
        if activations:
            return x
        x = self.layers[-1](x)
        return x
```

[ ]:
```python
def create_dataset(x, f, test_size=0.2):
    '''Create a dataset from a function f and input x. The function returns a␣
↪tuple of train and test datasets.'''
    y = f(x)

    x_train, x_test, y_train, y_test = train_test_split(x, y,␣
↪test_size=test_size, random_state=42)

    x_train, y_train, x_test, y_test = map(torch.tensor, (x_train, y_train,␣
↪x_test, y_test))
    train_dataset = TensorDataset(x_train.float(), y_train.float())
    test_dataset = TensorDataset(x_test.float(), y_test.float())

    return train_dataset, test_dataset
```

[ ]:
```python
def train_and_evaluate(net, criterion, optimizer, train_loader, test_loader,␣
↪num_epochs=1000, activations=False):
    '''Train and evaluate a network. Returns the outputs of the network and the␣
↪train losses.'''
    train_losses = []
    net.train()
    for epoch in range(num_epochs):
        epoch_loss = 0
        for inputs, targets in train_loader:
            optimizer.zero_grad()
            outputs = net(inputs)
            loss = criterion(outputs, targets)
            loss.backward(create_graph=True)
            optimizer.step()
            epoch_loss += loss.item()
        train_losses.append(epoch_loss / len(train_loader))

    net.eval()
    test_loss = 0
    all_outputs = []
    all_targets = []
    with torch.no_grad():
        for inputs, targets in test_loader:
            outputs = net(inputs, activations=activations)
            loss = criterion(outputs, targets)
            test_loss += loss.item()
            all_outputs.append(outputs)
            all_targets.append(targets)


    test_loss /= len(test_loader)
    print('Test Loss: %.6f' % test_loss)
```

```
    score = R2Score()
    score.update(torch.cat(all_targets).view(torch.cat(all_targets).shape[0],␣
↪1), torch.cat(all_outputs))
    r2score = score.compute()
    print('R2 Score: %.6f' % r2score)

    return torch.cat(all_outputs), train_losses, test_loss
```

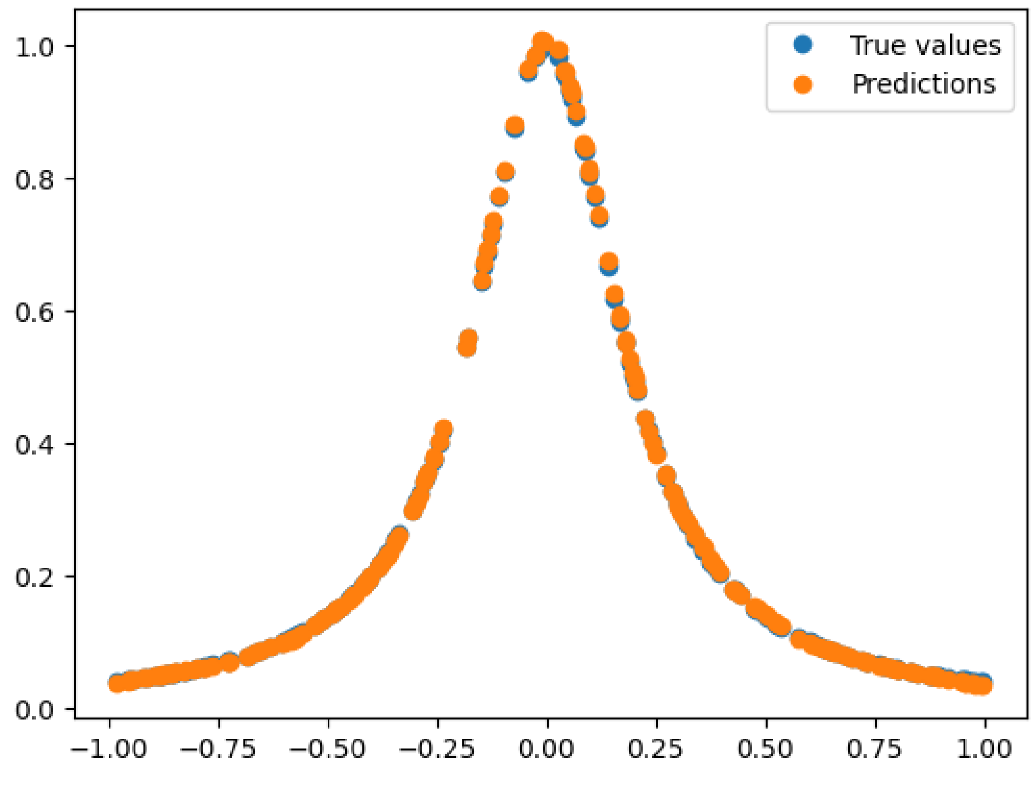
[ ]:
```
def plot_losses_and_predictions(test_dataset, train_losses, outputs):
    '''Plot the losses and predictions of a network.'''
    plt.plot(test_dataset.tensors[0].numpy(), test_dataset.tensors[1].numpy(),␣
↪'o' ,label='True values')
    plt.plot(test_dataset.tensors[0].numpy(), outputs.numpy(), 'o'␣
↪,label='Predictions')
    plt.legend()
    plt.show()

    plt.figure()
    plt.plot(train_losses)
    plt.xlabel('Epoch')
    plt.ylabel('Training Loss')
    plt.show()
```

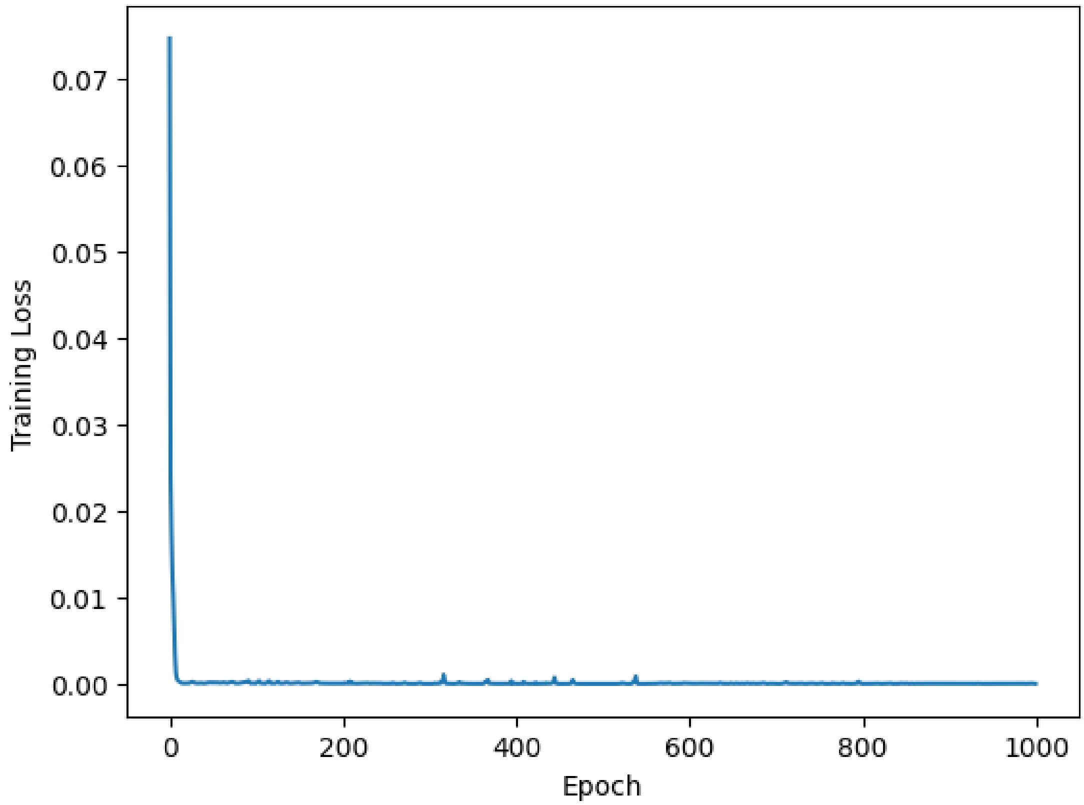
1 Q1 (equidistant sampling)

[ ]:
```
def f_q1(x):
    '''The function for question 1.'''
    return 1 / (1 + 25 * x**2)
```

[ ]:
```
train_dataset_q1_eq, test_dataset_q1_eq = create_dataset( np.linspace(-1, 1,␣
↪num_samples).reshape(-1, 1) ,f_q1)

train_loader_q1_eq = DataLoader(train_dataset_q1_eq, batch_size=32)
test_loader_q1_eq = DataLoader(test_dataset_q1_eq, batch_size=32)

net_q1_eq = Net_general(1,50,2)
criterion_q1_eq = nn.MSELoss()
optimizer_q1_eq = optim.Adam(net_q1_eq.parameters(), lr=0.01)

outputs_q1_eq, train_losses_q1_eq, test_loss_q1_eq =␣
↪train_and_evaluate(net_q1_eq, criterion_q1_eq, optimizer_q1_eq,␣
↪train_loader_q1_eq, test_loader_q1_eq)
print('Test loss: %.6f' % test_loss_q1_eq)
plot_losses_and_predictions(test_dataset_q1_eq, train_losses_q1_eq,␣
↪outputs_q1_eq)
```

```
Test Loss: 0.000010
R2 Score: 0.999859
Test loss: 0.000010
```

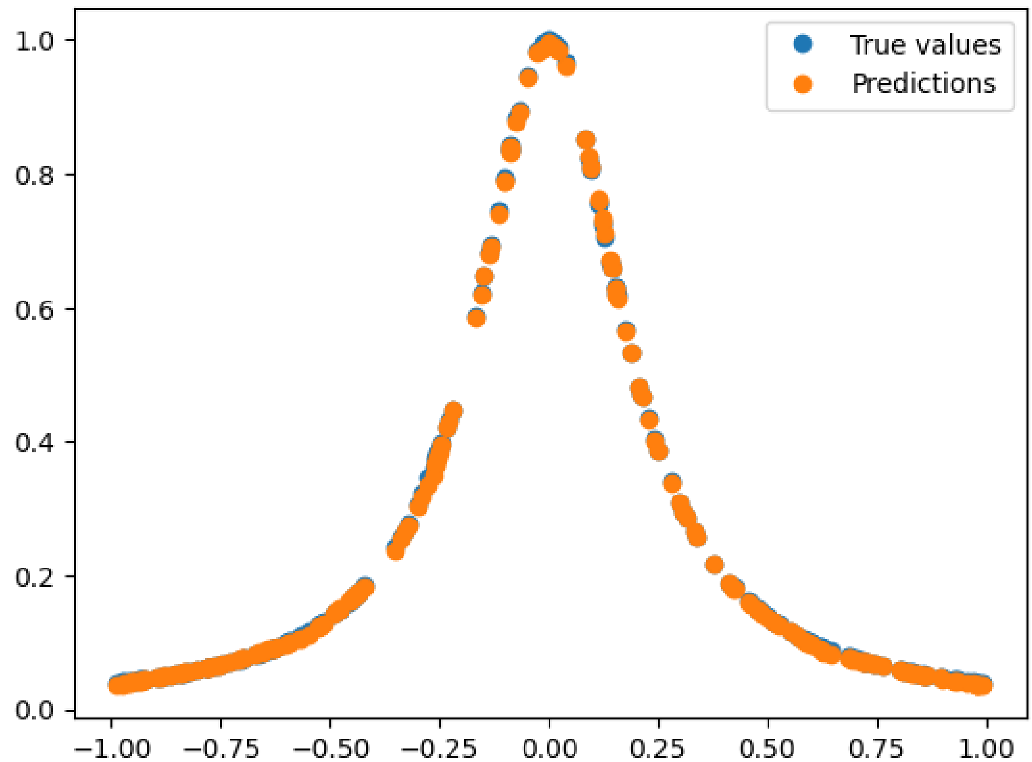


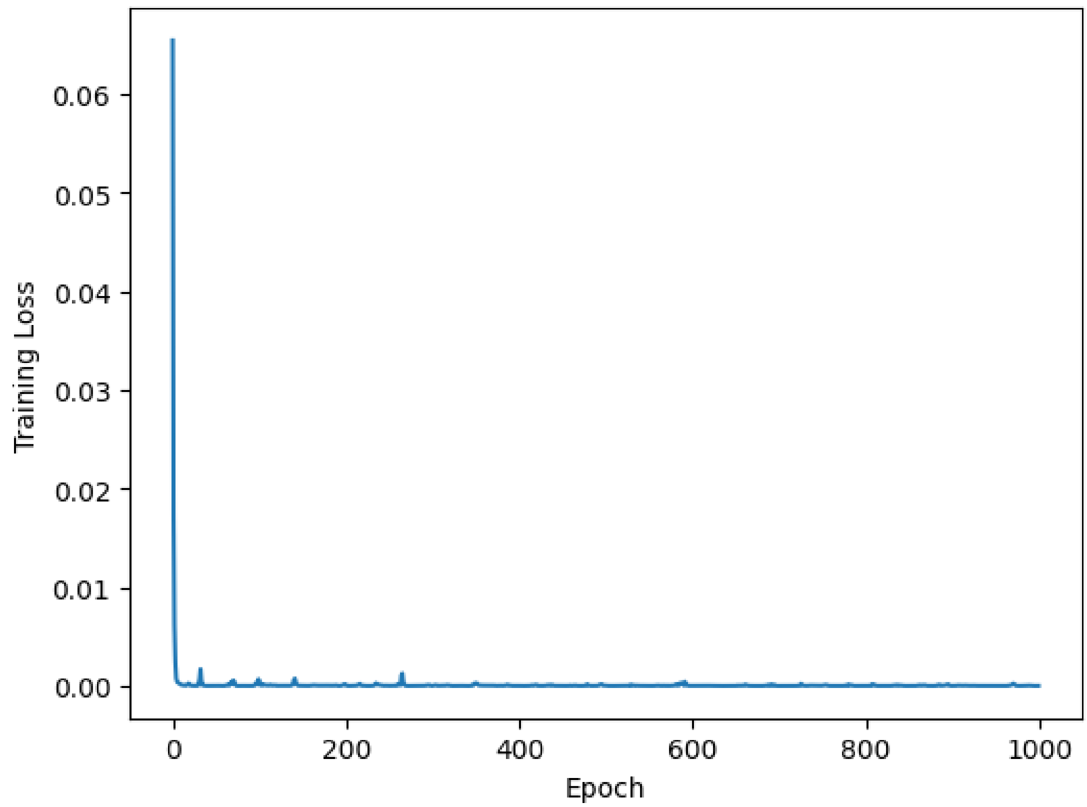


2 Q2 random sampling (from a uniform distribution)

[ ]:
```
train_dataset_q1_rand, test_dataset_q1_rand = create_dataset( np.random.
    ↪uniform(-1, 1, num_samples).reshape(-1, 1) ,f_q1)

train_loader_q1_rand = DataLoader(train_dataset_q1_rand, batch_size=32)
test_loader_q1_rand = DataLoader(test_dataset_q1_rand, batch_size=32)

net_q1_rand = Net_general(1,50,2)
criterion_q1_rand = nn.MSELoss()
optimizer_q1_rand = optim.Adam(net_q1_rand.parameters(), lr=0.01)

outputs_q1_rand, train_losses_q1_rand, test_loss_q1_rand = 
    ↪train_and_evaluate(net_q1_rand, criterion_q1_rand, optimizer_q1_rand, 
    ↪train_loader_q1_rand, test_loader_q1_rand)
print('Test loss: %.6f' % test_loss_q1_rand)

plot_losses_and_predictions(test_dataset_q1_rand, train_losses_q1_rand, 
    ↪outputs_q1_rand)
```

```
Test Loss: 0.000
```

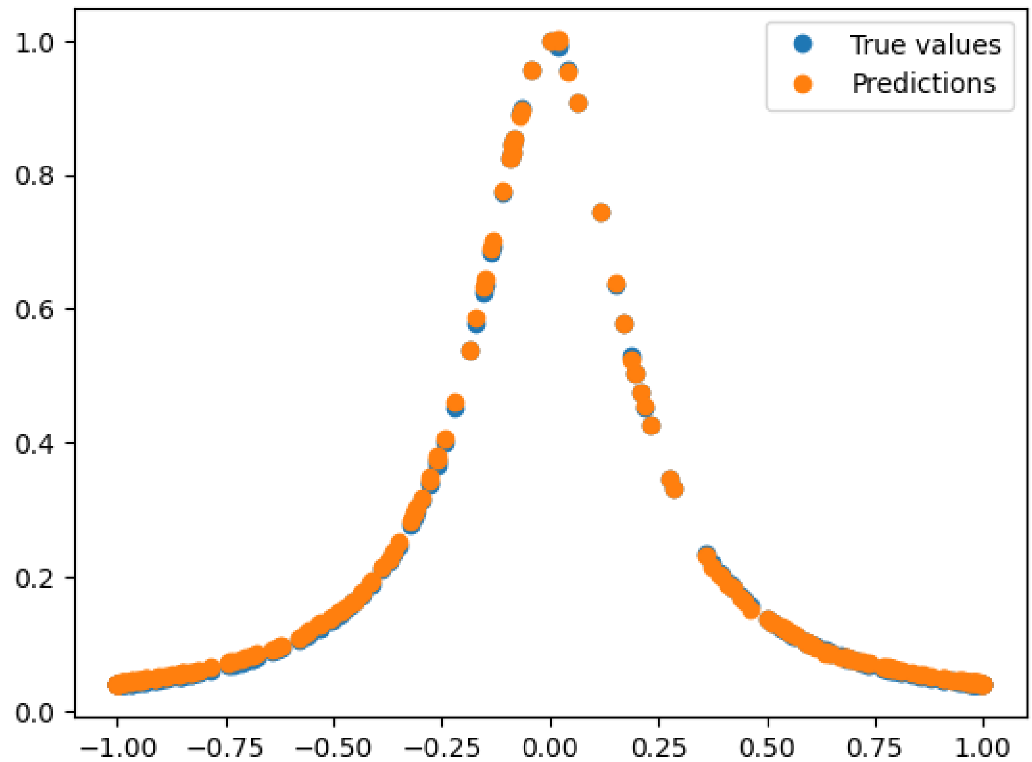


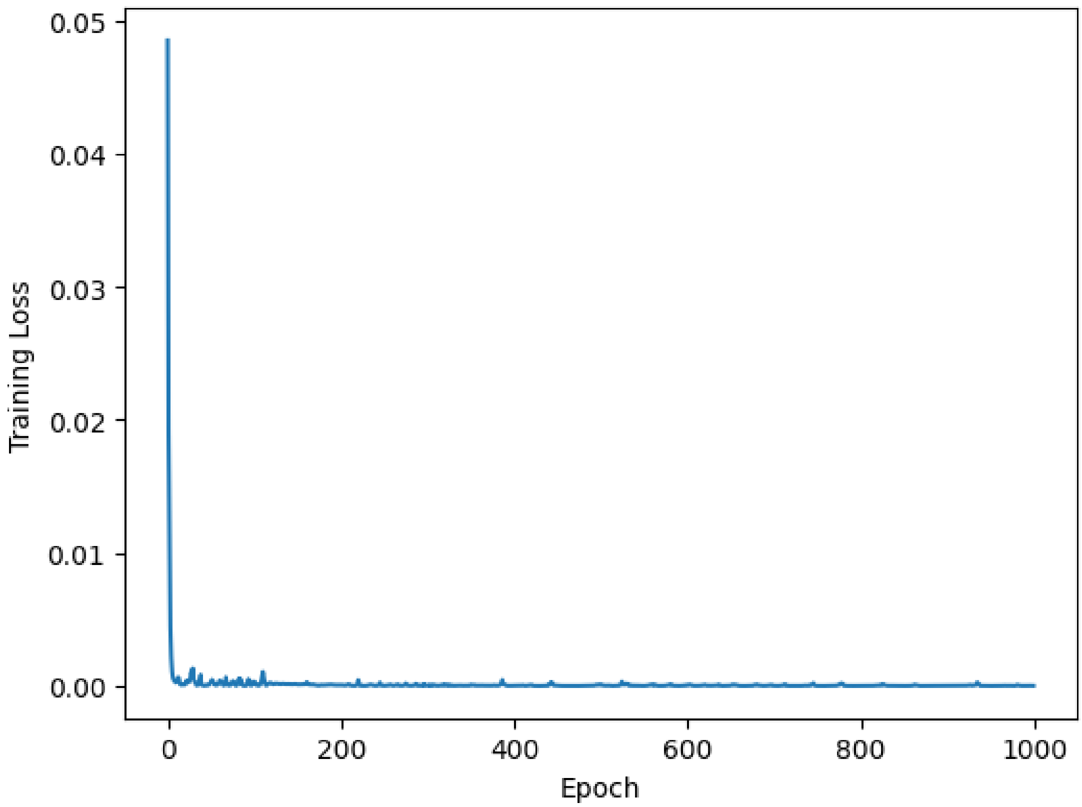


3 Q2 Chebyshev sampling

[ ]:
```
train_dataset_q1_cheb, test_dataset_q1_cheb = create_dataset( np.cos((2 * np.
↪arange(1, num_samples + 1) - 1) * np.pi / (2 * num_samples)).reshape(-1, 1)␣
↪,f_q1)

train_loader_q1_cheb = DataLoader(train_dataset_q1_cheb, batch_size=32)
test_loader_q1_cheb = DataLoader(test_dataset_q1_cheb, batch_size=32)

net_q1_cheb = Net_general(1,50,2)
criterion_q1_cheb = nn.MSELoss()
optimizer_q1_cheb = optim.Adam(net_q1_cheb.parameters(), lr=0.01)

outputs_q1_cheb, train_losses_q1_cheb, test_loss_q1_cheb =␣
↪train_and_evaluate(net_q1_cheb, criterion_q1_cheb, optimizer_q1_cheb,␣
↪train_loader_q1_cheb, test_loader_q1_cheb)
print('Test loss: %.6f' % test_loss_q1_cheb)

plot_losses_and_predictions(test_dataset_q1_cheb, train_losses_q1_cheb,␣
↪outputs_q1_cheb)
```

```
Test Loss: 0.000
```





4 Q3: Attached at the end and as a separate .ipynb file

5 Q4: Neural network approximation of hat function

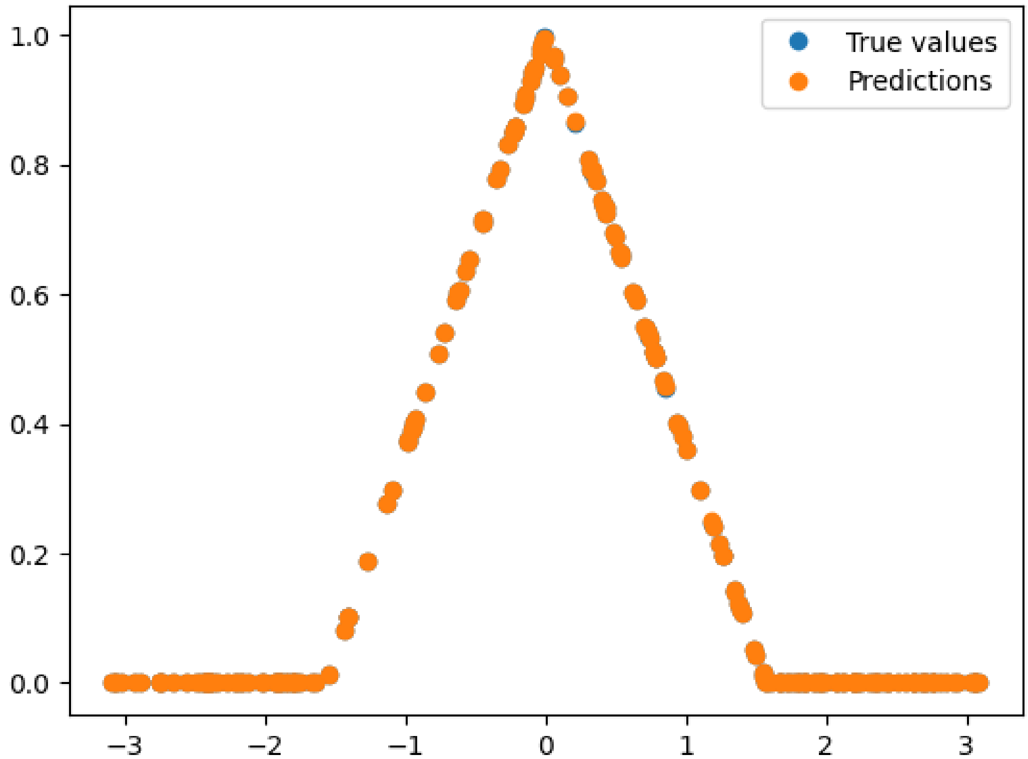
[ ]:
```
def hat_fn(x):
    '''The hat function for question 2.'''
    y_hat = 1.0 - np.abs(x)/(np.pi/2)
    y_hat[np.abs(x) > np.pi/2] = 0
    return y_hat
```

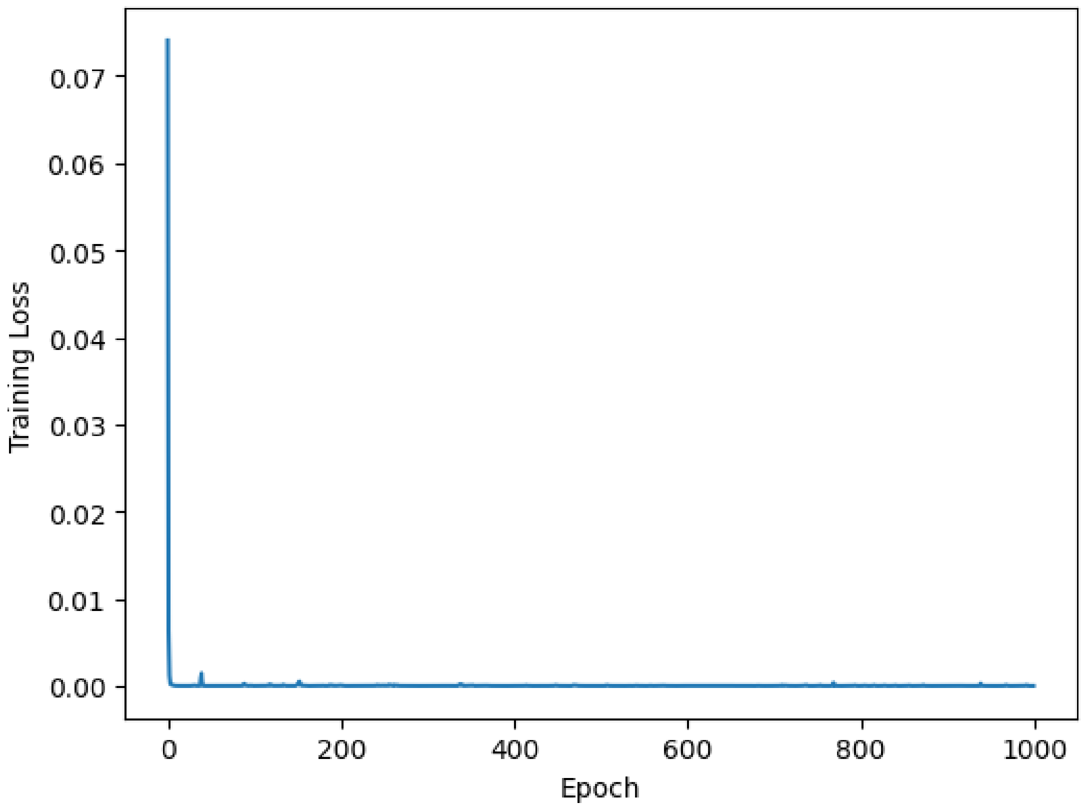
[ ]:
```
train_dataset_hat, test_dataset_hat = create_dataset( np.random.uniform(-np.pi,␣
 ↪np.pi, num_samples).reshape(-1, 1) , hat_fn)

train_loader_hat = DataLoader(train_dataset_hat, batch_size=32)
test_loader_hat = DataLoader(test_dataset_hat, batch_size=32)
```

[ ]:
```
net_q4 = Net_general(1,50,2)
criterion_q4 = nn.MSELoss()
optimizer_q4 = optim.Adam(net_q4.parameters(), lr=0.01)
```

```
outputs_q4_hat, train_losses_q4_hat, test_loss_q4_hat =␣
↪train_and_evaluate(net_q4, criterion_q4, optimizer_q4, train_loader_hat,␣
↪test_loader_hat)
print('Test loss: %.6f' % test_loss_q4_hat)

plot_losses_and_predictions(test_dataset_hat, train_losses_q4_hat,␣
↪outputs_q4_hat)
```

```
Test Loss: 0.000
```

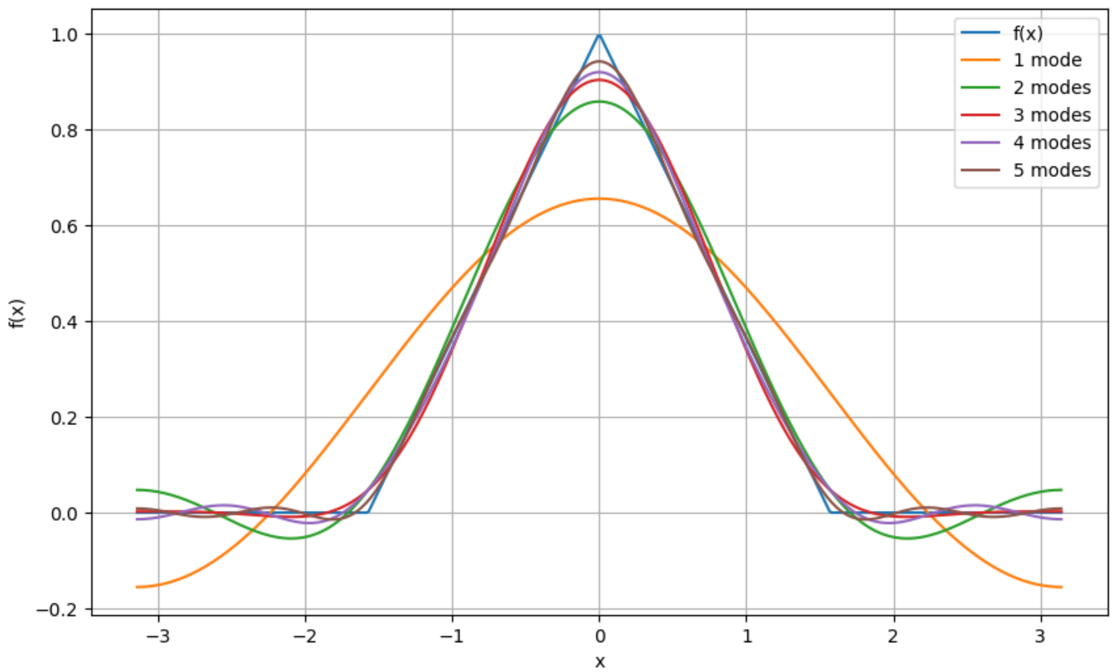




6 Q5: Fourier series expansion of f(x)

[ ]:
```
x = sp.symbols('x')
f = sp.Piecewise((1.0 - sp.Abs(x)/(sp.pi/2), sp.Abs(x) < sp.pi/2), (0, True))

F = sp.fourier_series(f, (x, -sp.pi, sp.pi))

f_np = sp.lambdify(x, f, 'numpy')
F_1 = sp.lambdify(x, F.truncate(n=2), 'numpy')
F_2 = sp.lambdify(x, F.truncate(n=3), 'numpy')
F_3 = sp.lambdify(x, F.truncate(n=4), 'numpy')
F_4 = sp.lambdify(x, F.truncate(n=5), 'numpy')
F_5 = sp.lambdify(x, F.truncate(n=6), 'numpy')

x_vals = np.linspace(-np.pi, np.pi, 400)

plt.figure(figsize=(10, 6))
plt.plot(x_vals, f_np(x_vals), label='f(x)')
plt.plot(x_vals, F_1(x_vals), label='1 mode')
plt.plot(x_vals, F_2(x_vals), label='2 modes')
```

```
plt.plot(x_vals, F_3(x_vals), label='3 modes')
plt.plot(x_vals, F_4(x_vals), label='4 modes')
plt.plot(x_vals, F_5(x_vals), label='5 modes')
plt.xlabel('x')
plt.ylabel('f(x)')
plt.legend()
plt.title('Fourier Series of f(x)')
plt.grid(True)
plt.show()
```

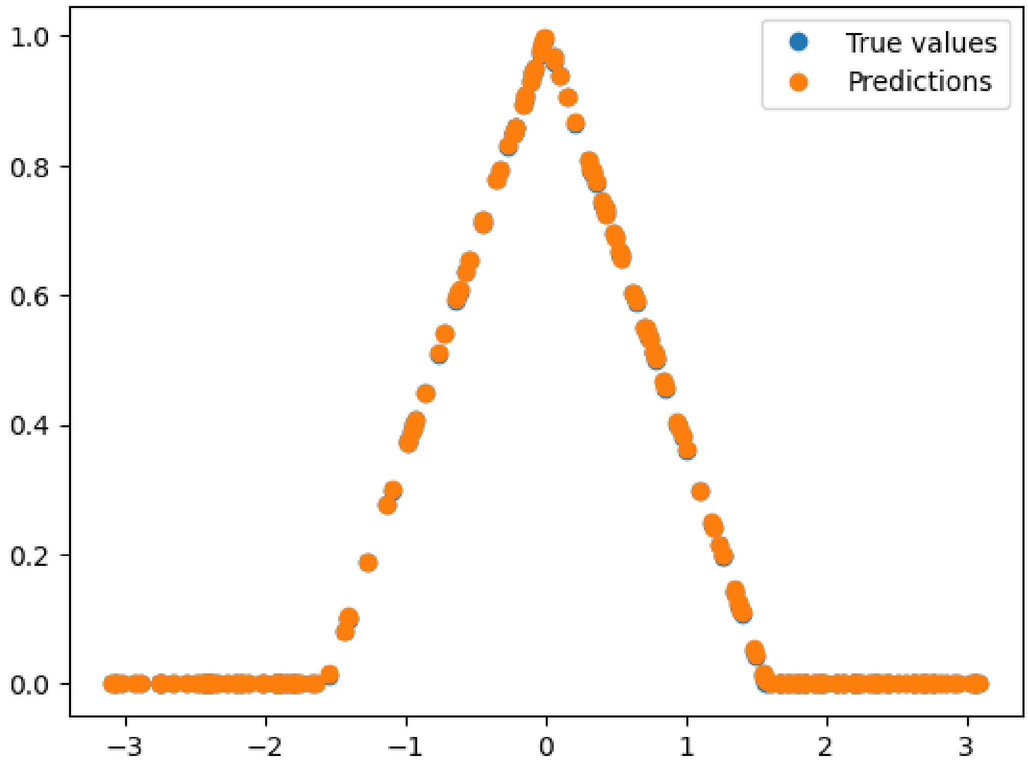


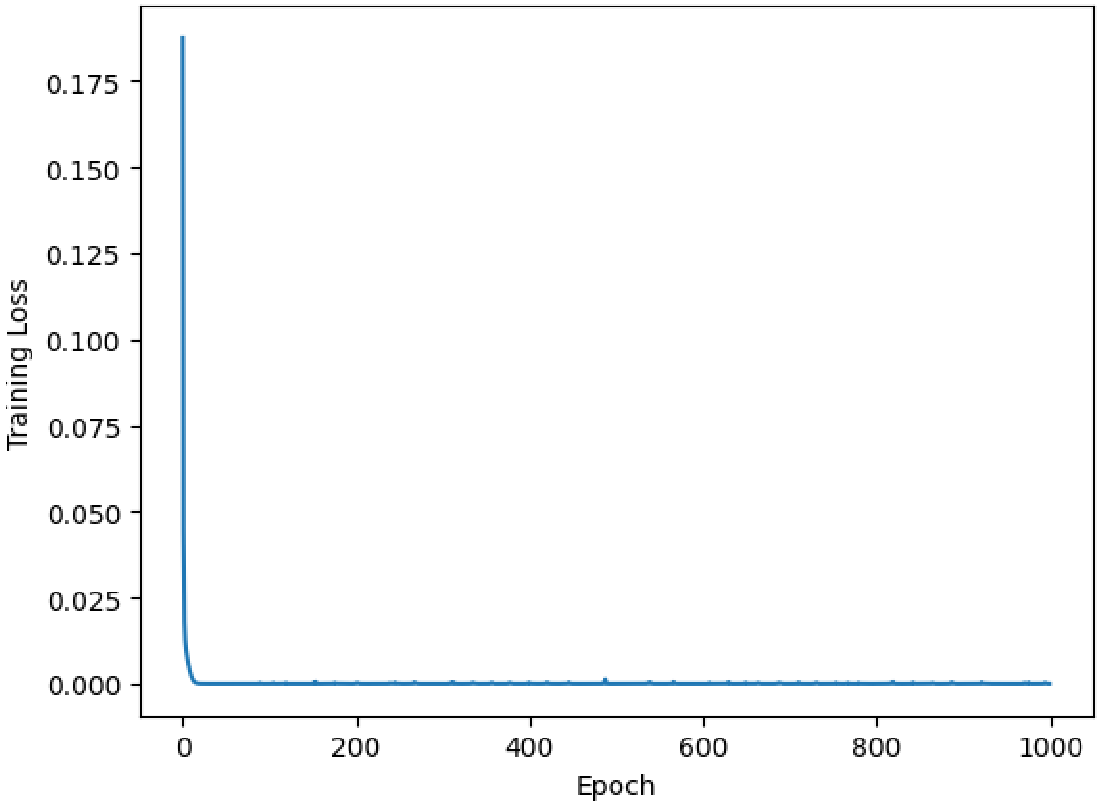
7 Q6: Accuracy with increasing neurons and number of hidden layers

[ ]:
```
for hidden_neurons in [10, 20, 50, 100]:
    for num_layers in [1, 2, 3]:
        n = Net_general(1, hidden_neurons, num_layers)
        c = nn.MSELoss()
        o = optim.Adam(n.parameters(), lr=0.01)
        preds, train_losses, test_loss = train_and_evaluate(n, c, o,␣
 ↪train_loader_hat, test_loader_hat)

        print(f'Hidden neurons: {hidden_neurons}, Num. layers: {num_layers},␣
 ↪Test Loss: {test_loss:.6f}')
```

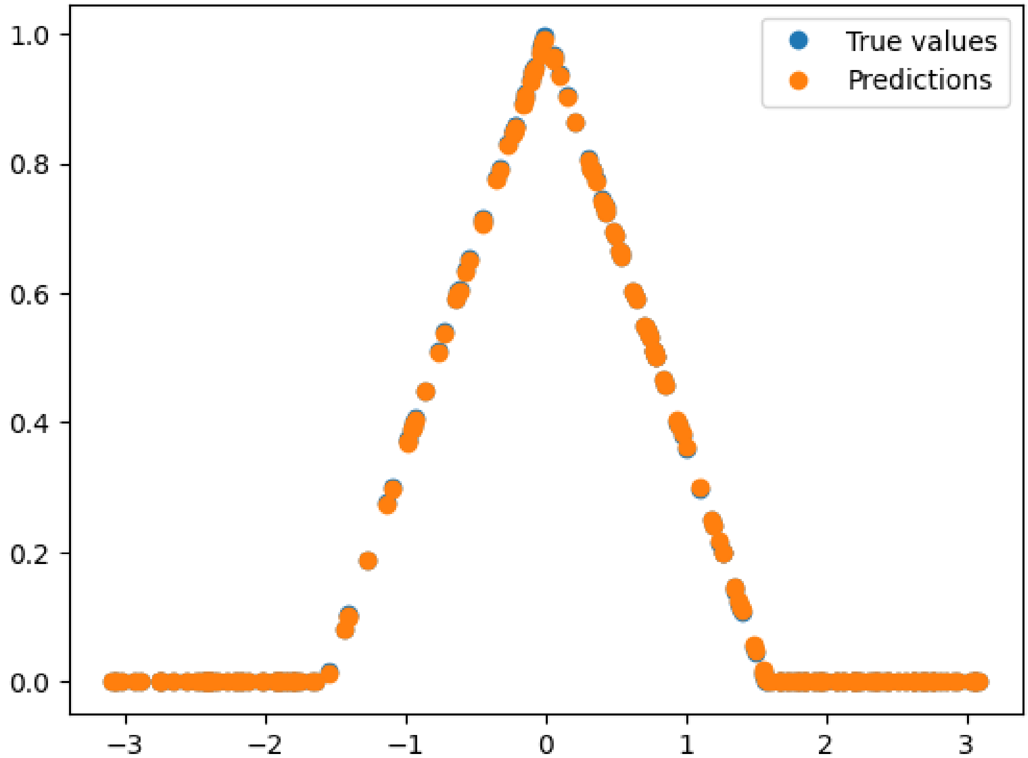
```python
        # plt.plot(train_losses, label=f'Hidden size: {hidden_neurons}, Num␣
↪layers: {num_layers}')
        plot_losses_and_predictions(test_dataset_hat, train_losses, preds)
```

```
Test Loss: 0.000002
R2 Score: 0.999983
Hidden neurons: 10, Num. layers: 1, Test Loss: 0.000002
```

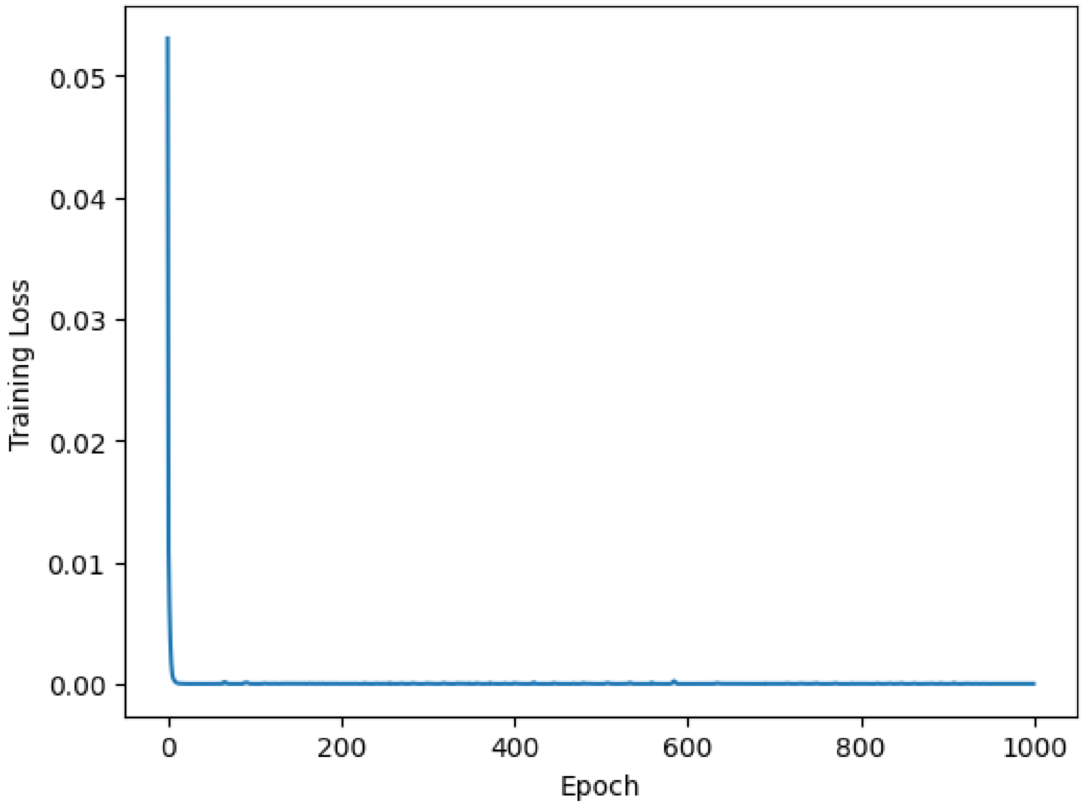




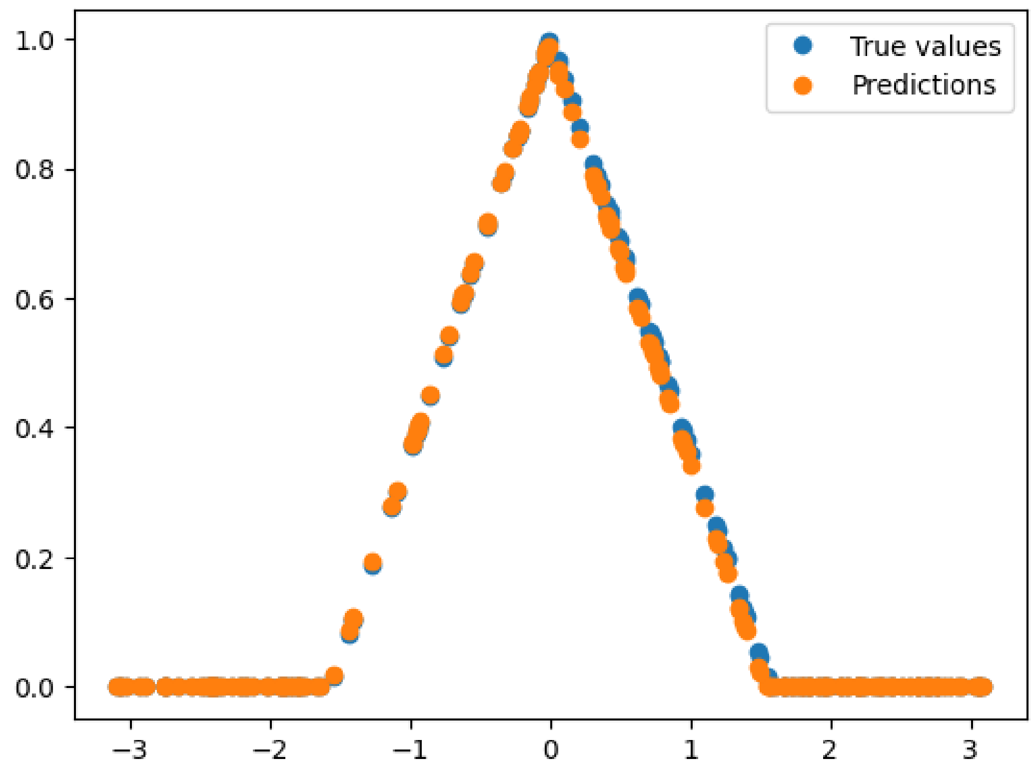

```
Test Loss: 0.000002
R2 Score: 0.999980
Hidden neurons: 10, Num. layers: 2, Test Loss: 0.000002
```



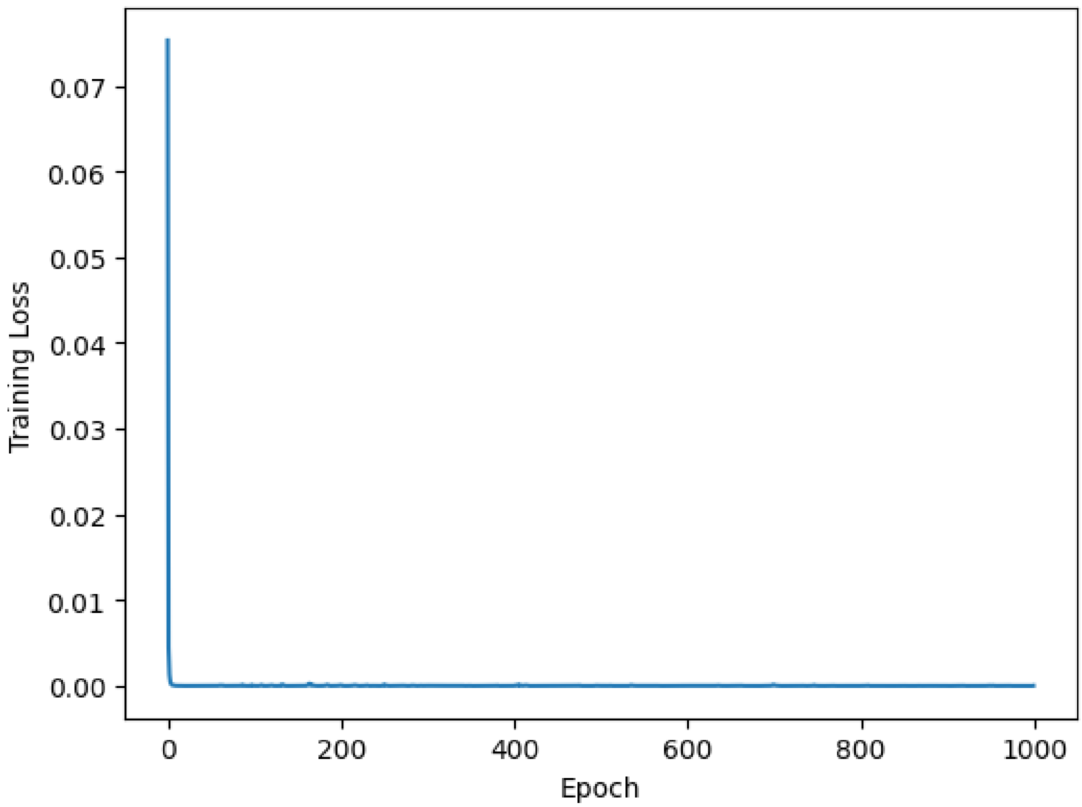
True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3



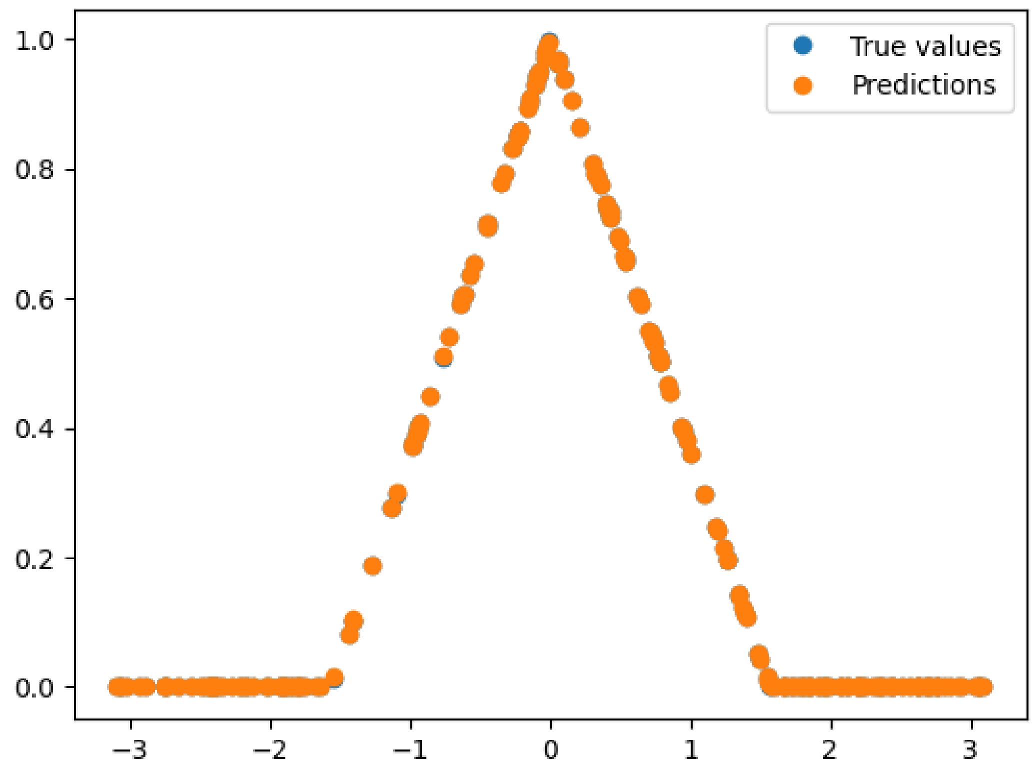

```
Test Loss: 0.000101
R2 Score: 0.999172
Hidden neurons: 10, Num. layers: 3, Test Loss: 0.000101
```

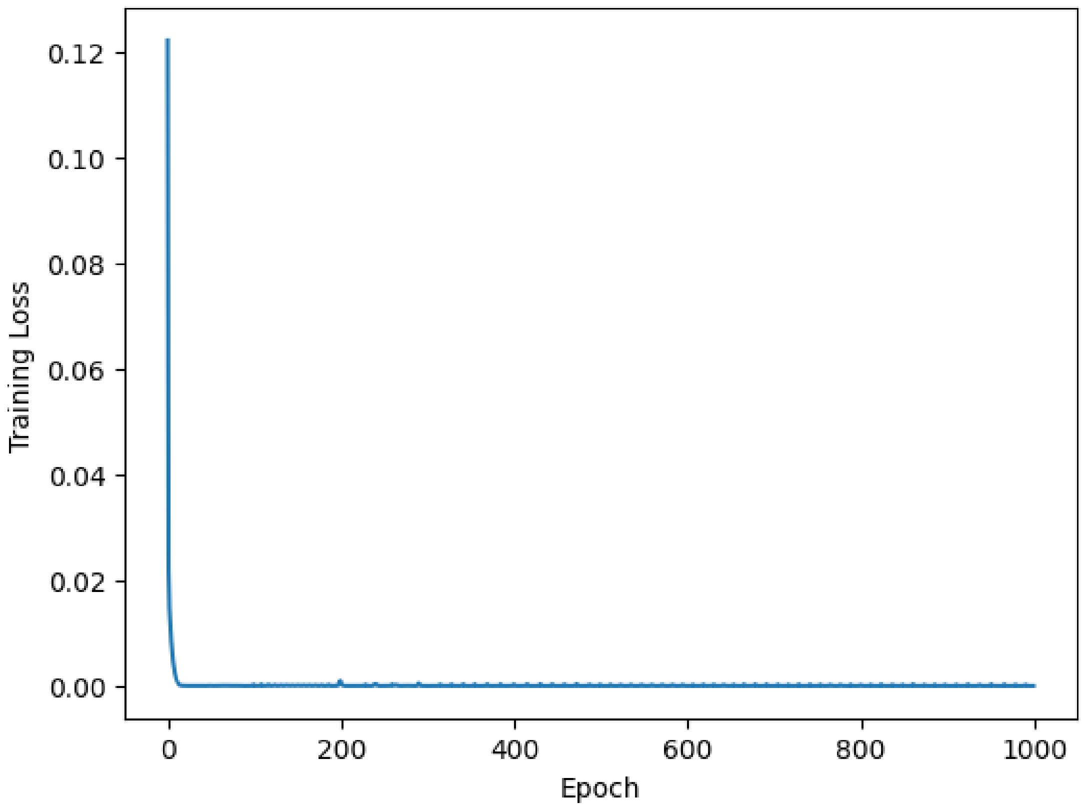


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

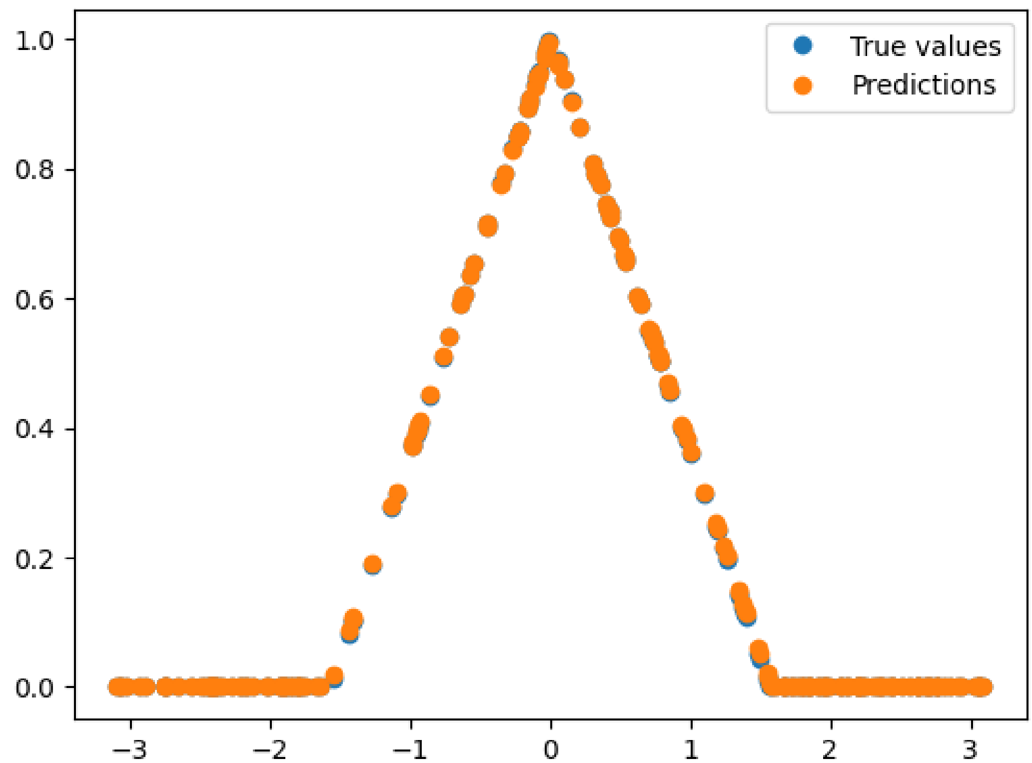


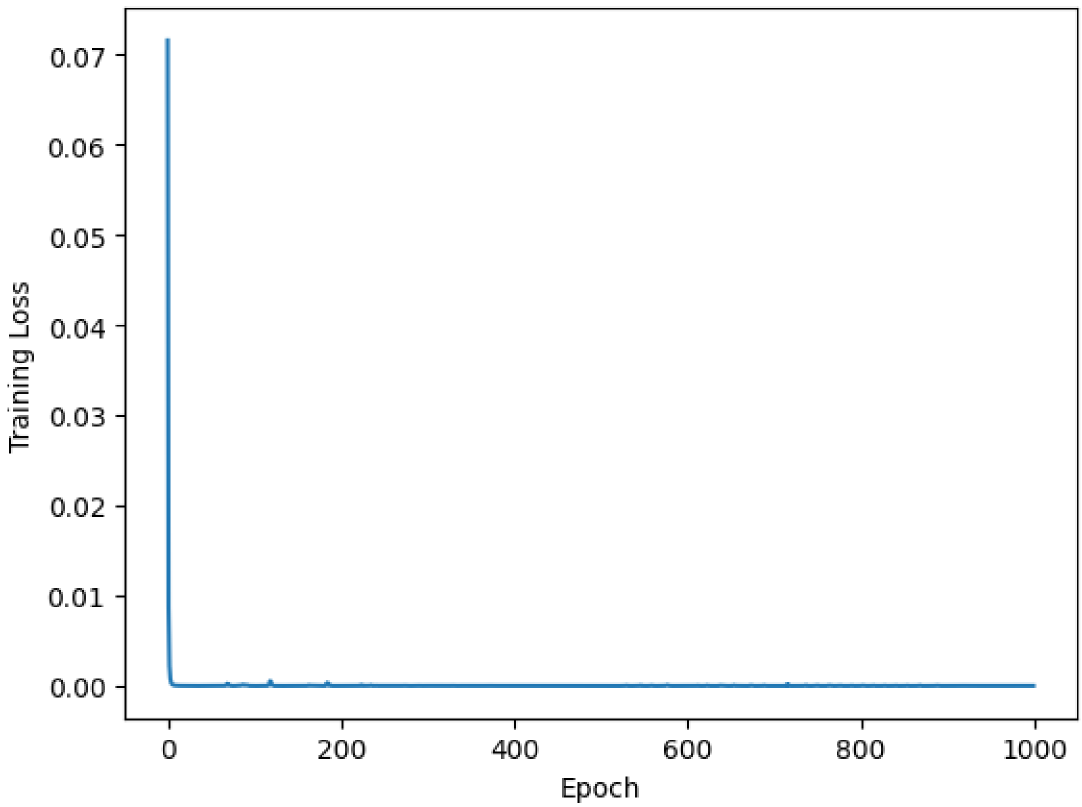

```
Test Loss: 0.000001
R2 Score: 0.999993
Hidden neurons: 20, Num. layers: 1, Test Loss: 0.000001
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

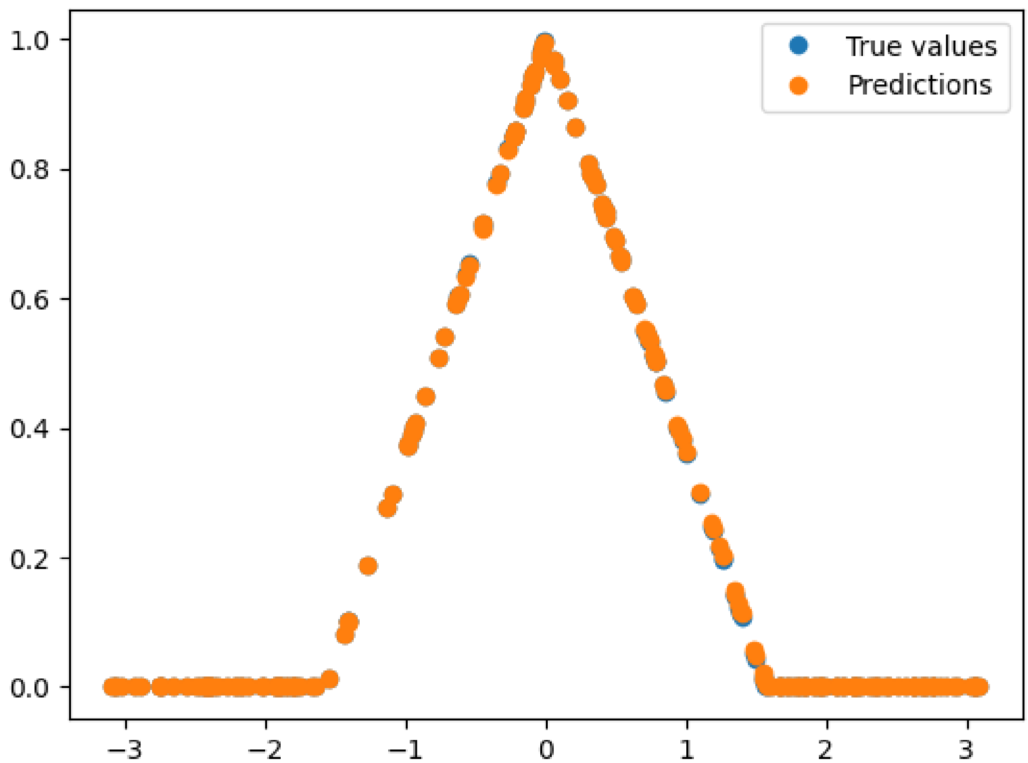


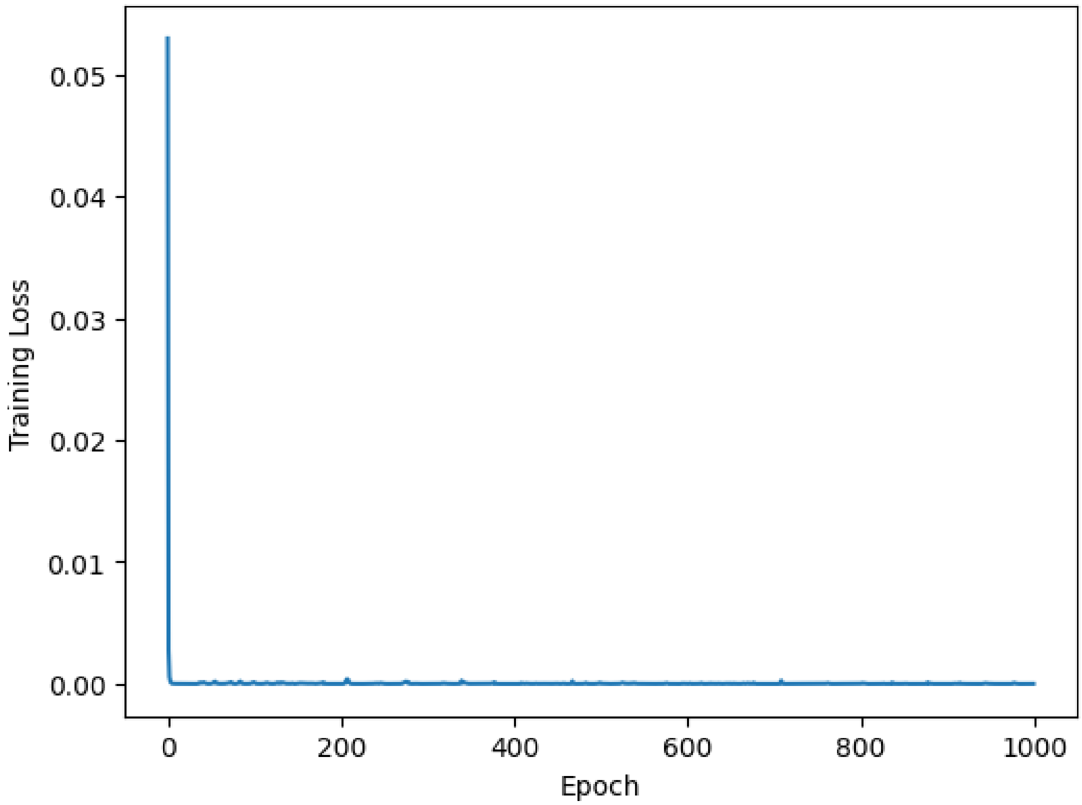

```
Test Loss: 0.000005
R2 Score: 0.999963
Hidden neurons: 20, Num. layers: 2, Test Loss: 0.000005
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

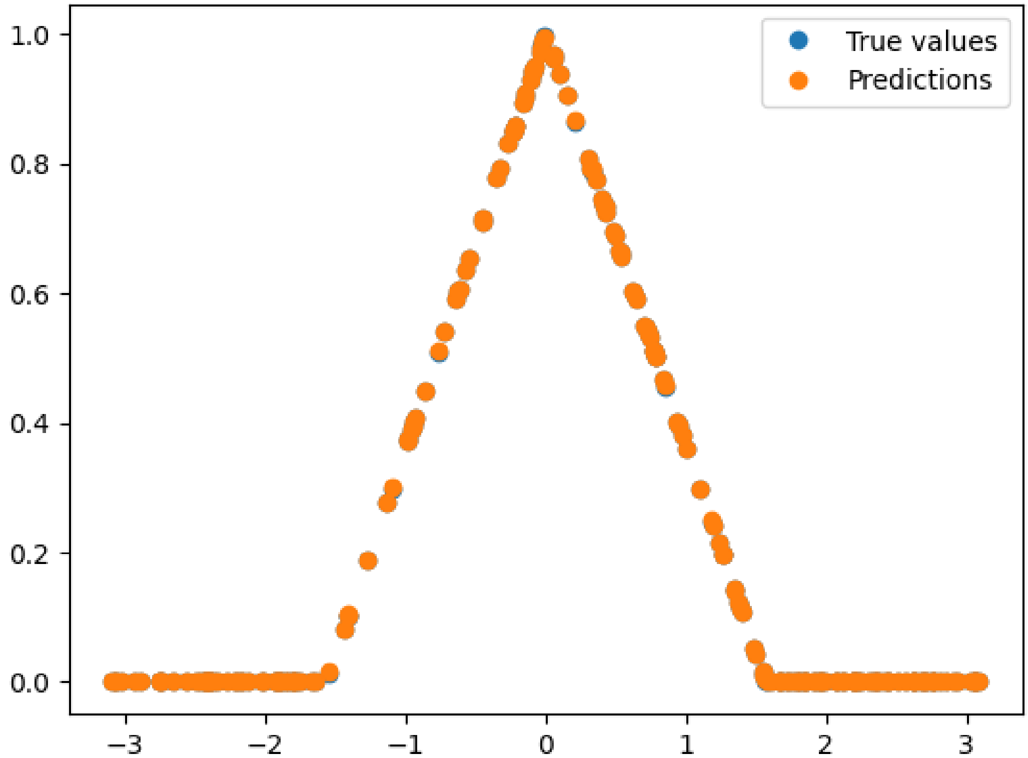


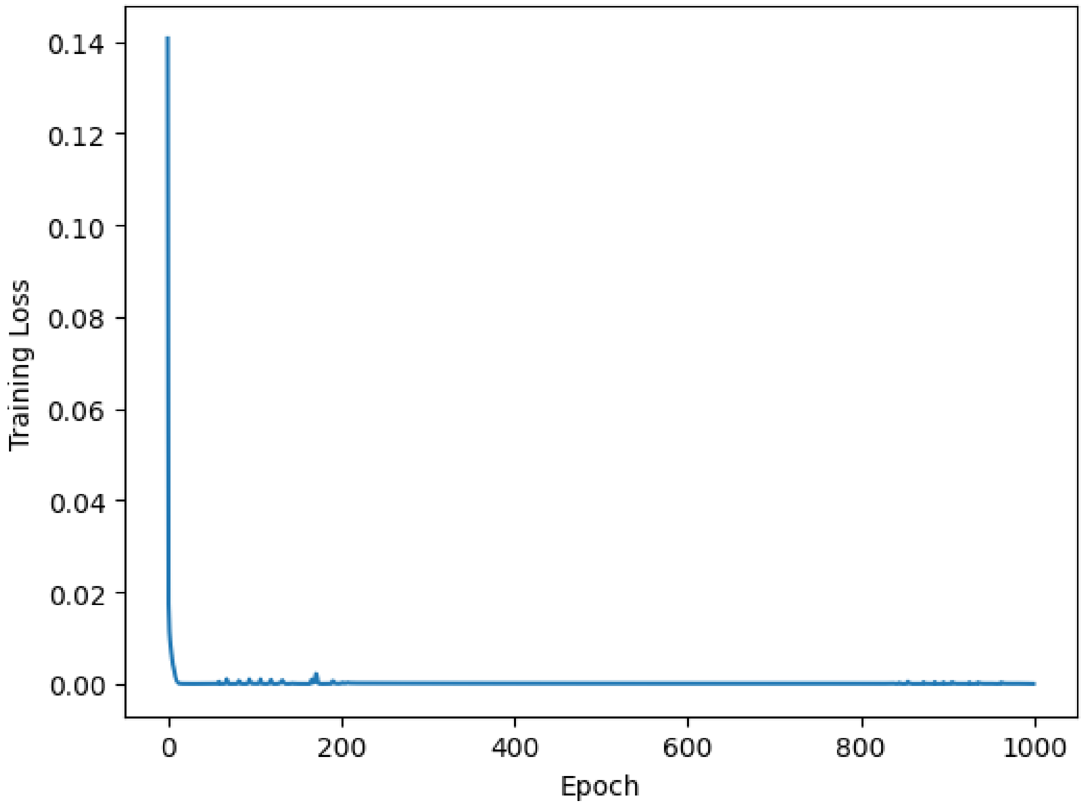

```
Test Loss: 0.000002
R2 Score: 0.999985
Hidden neurons: 20, Num. layers: 3, Test Loss: 0.000002
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

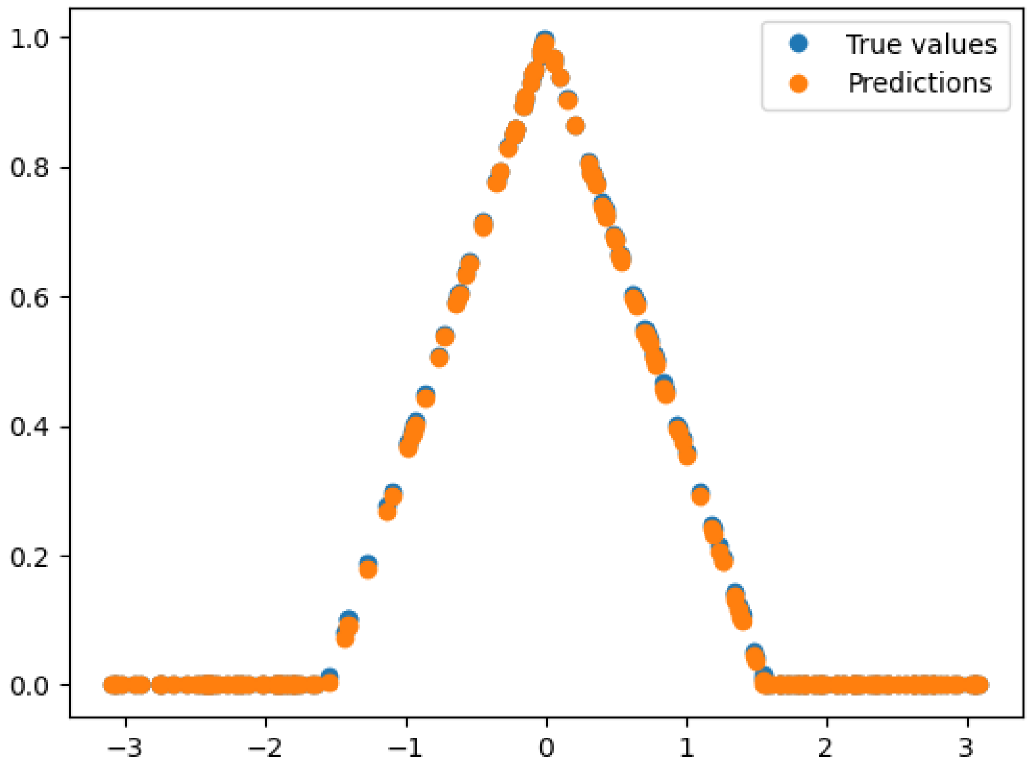


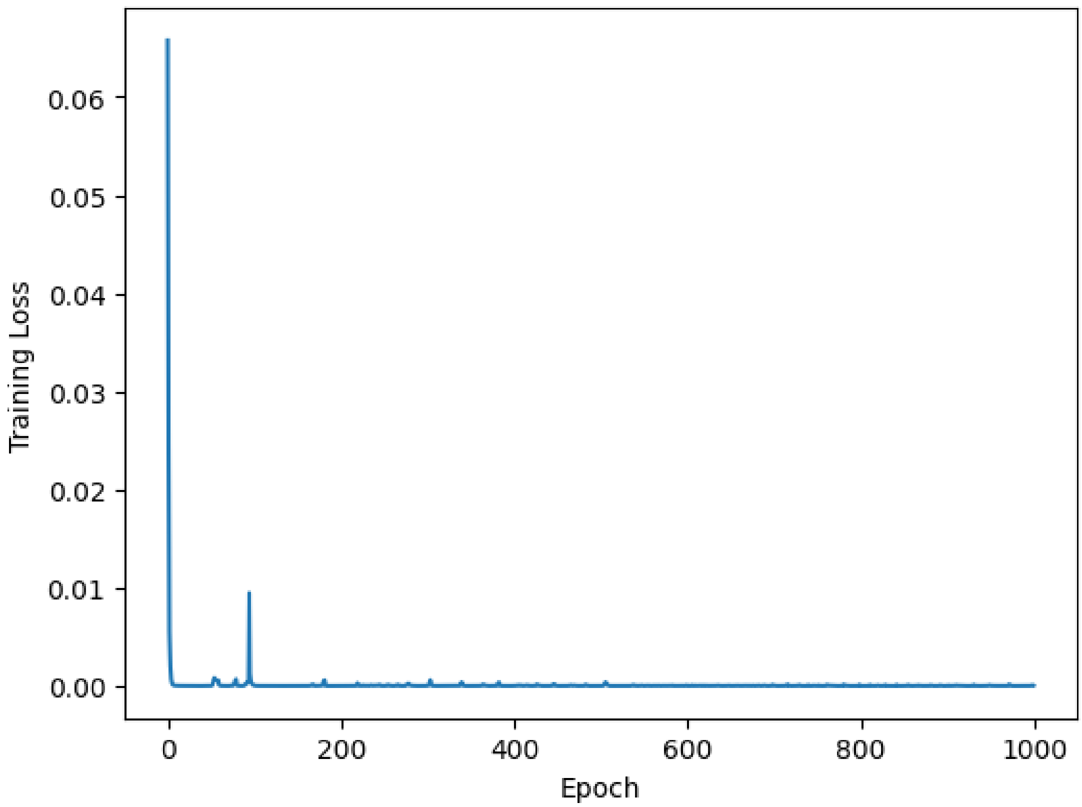

```
Test Loss: 0.000000
R2 Score: 0.999998
Hidden neurons: 50, Num. layers: 1, Test Loss: 0.000000
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

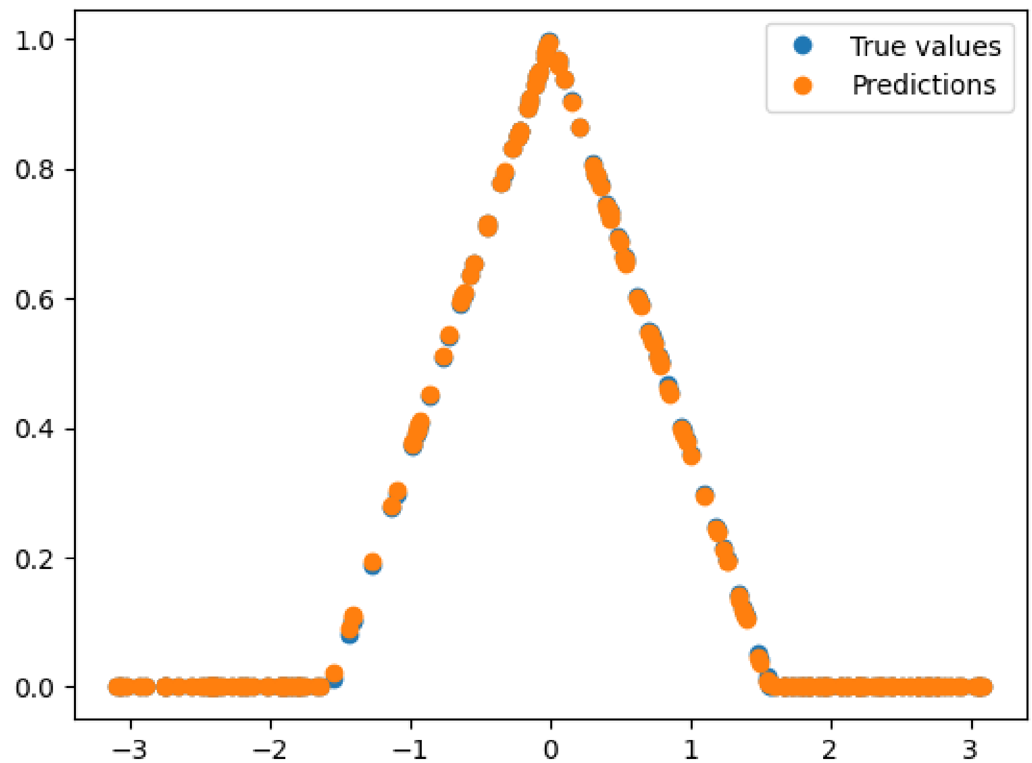


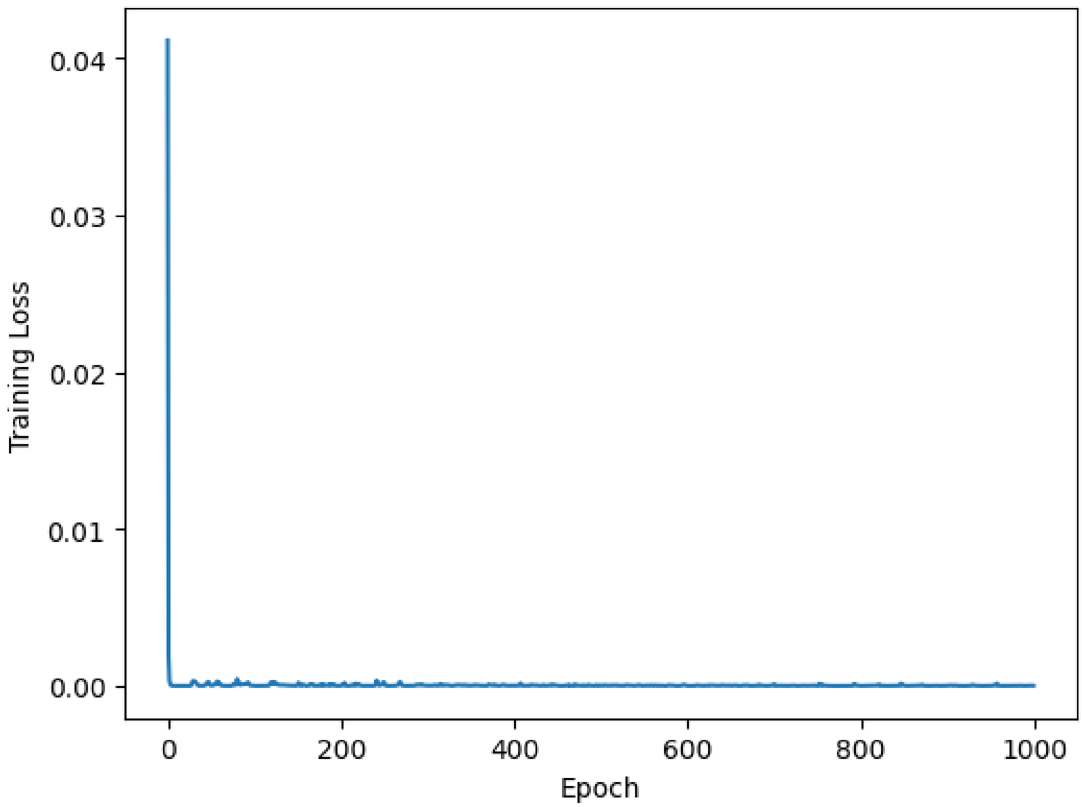

```
Test Loss: 0.000015
R2 Score: 0.999886
Hidden neurons: 50, Num. layers: 2, Test Loss: 0.000015
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

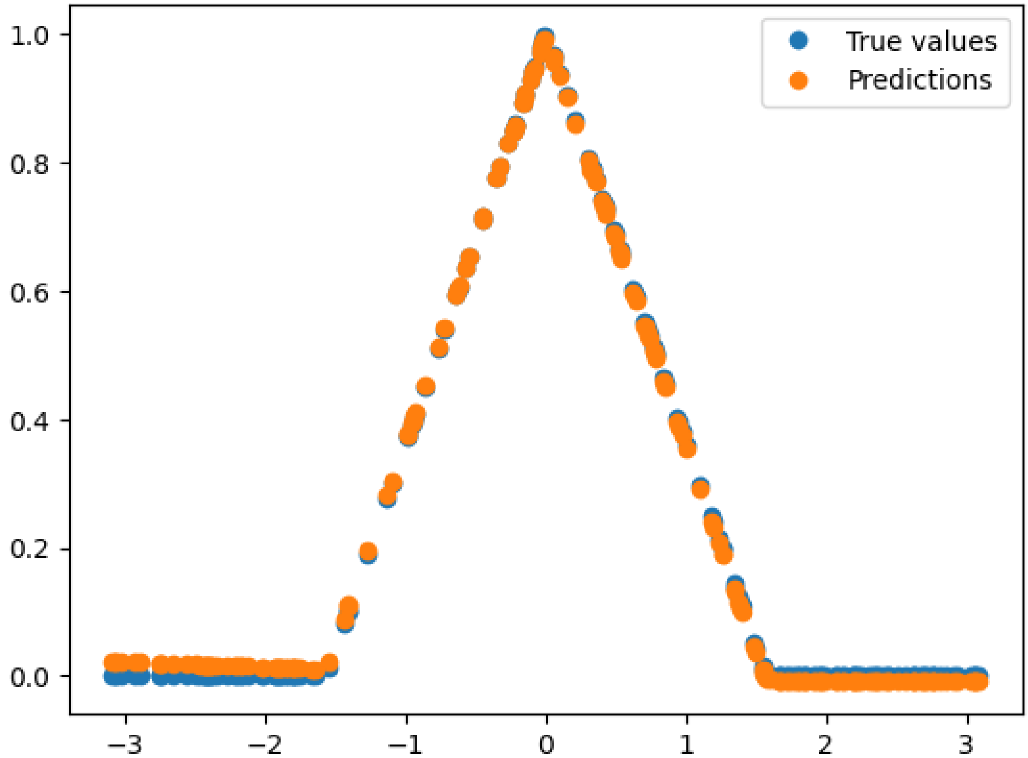


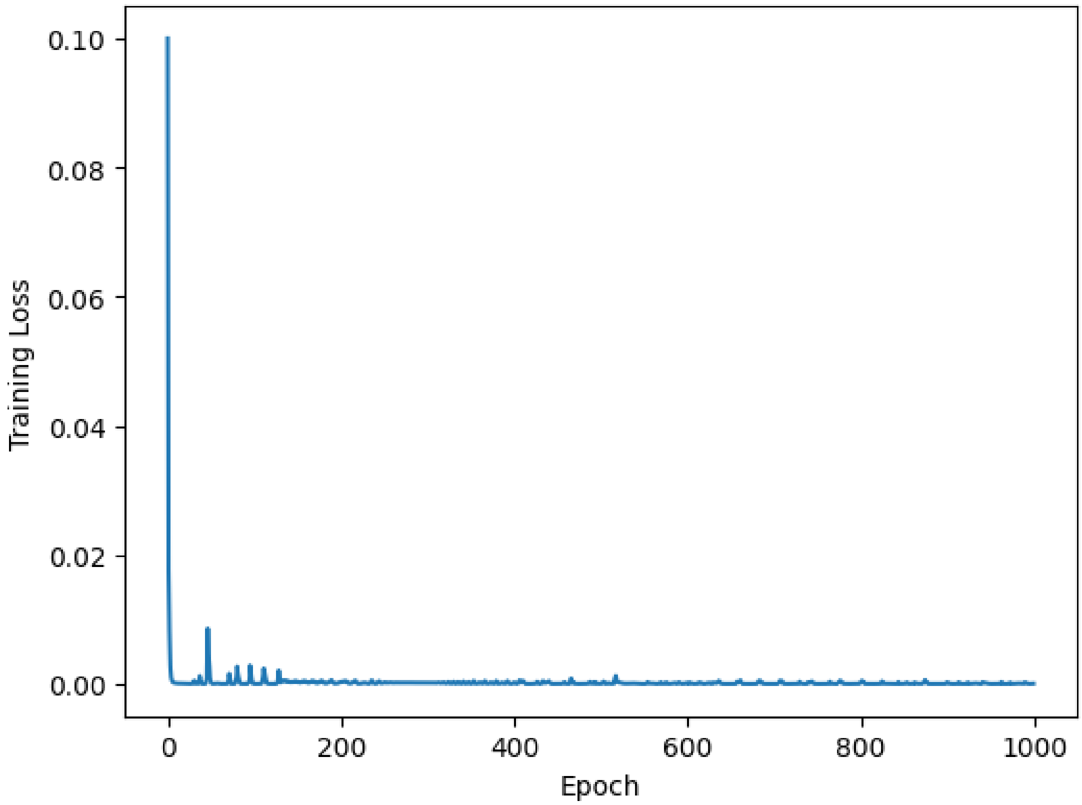

```
Test Loss: 0.000007
R2 Score: 0.999950
Hidden neurons: 50, Num. layers: 3, Test Loss: 0.000007
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3

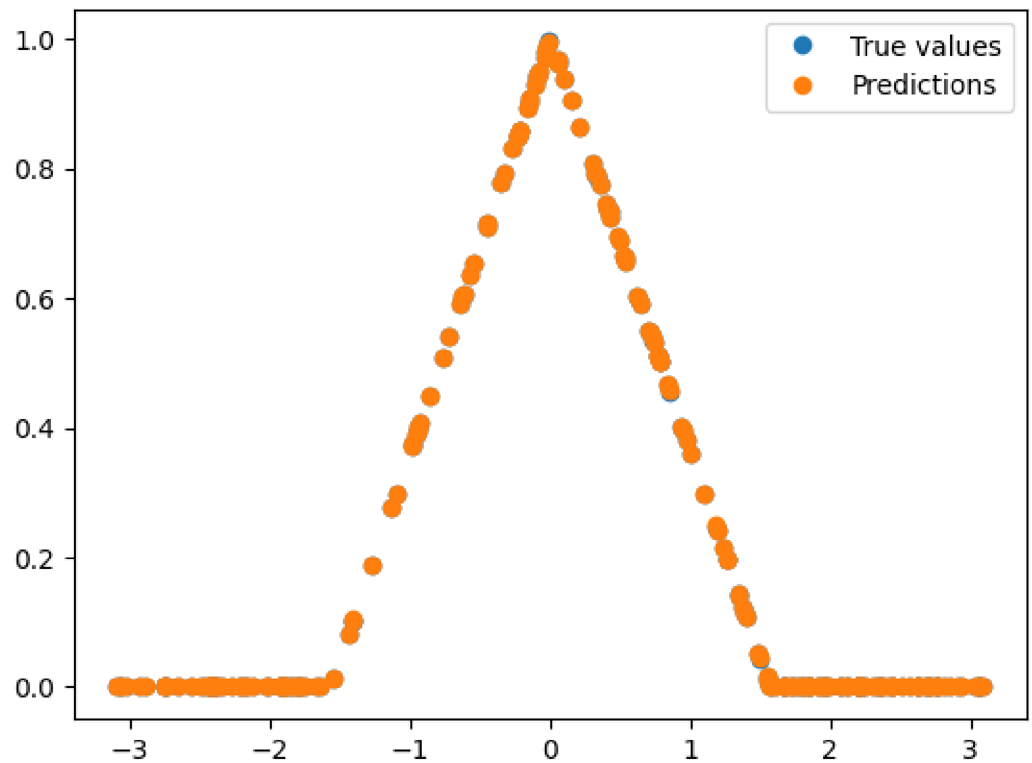



```
Test Loss: 0.000099
R2 Score: 0.999197
Hidden neurons: 100, Num. layers: 1, Test Loss: 0.000099
```

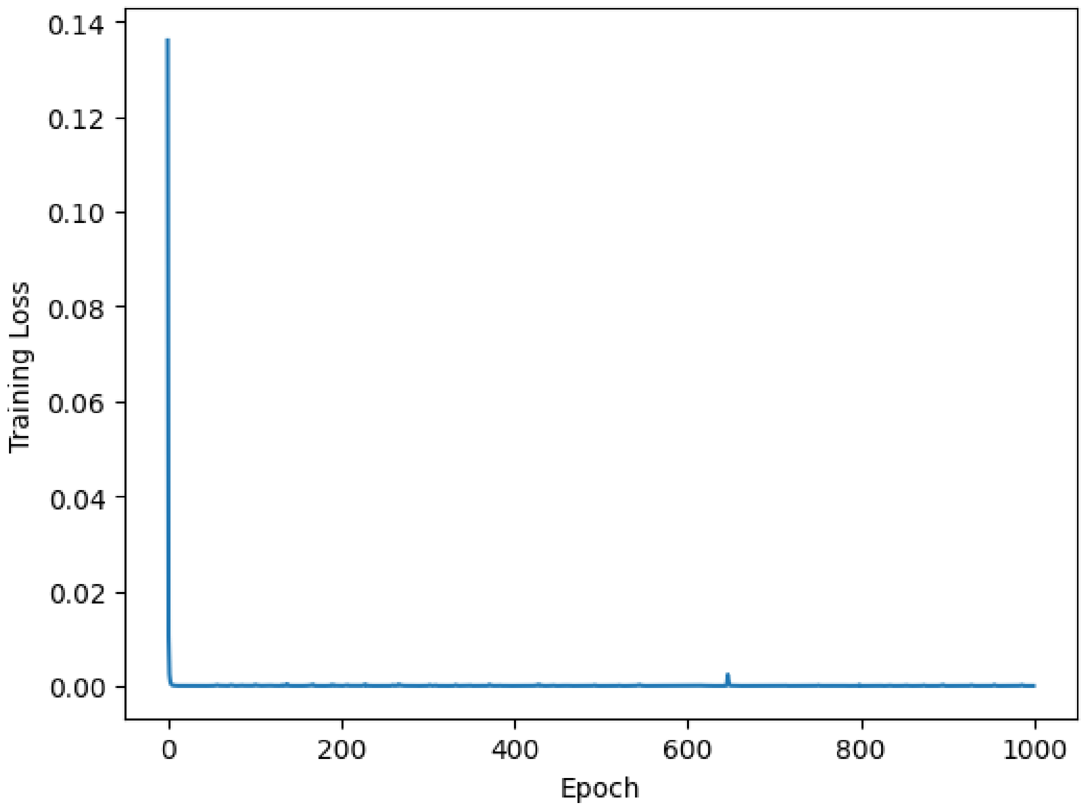

True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3



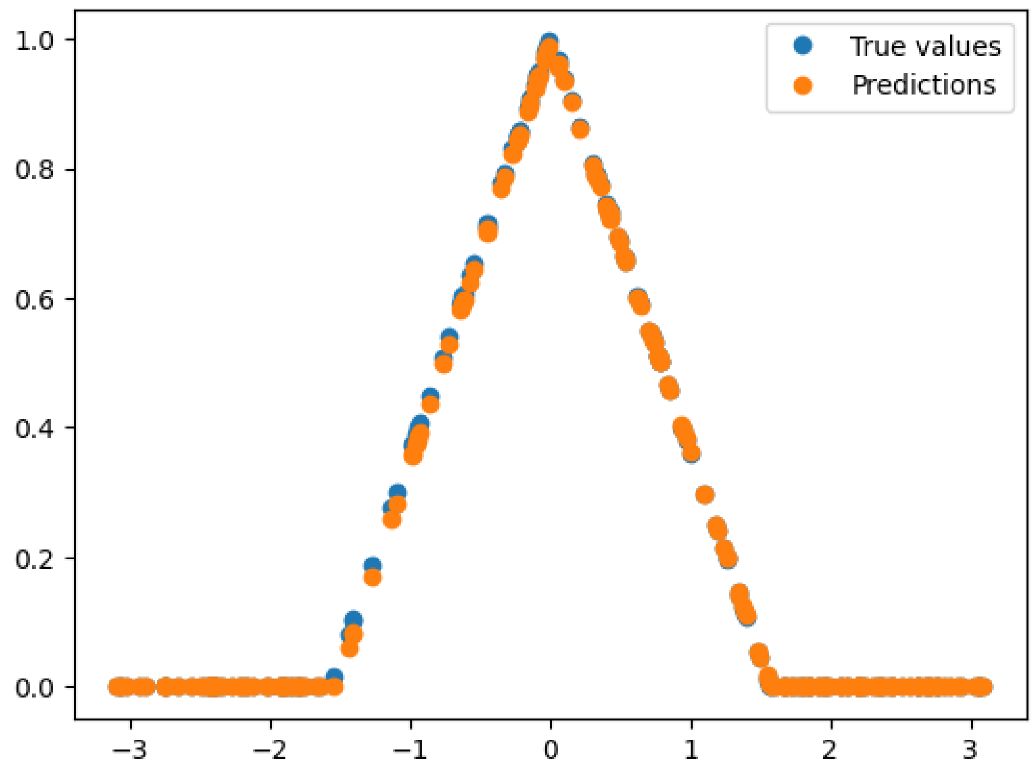

```
Test Loss: 0.000000
R2 Score: 1.000000
Hidden neurons: 100, Num. layers: 2, Test Loss: 0.000000
```

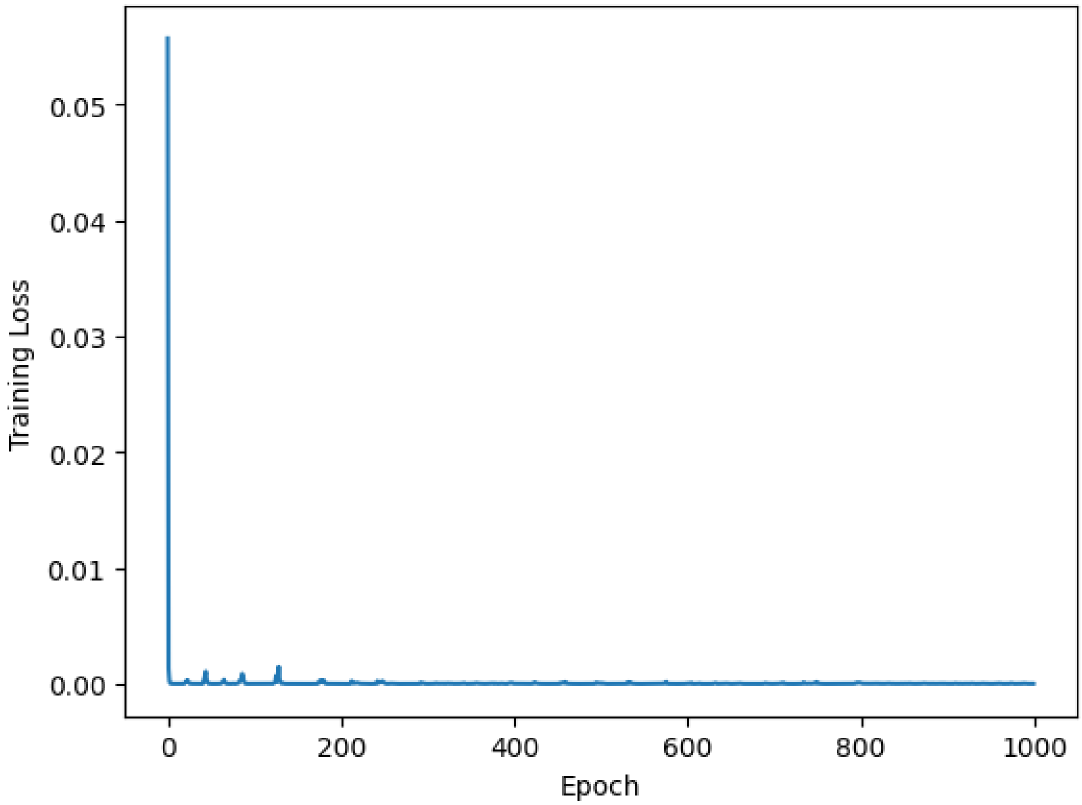


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3




```
Test Loss: 0.000032
R2 Score: 0.999751
Hidden neurons: 100, Num. layers: 3, Test Loss: 0.000032
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3



As the number of neurons in the hidden layers increases, the test loss decreases. It is also observed that the R2 score for the models also increases as the number of neurons increases.

8 Q7:

Similarity: Both neural networks and Fourier series are methods of approximating any complex function. They can both be looked at as a linear combination of different basis functions. In the Fourier series, the basis functions are sin(kx) and cos(kx). In the neural network, the basis functions are activation functions of the neurons. In both methods, the coefficients are determined by fitting the data to the model.

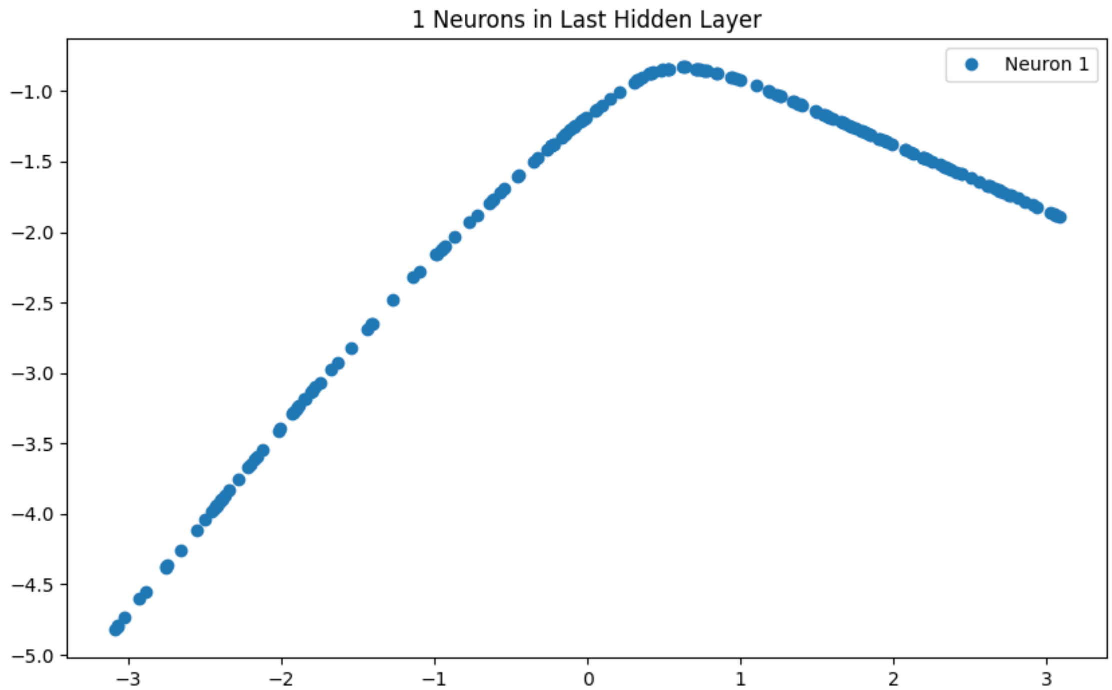
Differences: -In Fourier series, the sinusoidal basis functions are fixed and predefined, whereas, in the neural network the basis functions are learned by the model during training. With a flexible basis, neural networks are more flexible and can be used to learn more complex functions than Fourier series approximation can. -In additon, neural networks introduce non-linearity through activation functions, as compared to Fourier series that are inherently linear. -Fourier series basis functions are global. In contrast, neural networks have local basis/activation functions and the changes to the network are more localized.

9 Q8:

[ ]:
```
class NN_q8(nn.Module):
    def __init__(self, num_neurons_last_layer, num_layers=2, hidden_size=50,␣
 ↪input_size=1):
        super(NN_q8, self).__init__()
        self.layers = nn.ModuleList()
        self.layers.append(nn.Linear(input_size, hidden_size))
        for _ in range(num_layers - 1):
            self.layers.append(nn.Linear(hidden_size, hidden_size))
        self.layers.append(nn.Linear(hidden_size, num_neurons_last_layer))
        self.layers.append(nn.Linear(num_neurons_last_layer, 1))

    def forward(self, x, activations=False):
        for i, layer in enumerate(self.layers):
            x = layer(x)
            if i == len(self.layers) - 2 and activations:  # If this is the␣
 ↪last hidden layer and activations=True
                return x
            x = torch.relu(x)
        return x
```

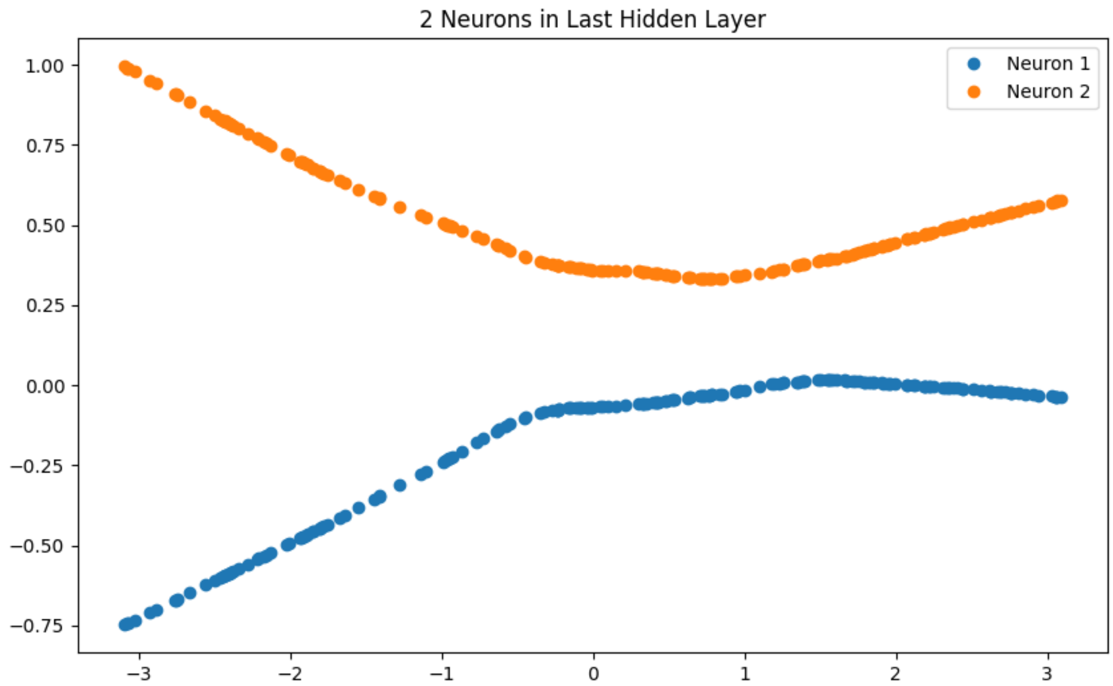
[ ]:
```
def create_model(num_neurons):
    model = NN_q8(num_neurons_last_layer=num_neurons, num_layers=2,␣
 ↪hidden_size=50, input_size=1)
    return model

# models = []
for i in range(1, 9):
    model = create_model(i)
    optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
    criterion = torch.nn.MSELoss()
    act_last, _, _ = train_and_evaluate(model, criterion, optimizer,␣
 ↪train_loader_hat, test_loader_hat, activations=True)
    print(act_last.shape)
    plt.figure(figsize=(10, 6))
    for j in range(act_last.shape[1]):
        plt.plot(test_dataset_hat.tensors[0].numpy(), act_last[:, j].numpy(),␣
 ↪'o' ,label=f'Neuron {j+1}')
    plt.title(f'{i} Neurons in Last Hidden Layer')
    plt.legend()
    plt.show()
```

```
Test Loss: 5.881685
torch.Size([200, 1])
```



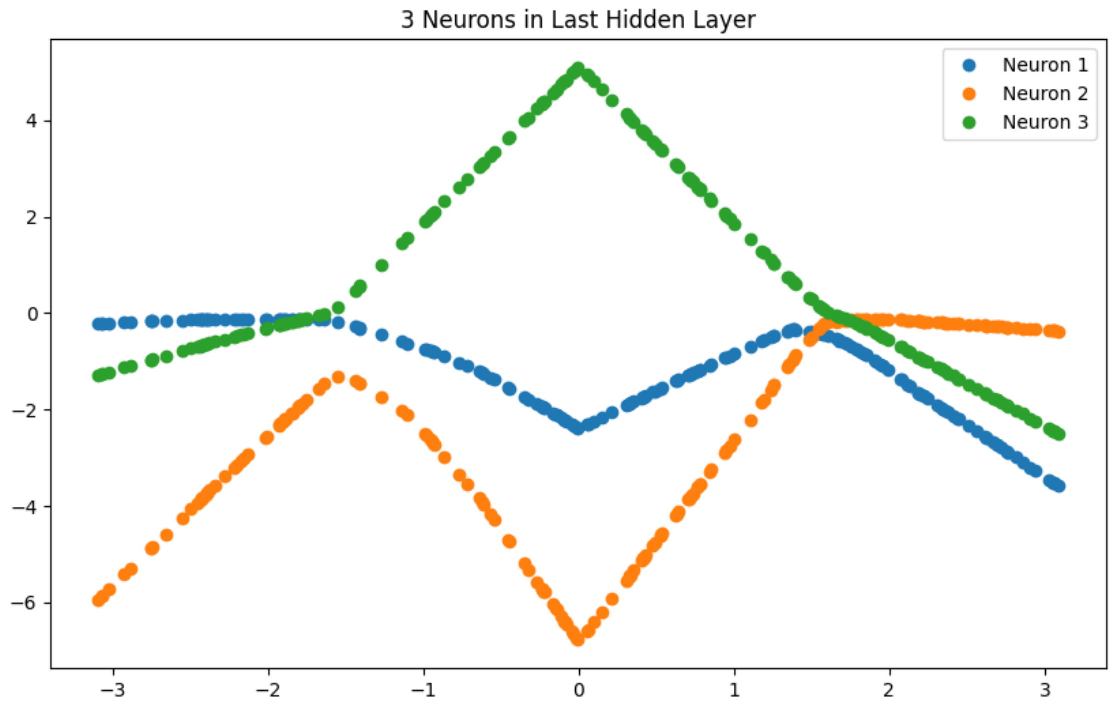

```
Test Loss: 0.292641
torch.Size([200, 2])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 2])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 2])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```



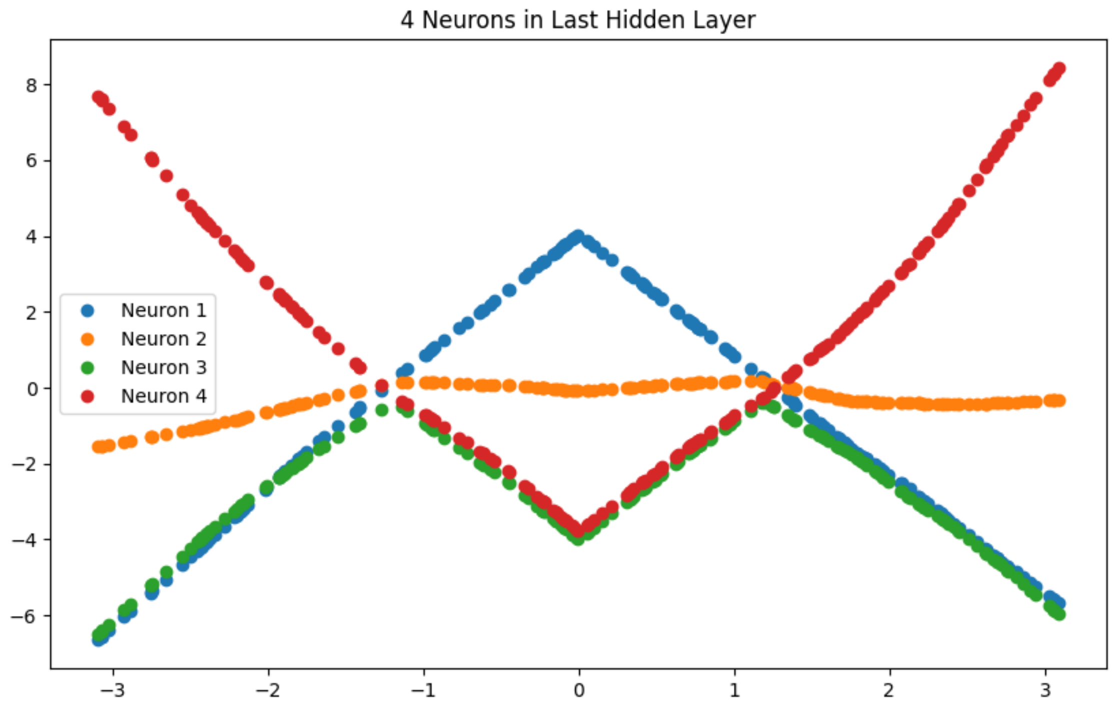

```
Test Loss: 7.100335
torch.Size([200, 3])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 3])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 3])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```



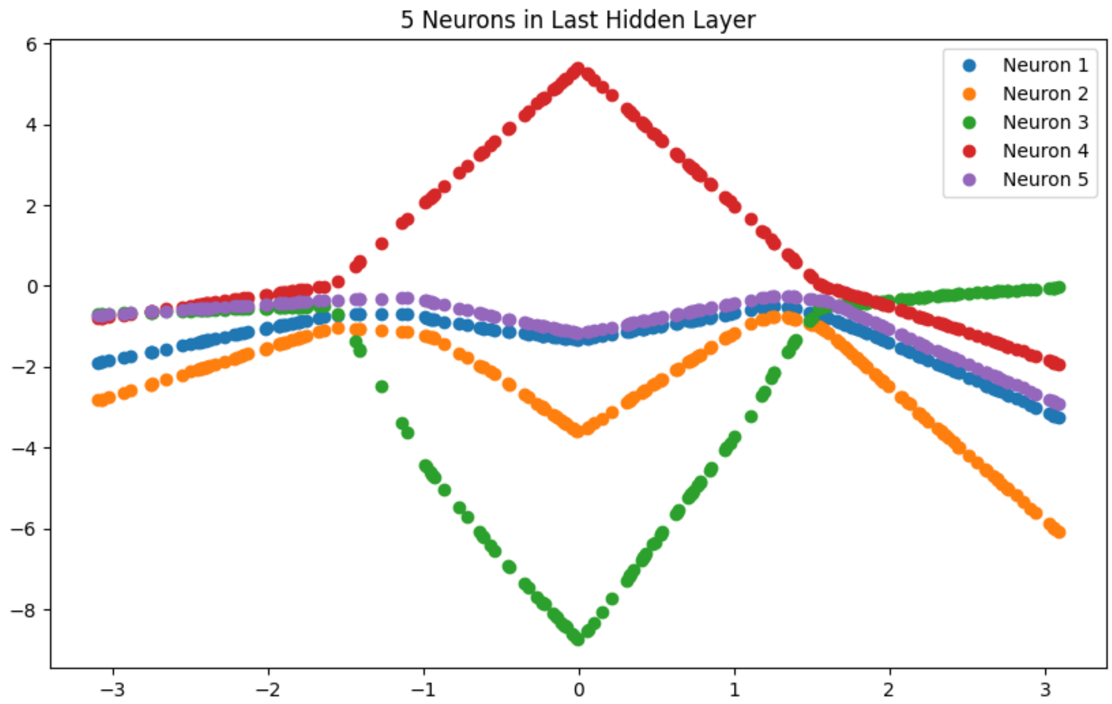

```
Test Loss: 8.906102
torch.Size([200, 4])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 4])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 4])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```



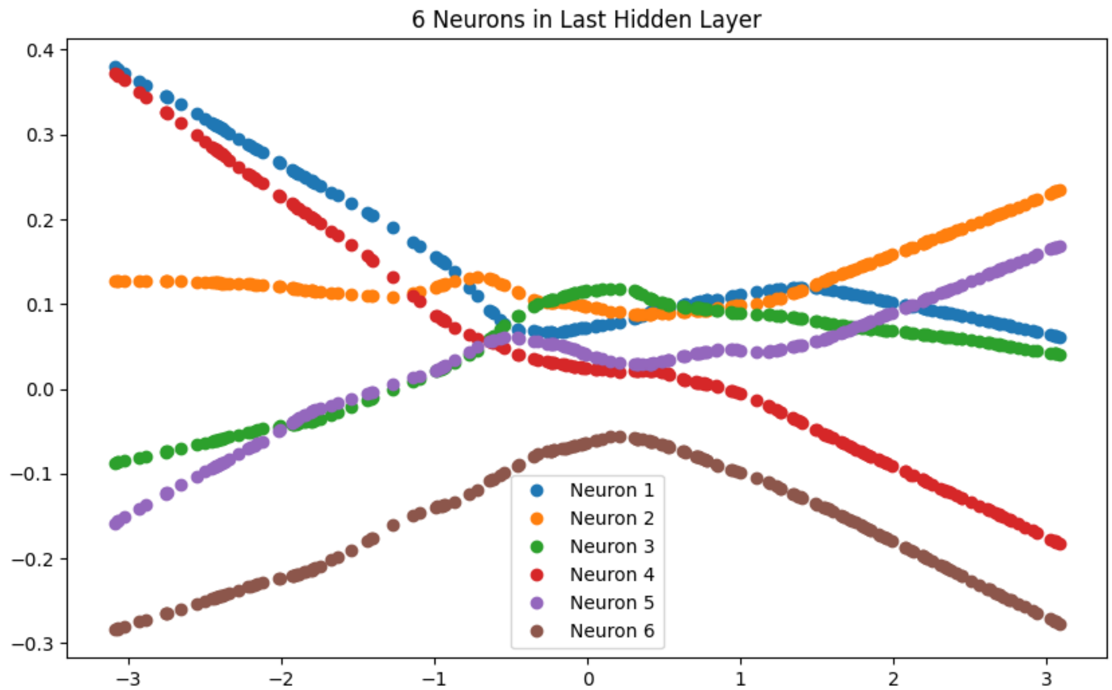

```
Test Loss: 7.273729
torch.Size([200, 5])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 5])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 5])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```



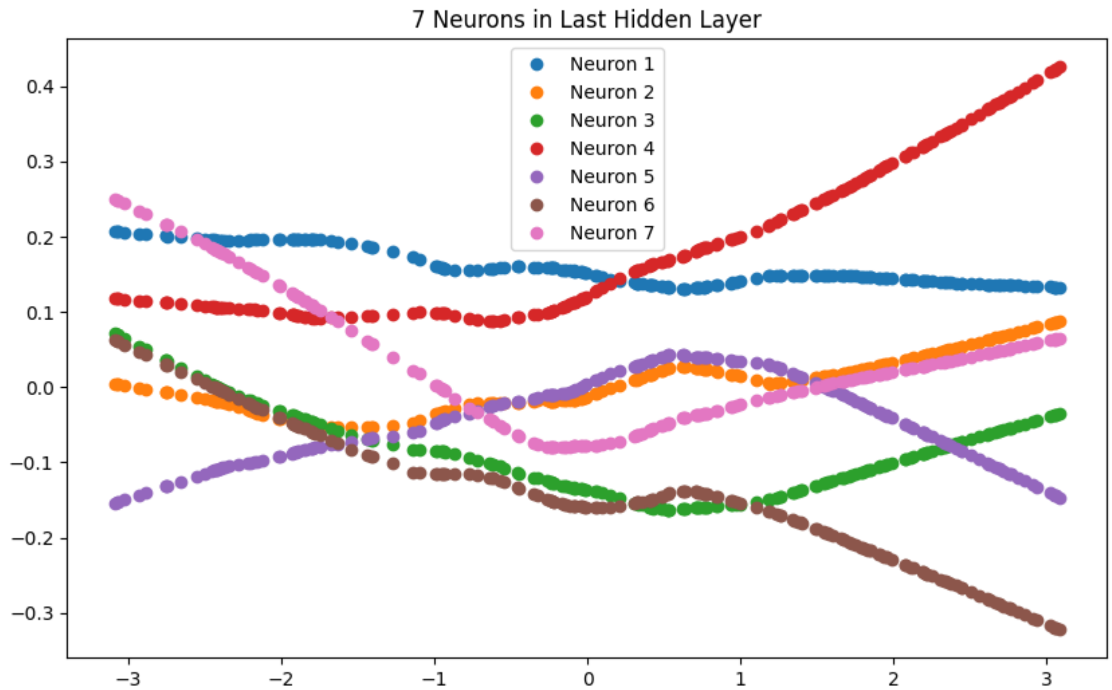

```
Test Loss: 0.174286
torch.Size([200, 6])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 6])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 6])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```



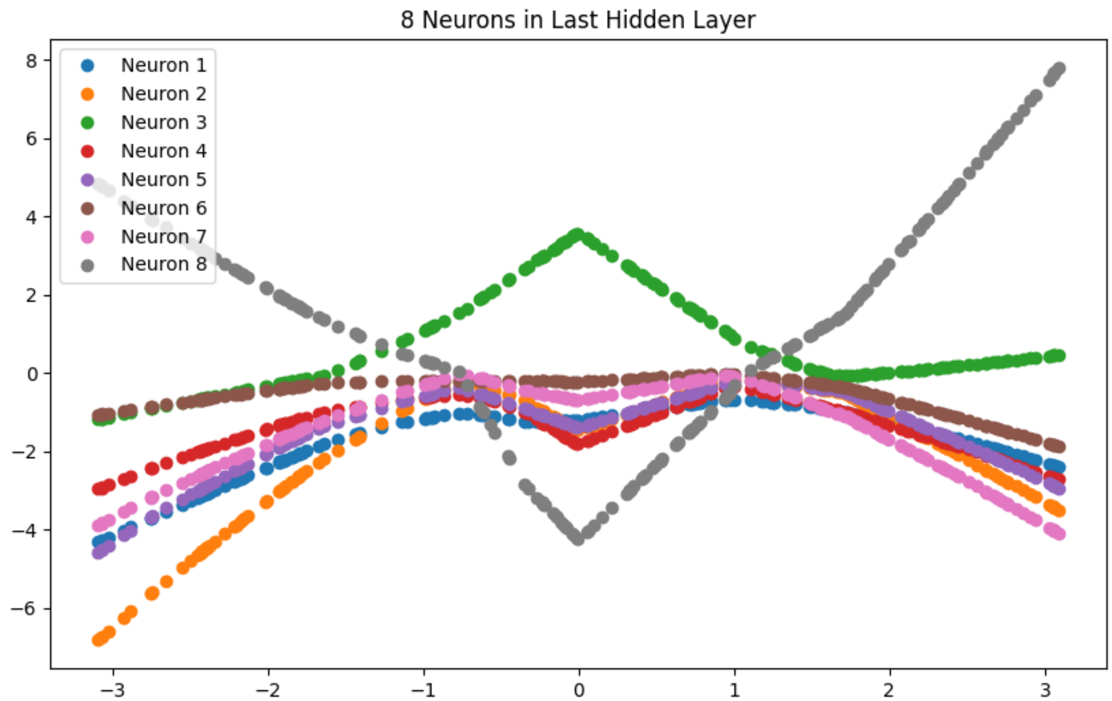

```
Test Loss: 0.200209
torch.Size([200, 7])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 7])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 7])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```




```
Test Loss: 4.434798
torch.Size([200, 8])
```

```
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([32, 1])) that is different to the input size (torch.Size([32, 8])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
/Users/purnavindhyakota/miniconda3/envs/bnn_trials/lib/python3.10/site-
packages/torch/nn/modules/loss.py:535: UserWarning: Using a target size
(torch.Size([8, 1])) that is different to the input size (torch.Size([8, 8])).
This will likely lead to incorrect results due to broadcasting. Please ensure
they have the same size.
  return F.mse_loss(input, target, reduction=self.reduction)
```



10 Q9

10.1 (i)

[ ]:
```
def fn_q9(x):
    return np.where(x < 0, 5 + np.sum([np.sin(k * x) for k in range(1, 7)],␣
 ↪axis=0), np.cos(10 * x))
```

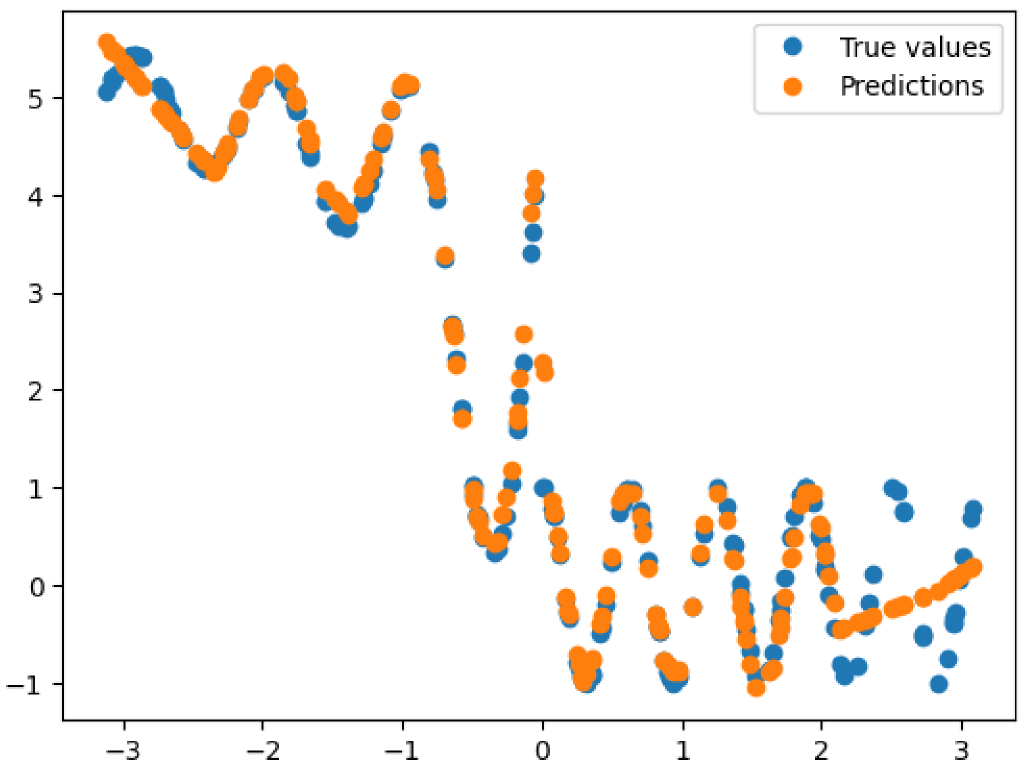
[ ]:
```
train_dataset_q9_i, test_dataset_q9_i = create_dataset(np.random.uniform(-np.
 ↪pi, np.pi, num_samples).reshape(-1, 1), fn_q9)

train_loader_q9_i = DataLoader(train_dataset_q9_i, batch_size=32)
test_loader_q9_i = DataLoader(test_dataset_q9_i, batch_size=32)
```

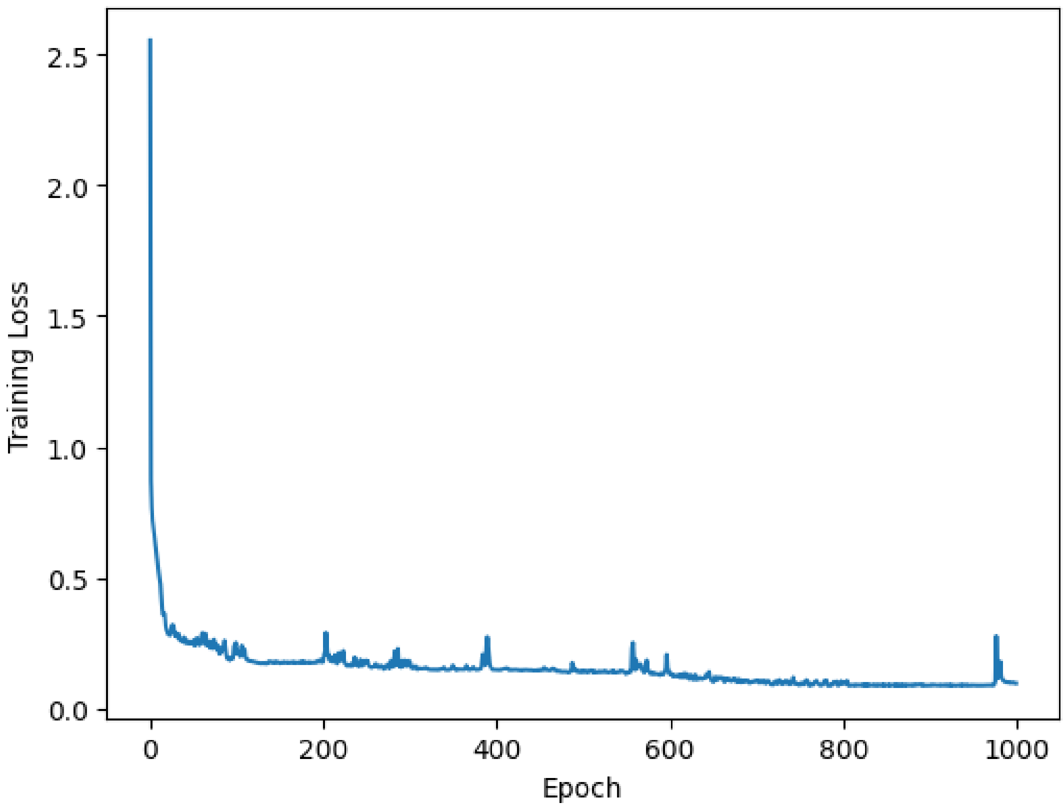
[ ]:
```
optimizers_all = {
    'Adam': lambda net: torch.optim.Adam(net.parameters(), lr=0.01),
    'SGD': lambda net: torch.optim.SGD(net.parameters(), lr=0.01),
    'RMSprop': lambda net: torch.optim.RMSprop(net.parameters(), lr=0.01),
    'Adagrad': lambda net: torch.optim.Adagrad(net.parameters(), lr=0.01),
    'Rprop': lambda net: torch.optim.RMSprop(net.parameters(), lr=0.01),
    'AdaHessian': lambda net: torch_optimizer.Adahessian(
    net.parameters(),
    lr= 0.7,
```

```
    betas= (0.9, 0.999),
    eps= 1e-4,
    weight_decay=0.0,
    hessian_power=1.0,
)
}
```

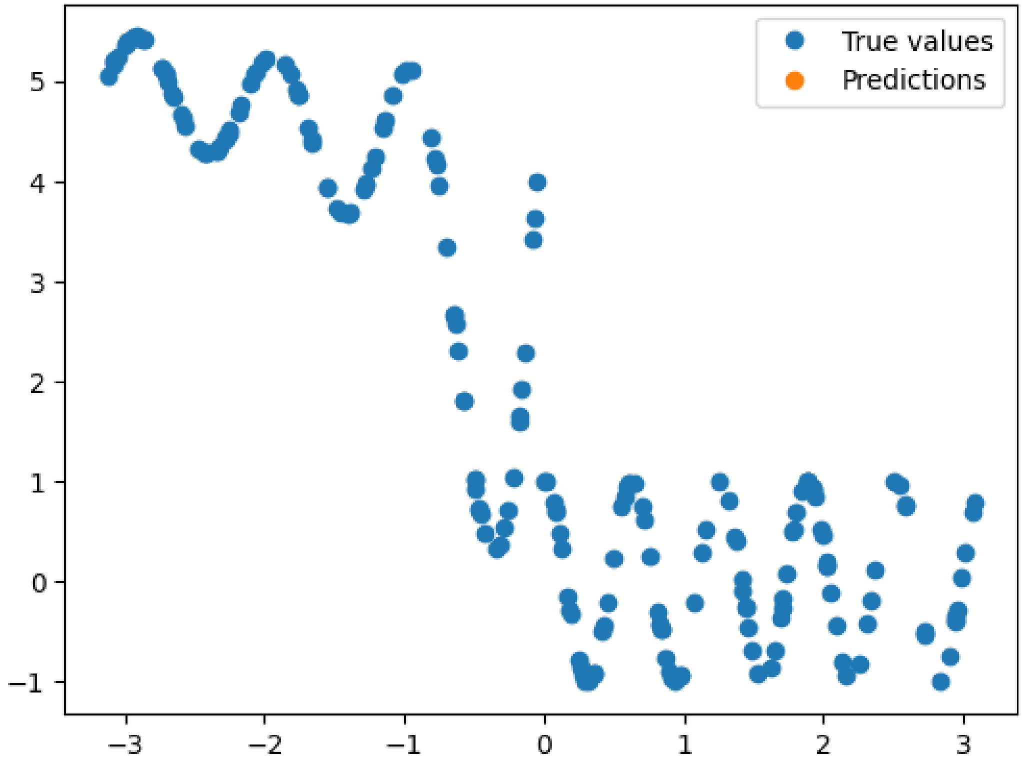
[ ]:
```
for name, optimizer in optimizers_all.items():
    n = Net_general(1, 50, 4)
    c = nn.MSELoss()
    o = optimizer(n)
    preds, train_losses, test_loss = train_and_evaluate( n, c, o,␣
 ↪train_loader_q9_i, test_loader_q9_i)
    print(f'Optimizer: {name}, Test Loss: {test_loss:.6f}')
    plot_losses_and_predictions(test_dataset_q9_i, train_losses, preds)
```

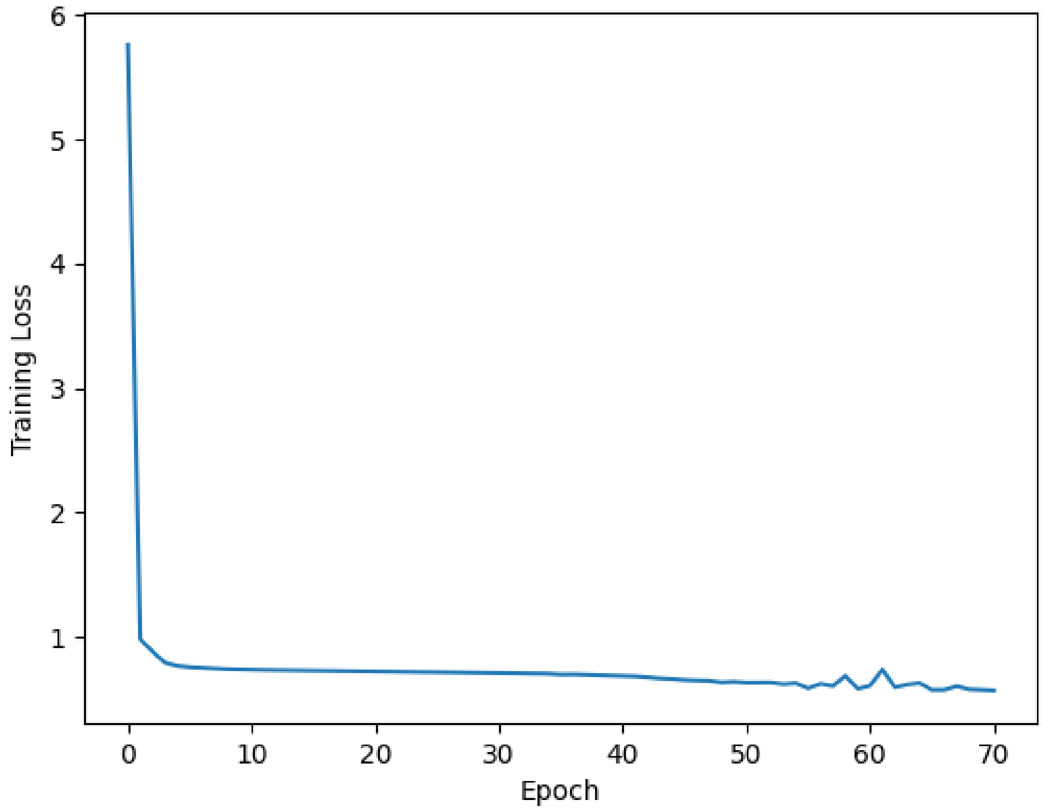
```
Test Loss: 0.069174
Optimizer: Adam, Test Loss: 0.069174
```



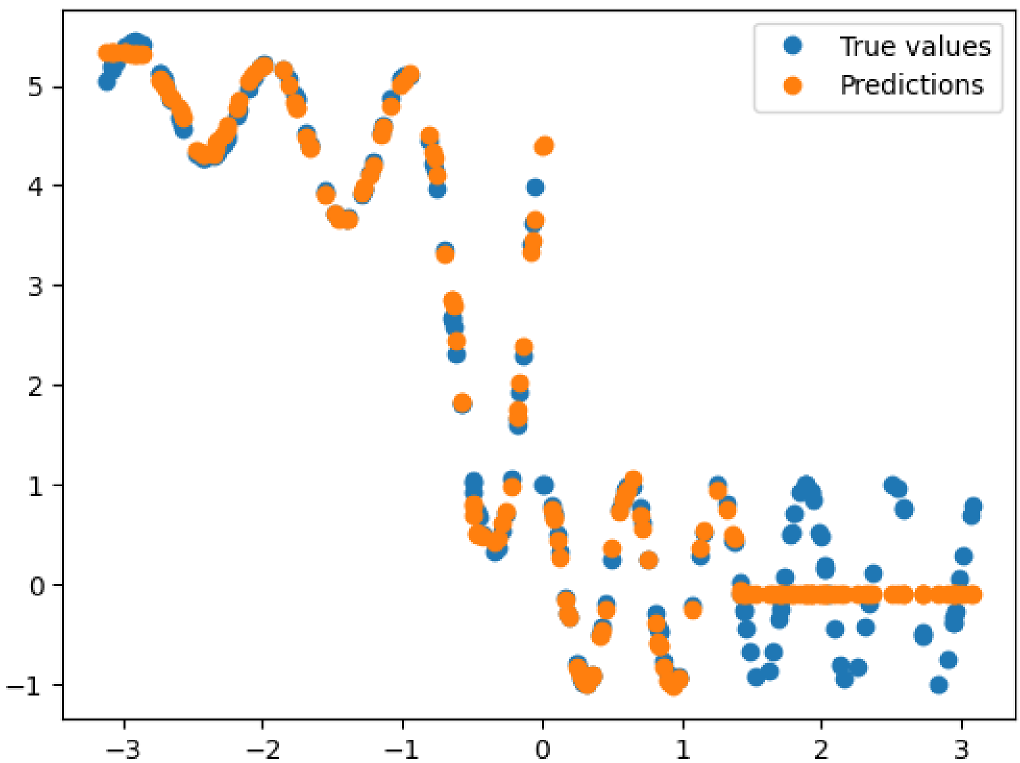


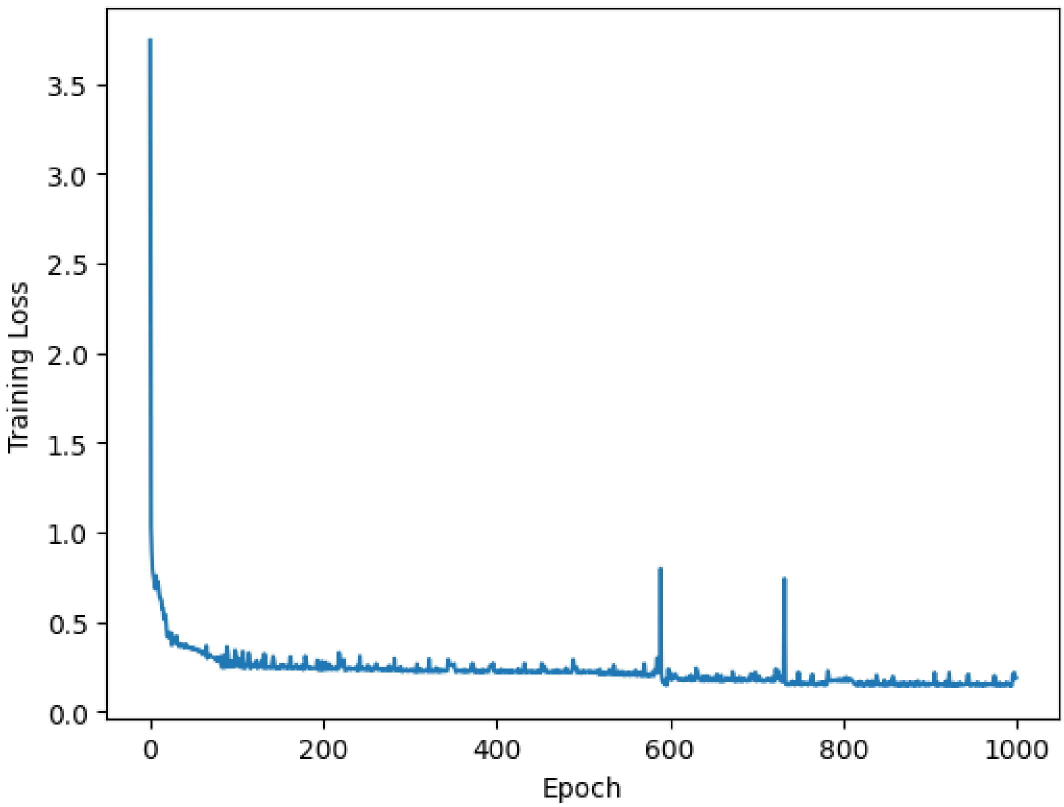

```
Test Loss: nan
Optimizer: SGD, Test Loss: nan
```


True values
Predictions
5
4
3
2
1
0
−1
−3
−2
−1
0
1
2
3

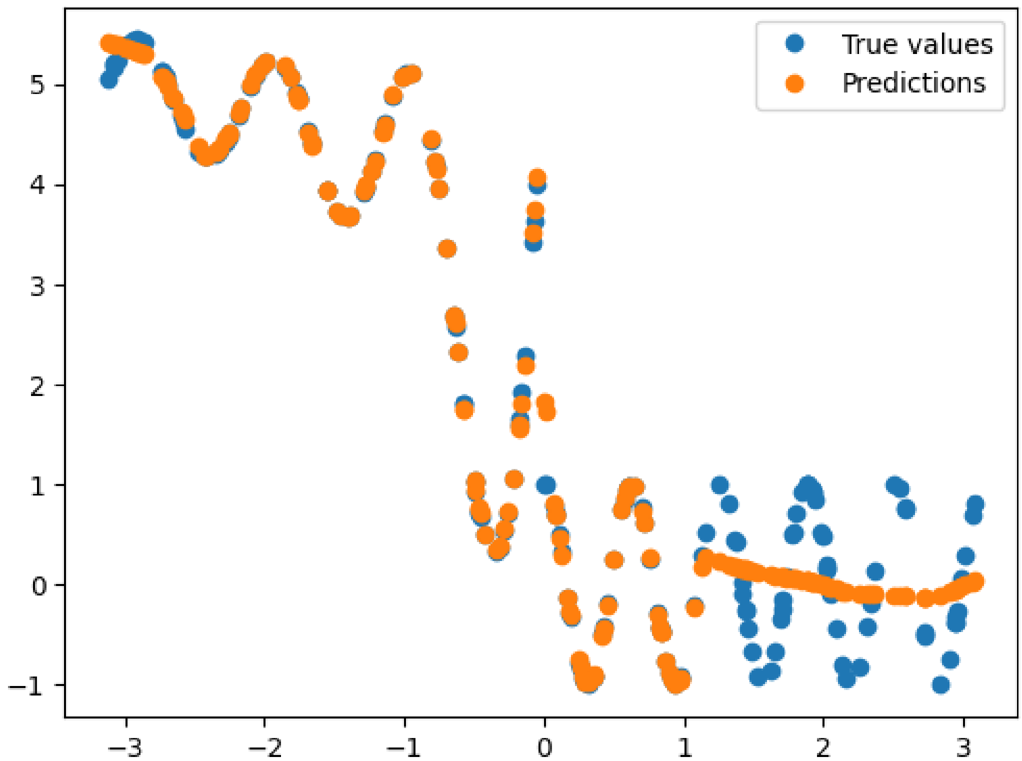



```
Test Loss: 0.226039
Optimizer: RMSprop, Test Loss: 0.226039
```

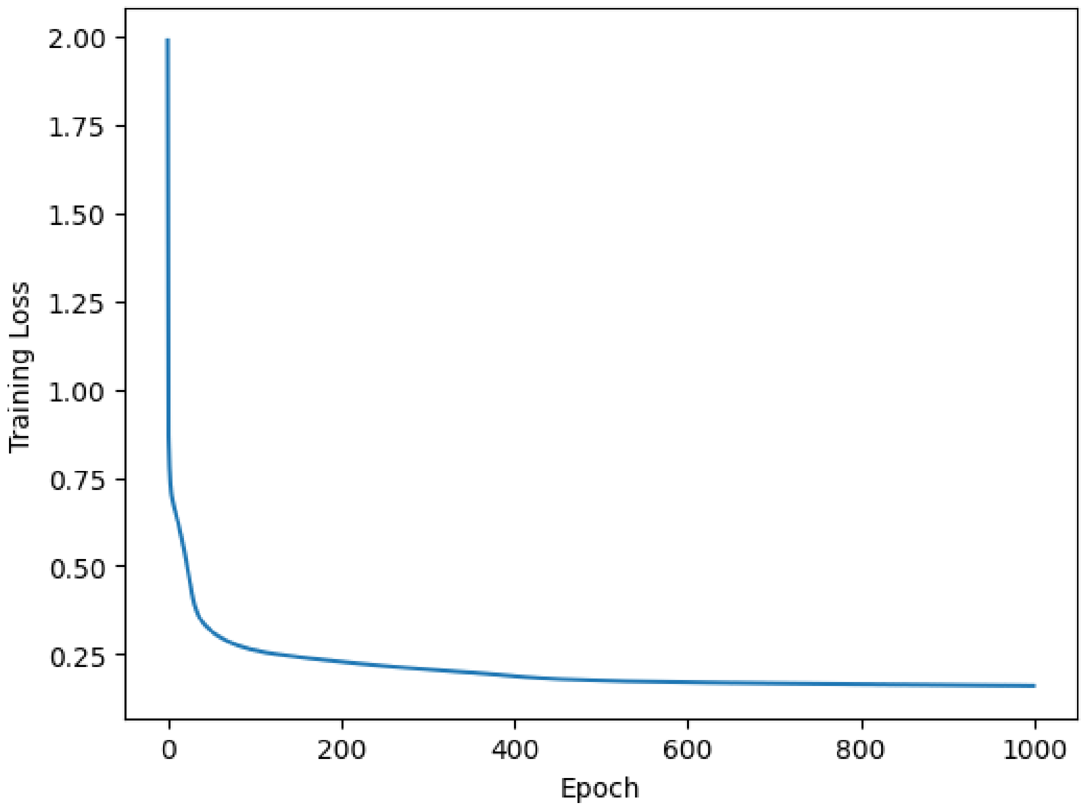

True values
Predictions
5
4
3
2
1
0
−1
−3
−2
−1
0
1
2
3



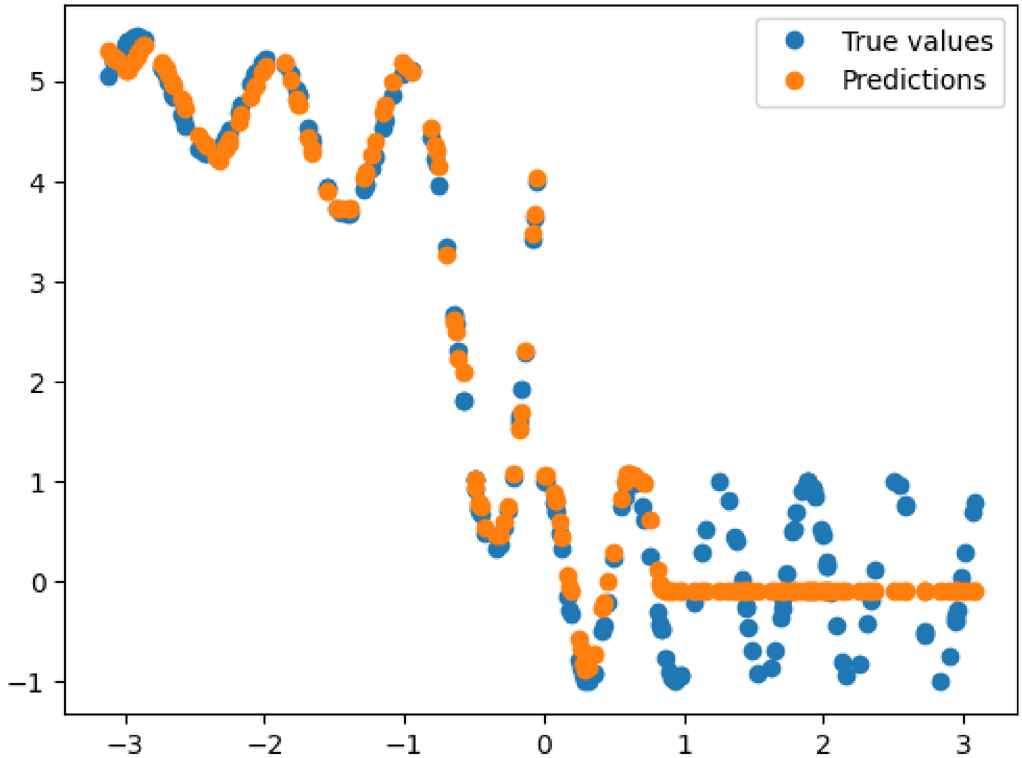

```
Test Loss: 0.121742
Optimizer: Adagrad, Test Loss: 0.121742
```

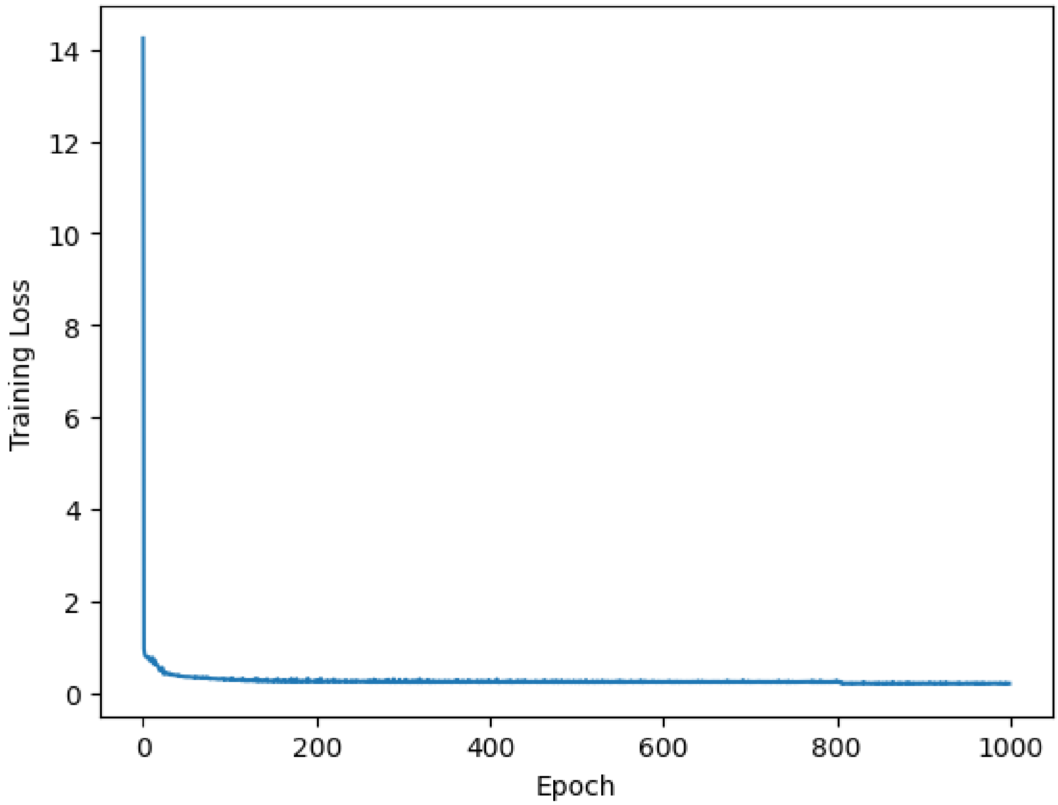


True values
Predictions
5
4
3
2
1
0
−1
−3
−2
−1
0
1
2
3

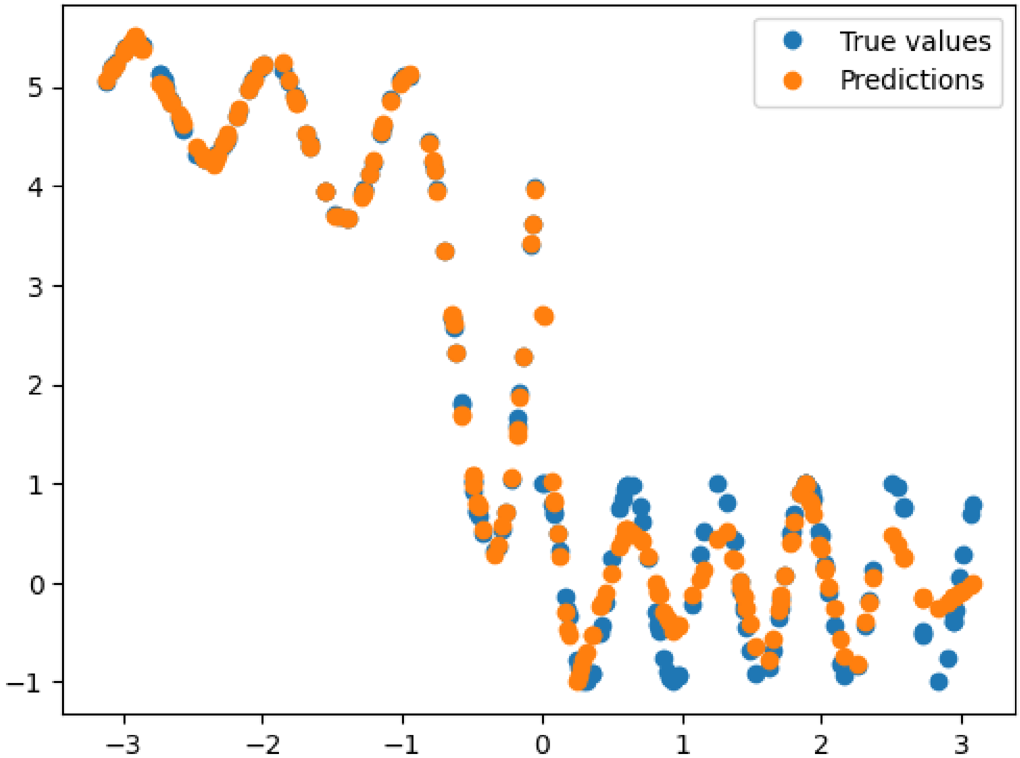


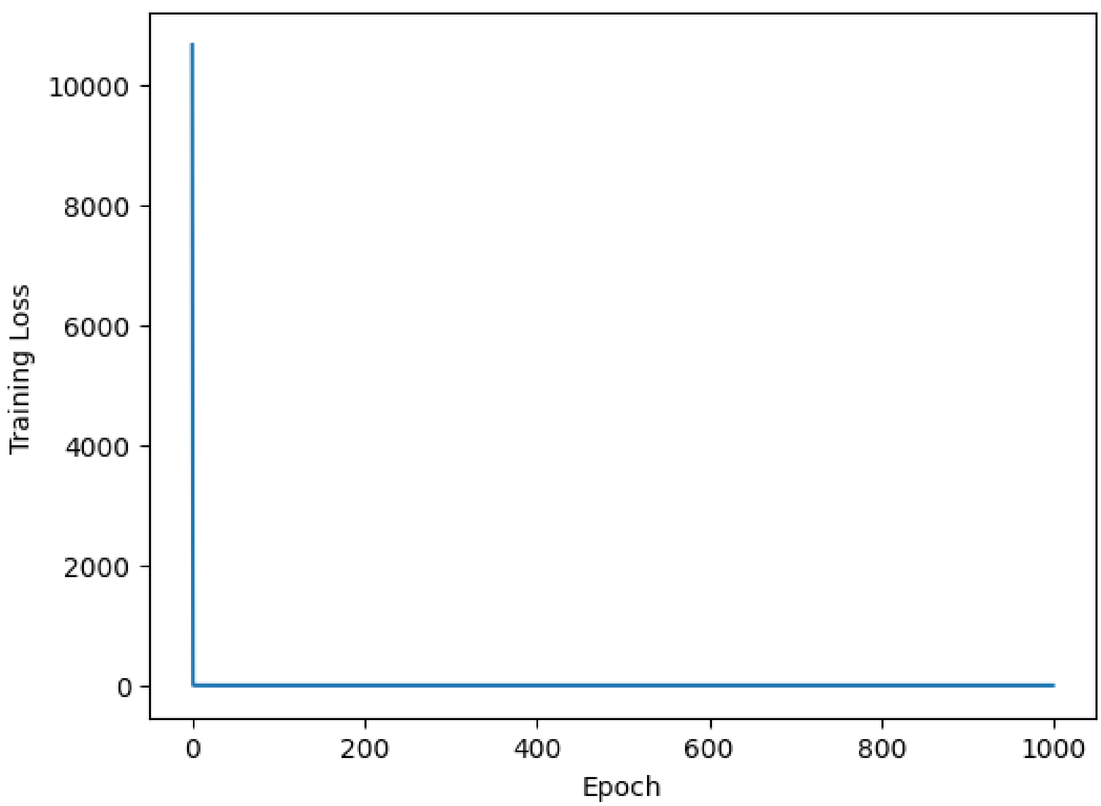

```
Test Loss: 0.171960
Optimizer: Rprop, Test Loss: 0.171960
```


True values
Predictions
5
4
3
2
1
0
−1
−3
−2
−1
0
1
2
3




```
Test Loss: 0.074262
Optimizer: AdaHessian, Test Loss: 0.074262
```


True values
Predictions
5
4
3
2
1
0
−1
−3
−2
−1
0
1
2
3


10000
8000
6000
4000
2000
0
Training Loss
0
200
400
600
800
1000
Epoch

10.2 (ii)

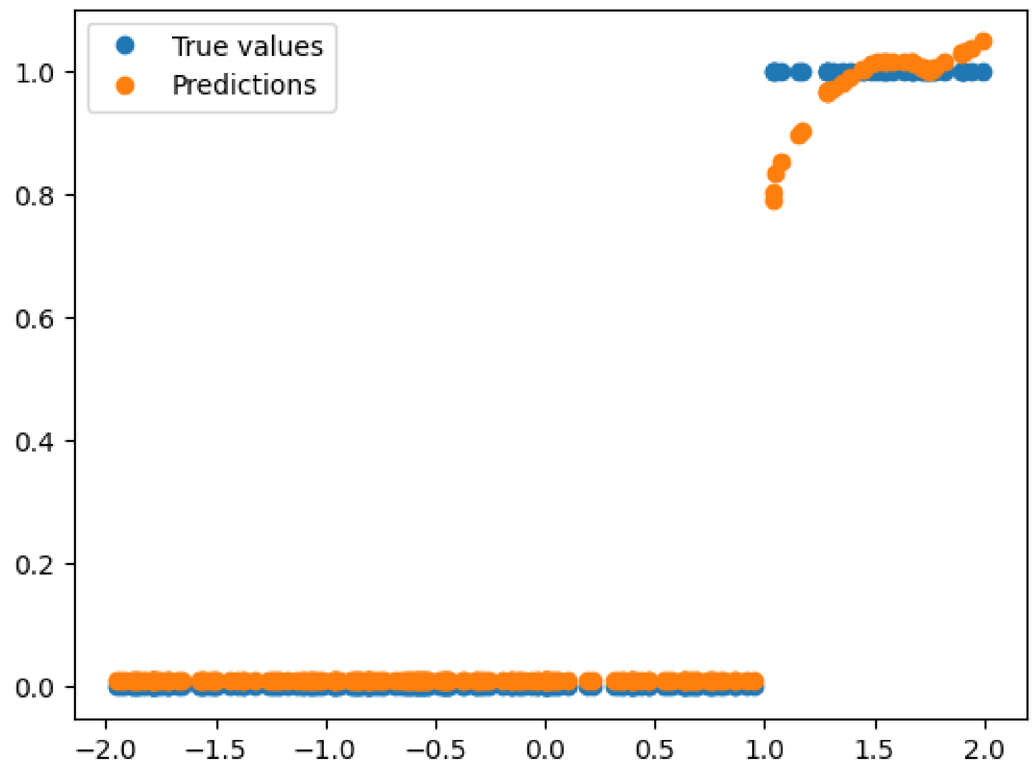
[ ]:
```
def fn_q9_ii(x):
    return np.where(x < 1.0, 0, 1)
```

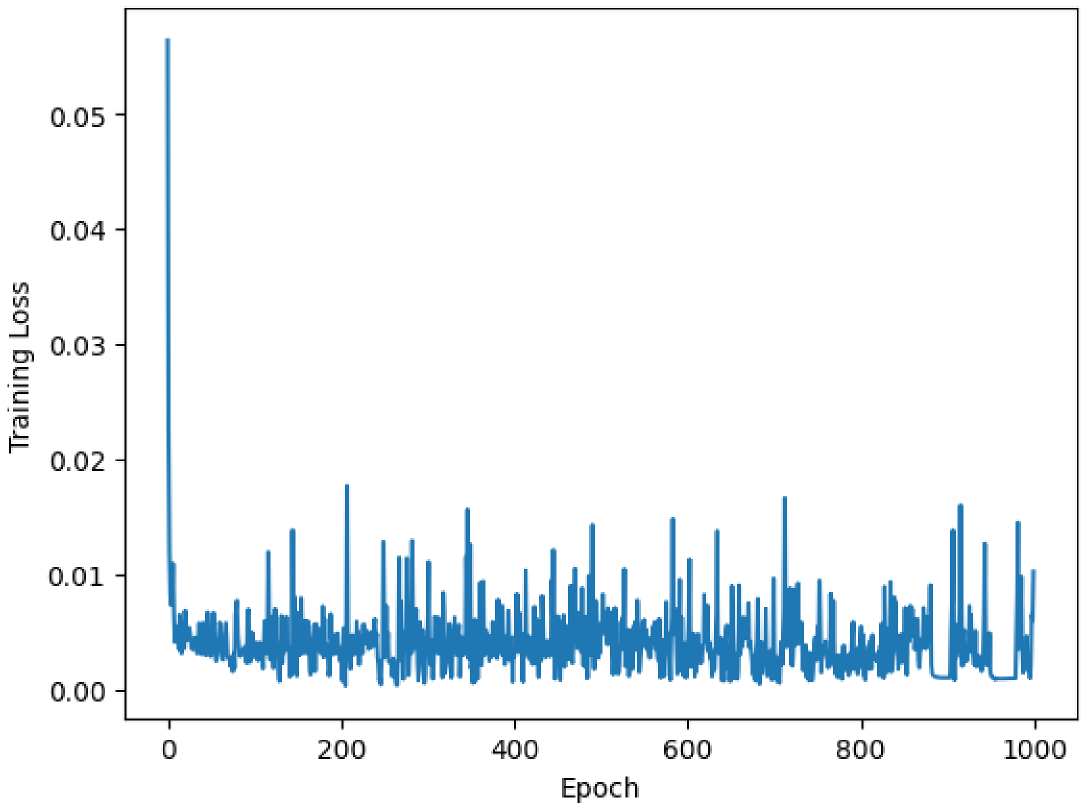
[ ]:
```
train_dataset_q9_ii, test_dataset_q9_ii = create_dataset(np.random.uniform(-2,␣
 ↪2, num_samples).reshape(-1, 1), fn_q9_ii)

train_loader_q9_ii = DataLoader(train_dataset_q9_ii, batch_size=32)
test_loader_q9_ii = DataLoader(test_dataset_q9_ii, batch_size=32)
```

[ ]:
```
optimizers_all_ii = {
    'Adam': lambda net: torch.optim.Adam(net.parameters(), lr=0.01),
    'SGD': lambda net: torch.optim.SGD(net.parameters(), lr=0.01),
    'RMSprop': lambda net: torch.optim.RMSprop(net.parameters(), lr=0.01),
    'Adagrad': lambda net: torch.optim.Adagrad(net.parameters(), lr=0.1),
    'Rprop': lambda net: torch.optim.RMSprop(net.parameters(), lr=0.002),
    'LBFGS': optim.LBFGS,
    'AdaHessian': lambda net: torch_optimizer.Adahessian(
    net.parameters(),
    lr= 0.01,
    betas= (0.9, 0.999),
    eps= 1e-4,
    weight_decay=1e-3,
    hessian_power=1.0,
)
}
```

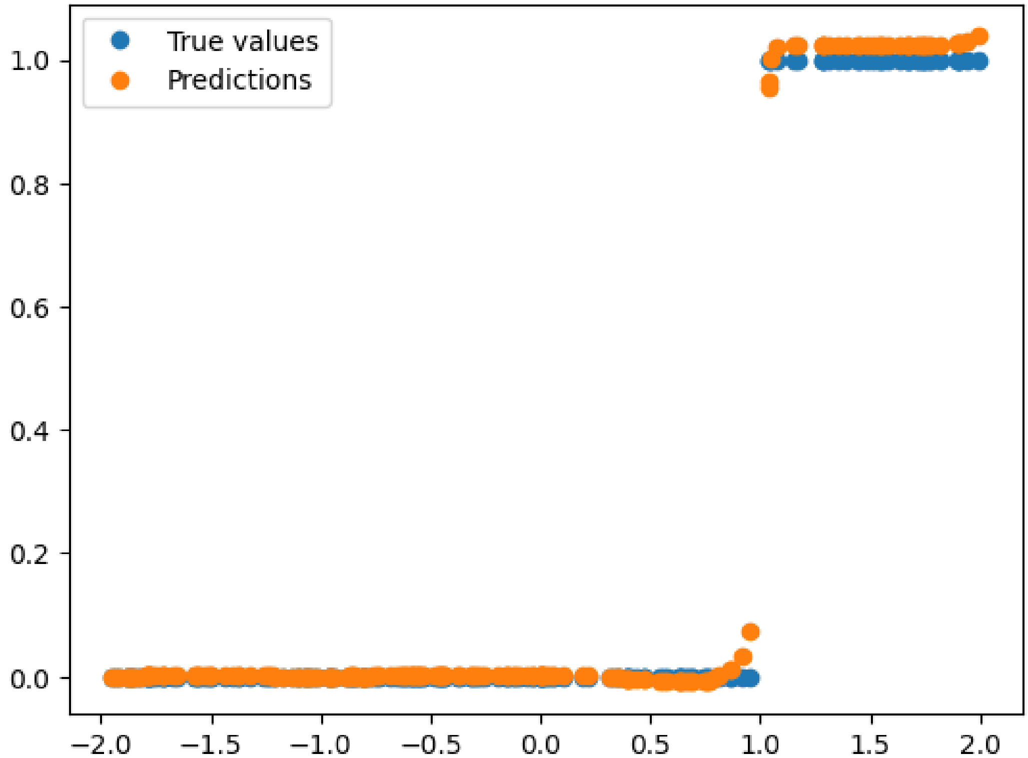
[ ]:
```
for name, optimizer in optimizers_all_ii.items():
    n = Net_general(1, 50, 4)
    c = nn.MSELoss()
    o = optimizer(n)
    preds, train_losses, test_loss = train_and_evaluate( n, c, o,␣
 ↪train_loader_q9_ii, test_loader_q9_ii)
    print(f'Optimizer: {name}, Test Loss: {test_loss:.6f}')
    # print(name)
    plot_losses_and_predictions(test_dataset_q9_ii, train_losses, preds)
```

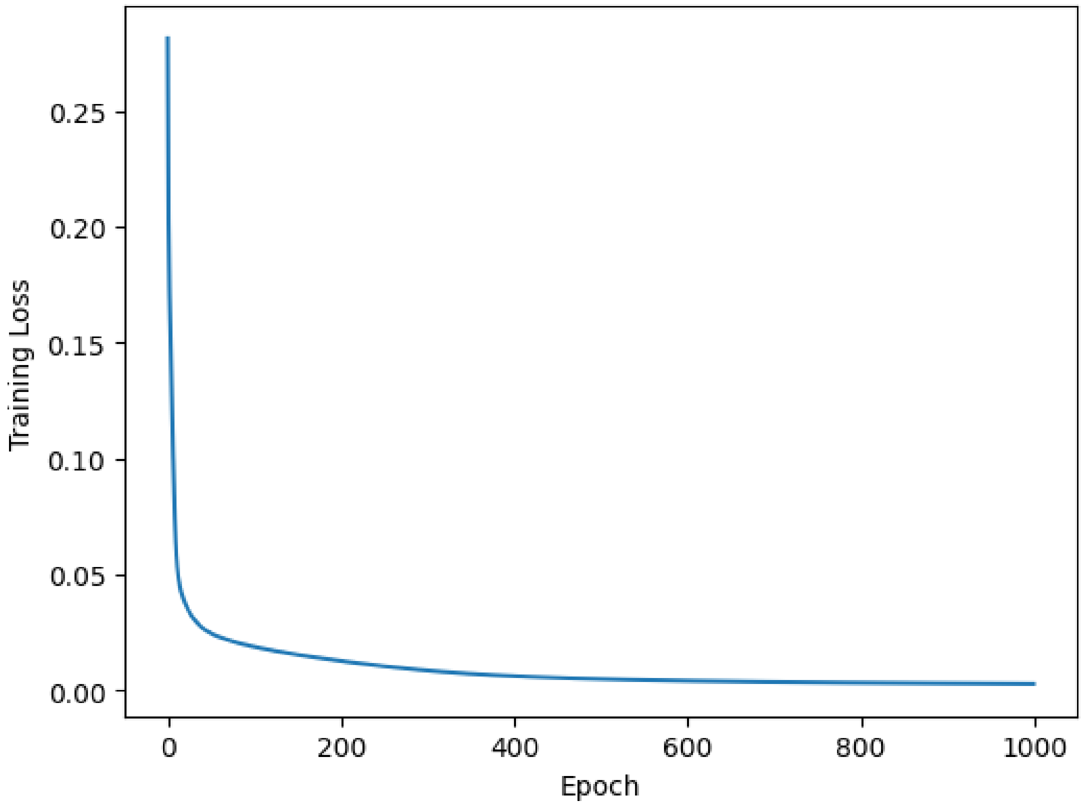
```
Test Loss: 0.000968
Optimizer: Adam, Test Loss: 0.000968
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

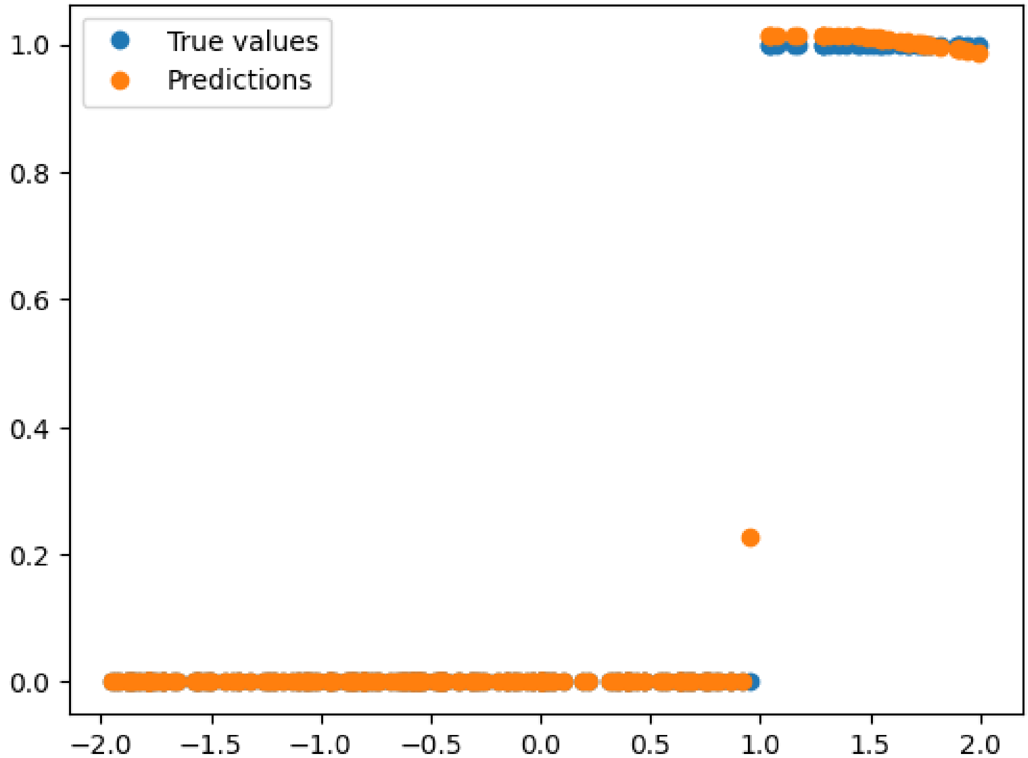


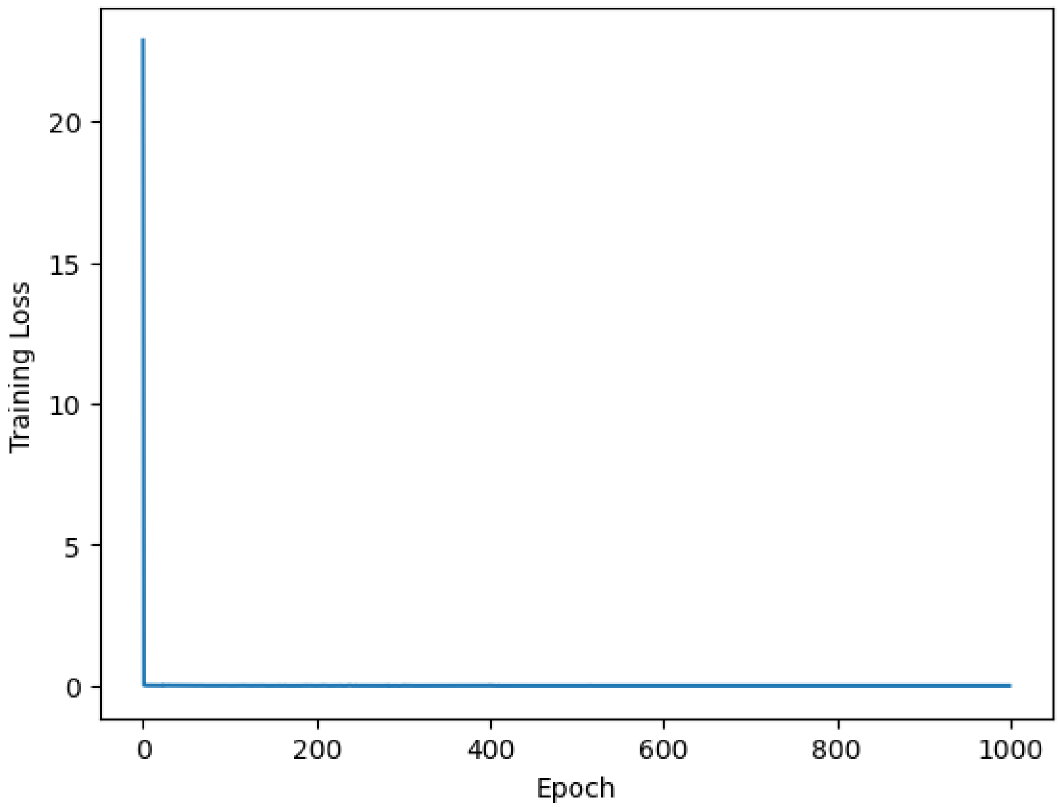

```
Test Loss: 0.000155
Optimizer: SGD, Test Loss: 0.000155
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

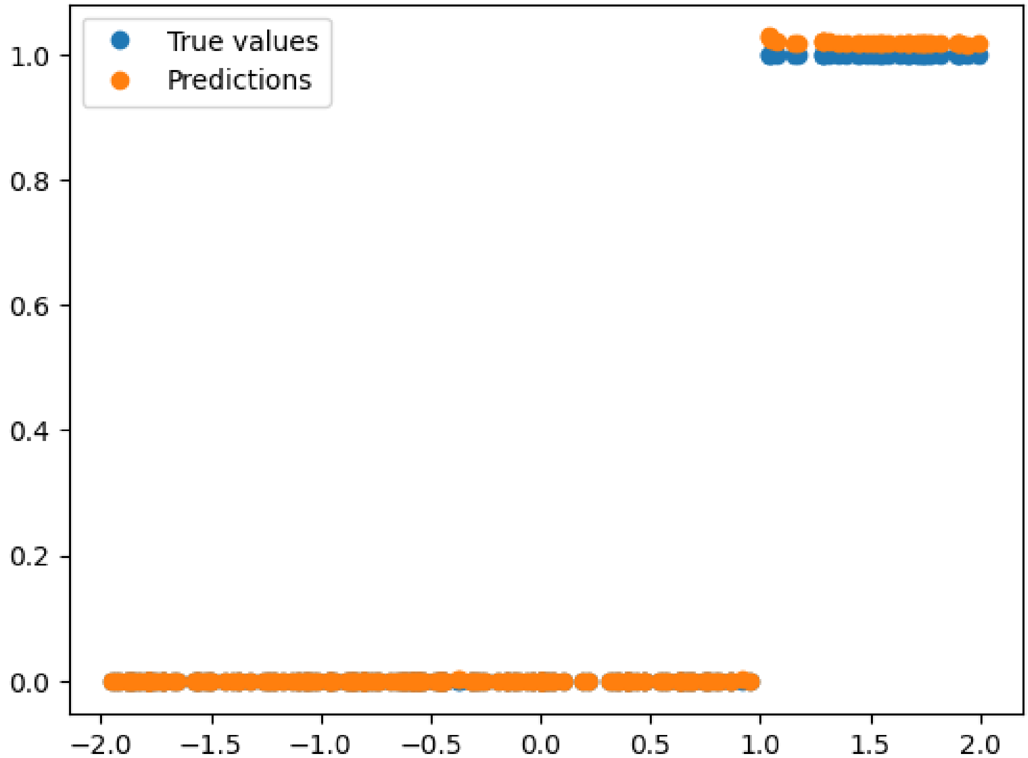


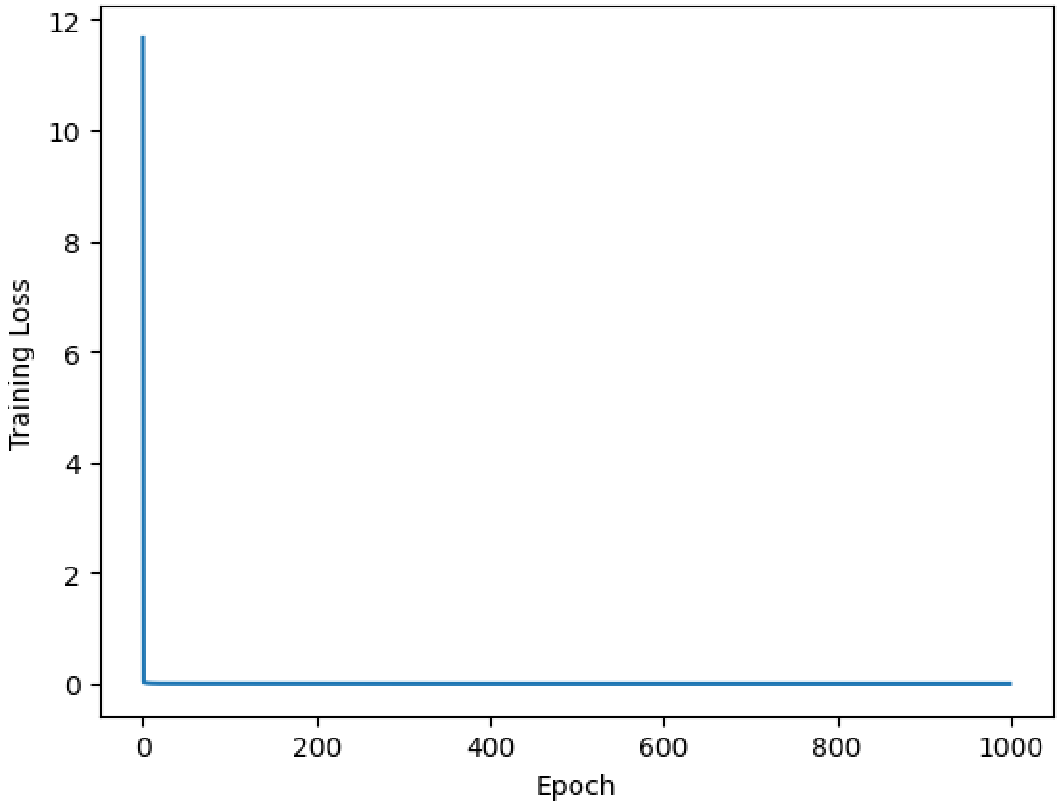

```
Test Loss: 0.000245
Optimizer: RMSprop, Test Loss: 0.000245
```


True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

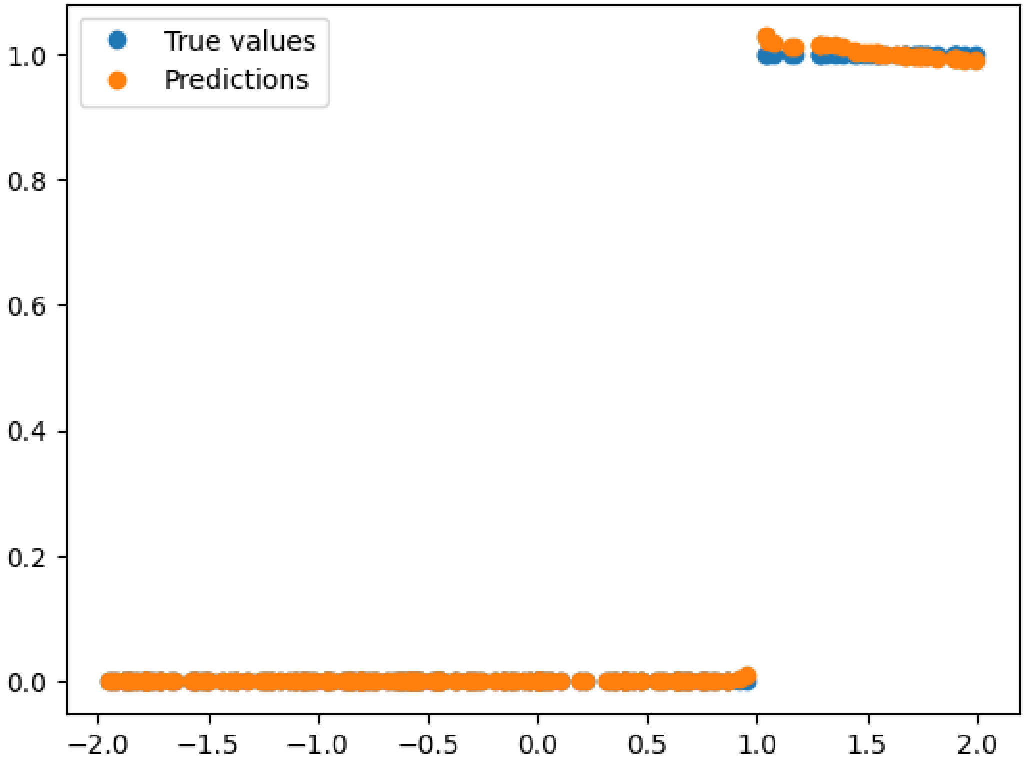



```
Test Loss: 0.000066
Optimizer: Adagrad, Test Loss: 0.000066
```

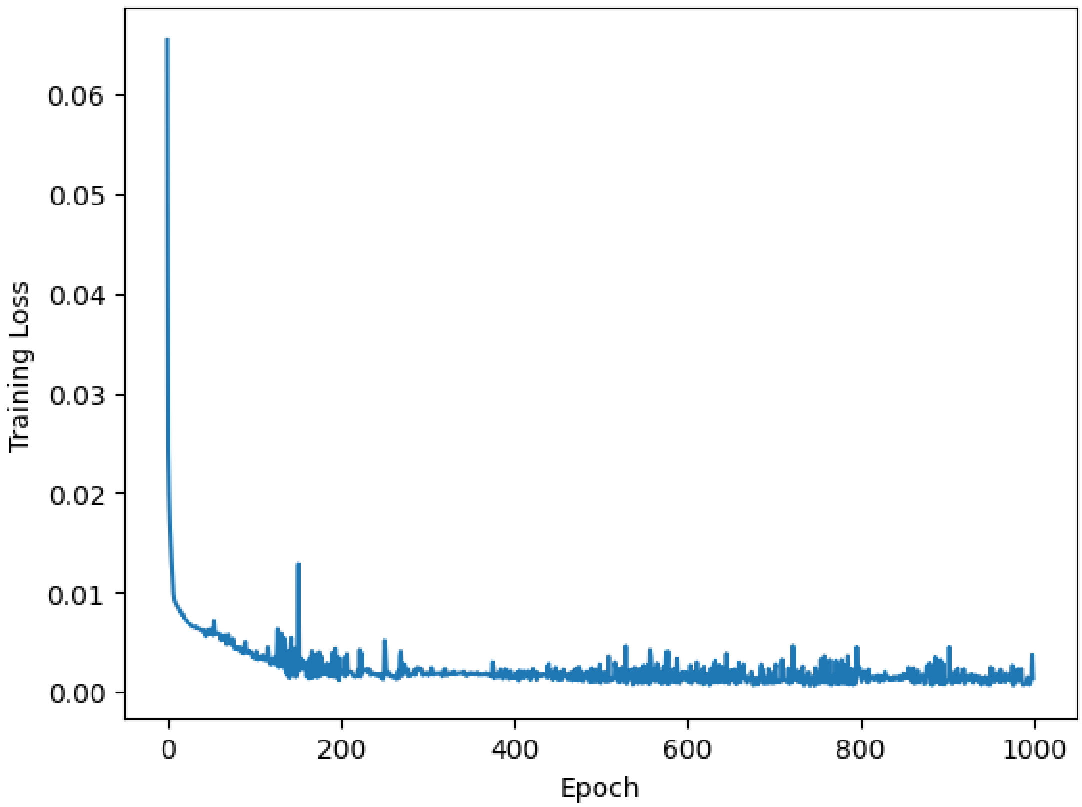

True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0




```
Test Loss: 0.000024
Optimizer: Rprop, Test Loss: 0.000024
```



True values
Predictions
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0




```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[190], line 4
      2 n = Net_general(1, 50, 4)
      3 c = nn.MSELoss()
----> 4 o = optimizer(n)
      5 preds, train_losses, test_loss = train_and_evaluate( n, c, o,␣
 ↪train_loader_q9_ii, test_loader_q9_ii)
      6 print(f'Optimizer: {name}, Test Loss: {test_loss:.6f}')

File ~/miniconda3/envs/bnn_trials/lib/python3.10/site-packages/torch/optim/lbfgs.
 ↪py:236, in LBFGS.__init__(self, params, lr, max_iter, max_eval,␣
 ↪tolerance_grad, tolerance_change, history_size, line_search_fn)
    227     max_eval = max_iter * 5 // 4
    228 defaults = dict(
    229     lr=lr,
    230     max_iter=max_iter,
   (…)
    234     history_size=history_size,
    235     line_search_fn=line_search_fn)
--> 236 super().__init__(params, defaults)
```

```
    238 if len(self.param_groups) != 1:
    239     raise ValueError("LBFGS doesn't support per-parameter options "
    240                      "(parameter groups)")

File ~/miniconda3/envs/bnn_trials/lib/python3.10/site-packages/torch/optim/
  ↪optimizer.py:271, in Optimizer.__init__(self, params, defaults)
    268 self.state: DefaultDict[torch.Tensor, Any] = defaultdict(dict)
    269 self.param_groups: List[Dict[str, Any]] = []
--> 271 param_groups = list(params)
    272 if len(param_groups) == 0:
    273     raise ValueError("optimizer got an empty parameter list")

TypeError: 'Net_general' object is not iterable
```

11 Q10

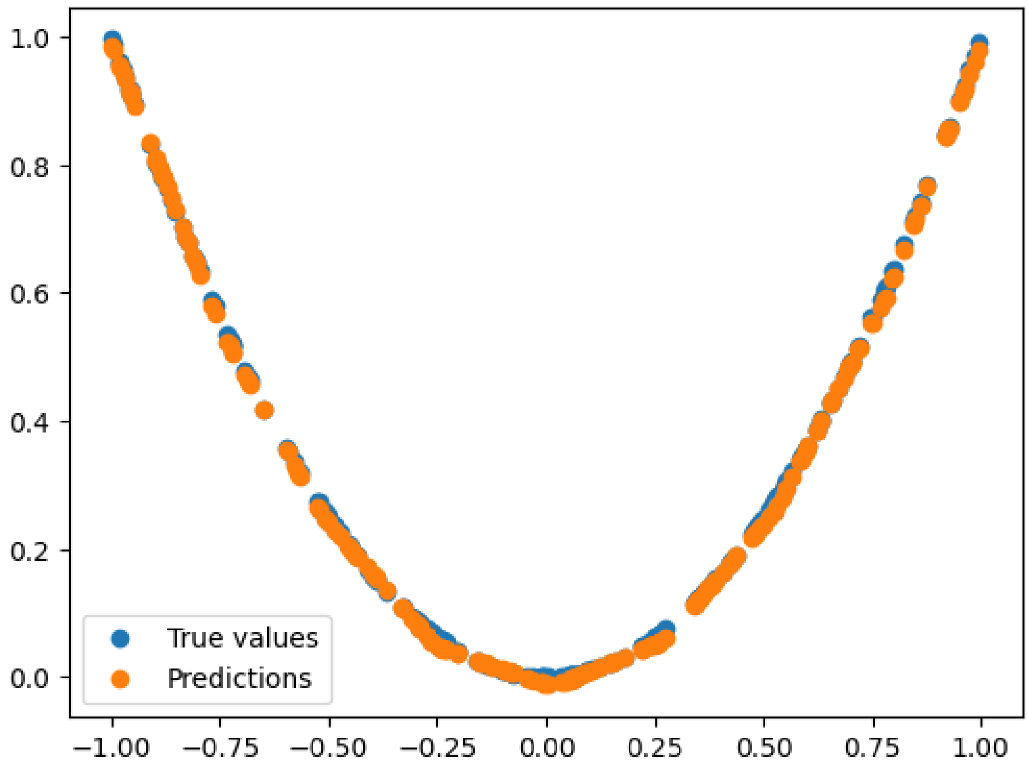
11.1 1D

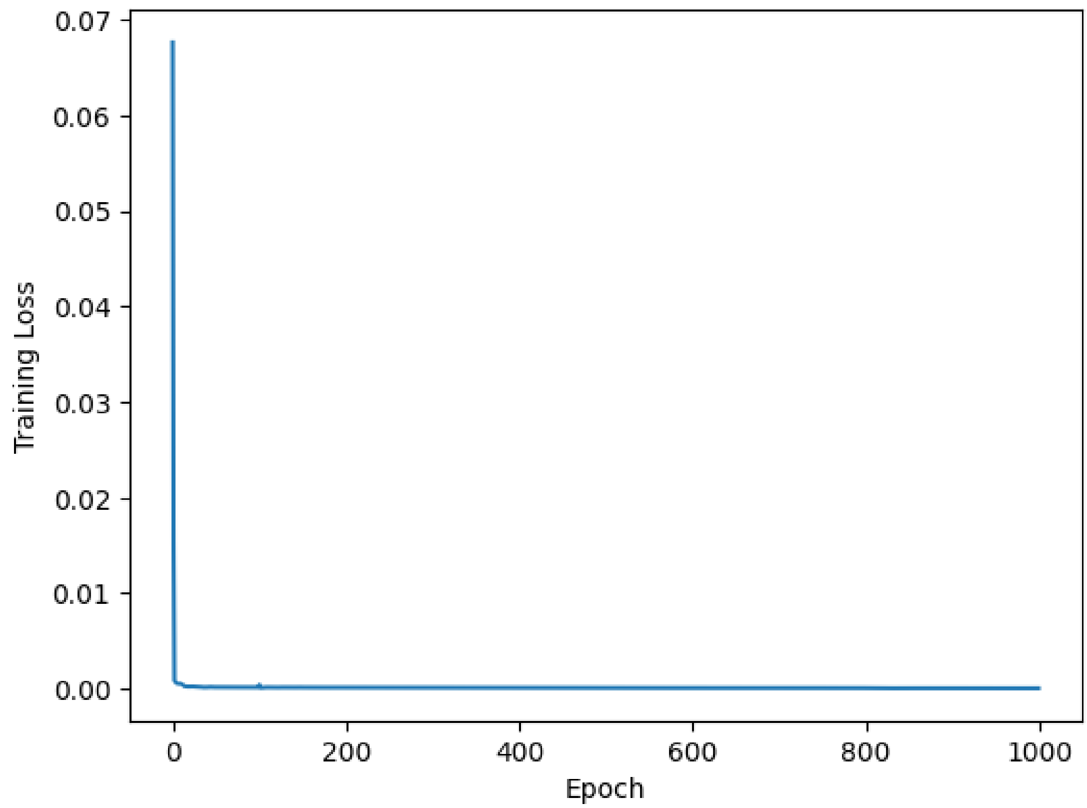
[ ]:
```
def fn_q10(x):
    return x**2
```

[ ]:
```
train_dataset_q10, test_dataset_q10 = create_dataset(np.random.uniform(-1, 1,␣
 ↪num_samples).reshape(-1, 1), fn_q10)

train_loader_q10 = DataLoader(train_dataset_q10, batch_size=16)
test_loader_q10 = DataLoader(test_dataset_q10, batch_size=16)
```

[ ]:
```
net_q10 = Net_general(1, 5, 2)
criterion_q10 = nn.MSELoss()
optimizer_q10 = torch.optim.Adam(net_q10.parameters(), lr=0.01)
outputs_q10, train_losses_q10, test_losses_q10 = train_and_evaluate(optimizer=␣
 ↪optimizer_q10, net= net_q10, criterion= criterion_q10, train_loader=␣
 ↪train_loader_q10, test_loader= test_loader_q10)

# Plot the test predictions vs true values
print(f'Test Loss: {test_losses_q10:.6f}')
plot_losses_and_predictions(test_dataset_q10, train_losses_q10, outputs_q10)
```

```
Test Loss: 0.000049
R2 Score: 0.999491
Test Loss: 0.000049
```


True values
Predictions
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
1.00



[ ]:
```
def get_direction_vector(net):
    directions=[torch.randn(w.size()) for w in net.parameters()]
    directions_dict={name:direction.to(device) for name, direction in␣
 ↪zip(dict(net.named_parameters()).keys(), directions)}
    for (name, direction),param in zip(directions_dict.items(), net.
 ↪named_parameters()):
        if "bias" in name:
            directions_dict[name] = param[1]
            continue
        direction = direction / torch.norm(direction, dim=1,␣
 ↪keepdim=True)*torch.norm(param[1], dim=1, keepdim=True)
        directions_dict[name] = direction
    directions_vec = torch.cat([v.flatten() for v in directions_dict.values()])
    return directions_vec
```

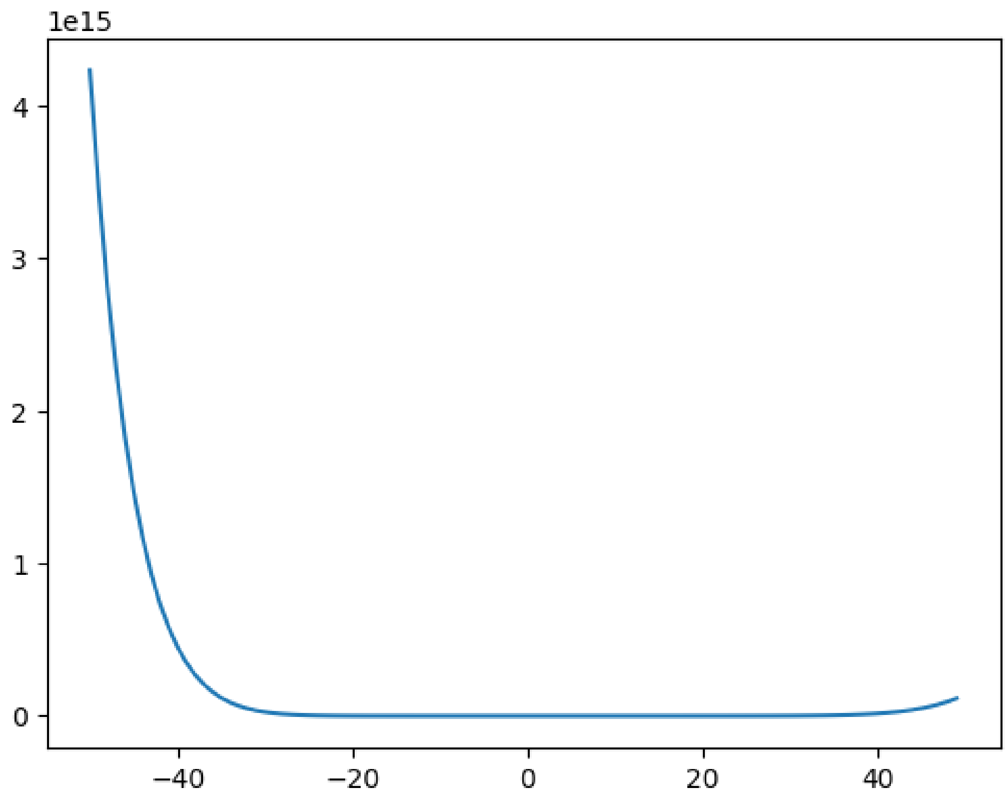
[ ]:
```
params_learnt_q10 = Params2Vec(net_q10.parameters())
directions_vec = get_direction_vector(net_q10)
```

[ ]:
```
losses_q10_1d = []
eval_net_q10 = Net_general(1, 5, 4)
criterion_q10 = nn.MSELoss()
```

```
test_loss = 0.0
for alpha in torch.arange(-50, 50, 1):
    test_loss = 0.0
    with torch.no_grad():
      for inputs, targets in test_loader_q10:
        Vec2Params( alpha * directions_vec + params_learnt_q10 ,  eval_net_q10.
 ↪parameters())
        eval_net_q10.eval()
        preds_1d = eval_net_q10(inputs.float())
        loss = criterion_q10(preds_1d, targets)
        test_loss += loss.item()
      losses_q10_1d.append(test_loss)
```

[ ]:
```
plt.plot(torch.arange(-50, 50, 1), losses_q10_1d)
```

[ ]: [<matplotlib.lines.Line2D at 0x1a71459f0>]



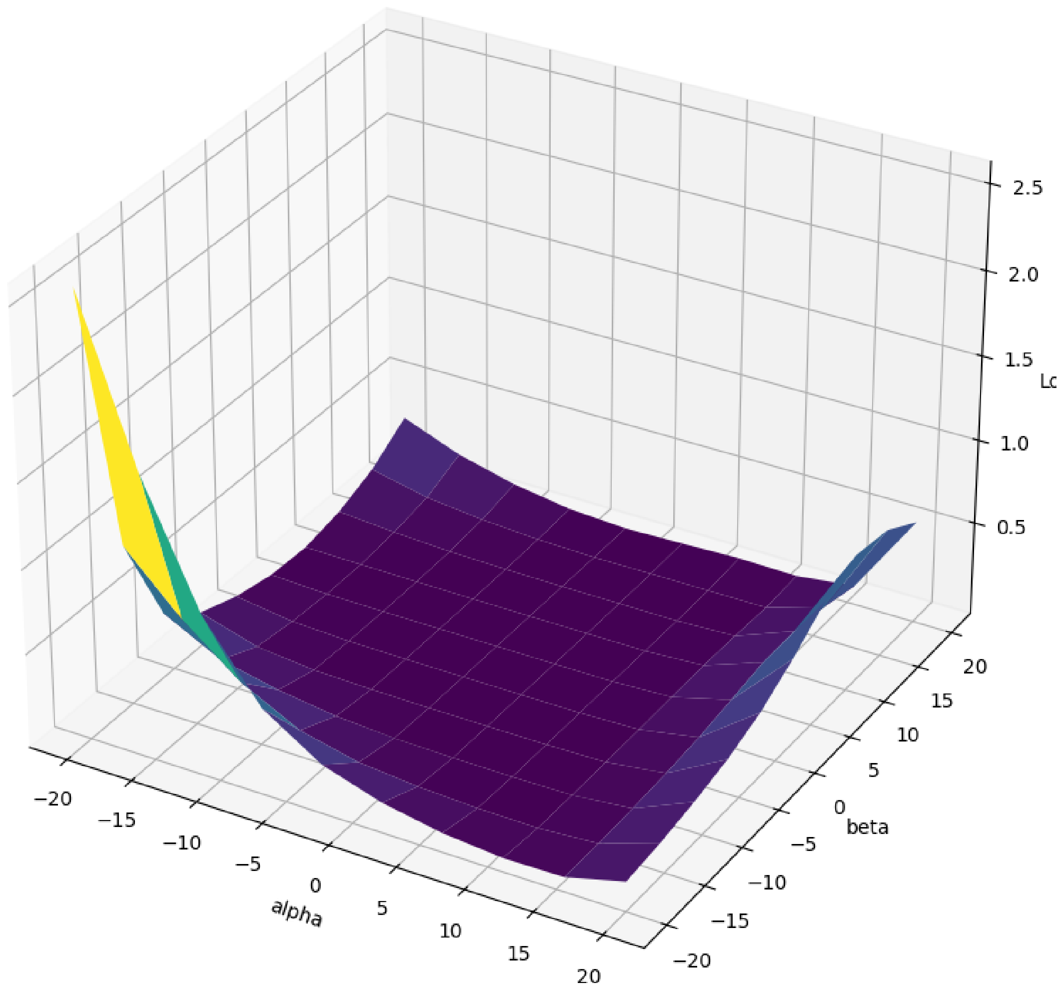
11.2 2D

[ ]:
```
directions_vec_1 = get_direction_vector(net_q10)
directions_vec_2 = get_direction_vector(net_q10)
```

11.2.1 method 1

[ ]:
```
range_q10_dim_2 = torch.linspace(-20, 20, 10)
alpha, beta = torch.meshgrid(range_q10_dim_2, range_q10_dim_2)

eval_2_net_q10 = Net_general(1, 5, 2)
criterion_q10 = nn.MSELoss()
test_loss = 0.0
losses_q10_dim_2 = []
for i,a in enumerate(alpha.flatten()):
        test_loss = 0.0
        with torch.no_grad():
          for inputs, targets in test_loader_q10:
            Vec2Params(  params_learnt_q10 + a * directions_vec_1 + beta.
 ↪flatten()[i] * directions_vec_2,  eval_2_net_q10.parameters())
            eval_2_net_q10.eval()
            pred_2d = eval_2_net_q10(inputs)
            loss = criterion_q10(pred_2d, targets)
            test_loss += loss.item()
          losses_q10_dim_2.append(test_loss)
```

[ ]:
```
fig = plt.figure(figsize=(20, 10))
ax = fig.add_subplot(111, projection='3d')
ax.plot_surface(alpha, beta, np.array(losses_q10_dim_2).reshape( alpha.shape ),␣
 ↪cmap='viridis')
ax.set_xlabel('alpha')
ax.set_ylabel('beta')
ax.set_zlabel('Loss')
plt.show()
```



12 Q11

[ ]:
```
nu = 0.01/np.pi # Viscosity
N_u = 100 # Number of Initial and Boundary data points
N_f = 10000 # Number of residual point
Nmax=  5 #20000


dat = scipy.io.loadmat('./burgers_shock.mat')

t = dat['t'].flatten()[:,None]
x = dat['x'].flatten()[:,None]
```

```python
Exact = np.real(dat['usol']).T
X, T = np.meshgrid(x,t)
X_star = np.hstack((X.flatten()[:,None], T.flatten()[:,None]))
u_star = Exact.flatten()[:,None]

X_star = torch.from_numpy(X_star) # t.tensor(X_star).float()
u_star = torch.from_numpy(u_star) # t.tensor(u_star).float()

X_star.requires_grad = True
u_star.requires_grad = True

lb = X_star.min(0)
ub = X_star.max(0)

xx1 = np.hstack((X[0:1,:].T, T[0:1,:].T))
uu1 = Exact[0:1,:].T

xx1= torch.from_numpy(xx1).float() # t.tensor(xx1).float()
uu1= torch.from_numpy(uu1).float() # t.tensor(uu1).float()

xx2 = np.hstack((X[:,0:1], T[:,0:1]))
uu2 = Exact[:,0:1]

xx2= torch.from_numpy(xx2).float() # t.tensor(xx2).float()
uu2= torch.from_numpy(uu2).float() # t.tensor(uu2).float()

xx3 = np.hstack((X[:,-1:], T[:,-1:]))
uu3 = Exact[:,-1:]

xx3= torch.from_numpy(xx3).float() # t.tensor(xx3).float()
uu3= torch.from_numpy(uu3).float() # t.tensor(uu3).float()
```

[ ]:
```python
def get_derivative(y, x):
    dydx = torch.autograd.grad(
        y, x, torch.ones(x.size()[0], 1), create_graph=True, retain_graph=True
    )[0]

    return dydx

def train_pinn(net, criterion, optimizer, train_loader, num_epochs=100):
    train_losses = []
    net.train()
    for epoch in range(num_epochs):
        epoch_loss = 0
        for inputs, targets in train_loader:
            optimizer.zero_grad()
            outputs = net(inputs)
```

```
            dy_dx = get_derivative(outputs, inputs)
            dy_dx_dx = get_derivative(dy_dx[:,0].reshape(-1,1), inputs)
            op_1 = net(xx1)
            op_2 = net(xx2)
            op_3 = net(xx3)

            loss = criterion( outputs, targets) + \
                    criterion(op_1, uu1) + \
                    criterion(op_2, uu2) + \
                    criterion(op_3, uu3) + \
                    criterion(
                        ( dy_dx[:,1] + outputs.reshape(-1) * dy_dx[:,0] - (0.1/
 ↪torch.pi) * dy_dx_dx[:,0] ).reshape(-1,1),
                        torch.zeros( dy_dx[:,0].size()[0], 1 )
                     )
            loss.backward(retain_graph=True)
            optimizer.step()
            epoch_loss += loss.item()

        if epoch % 10 == 0:
            print(f'Epoch {epoch} Loss: {epoch_loss}')
        train_losses.append(epoch_loss / len(train_loader))

    return train_losses

def test_pinn(net, criterion, test_loader, activations=False):
    net.eval()
    test_loss = 0
    all_outputs = []
    with torch.no_grad():
        for inputs, targets in test_loader:
            outputs = net(inputs, activations=activations)
            loss = criterion(outputs, targets)
            test_loss += loss.item()
            all_outputs.append(outputs)
            # all_targets.append(targets)
    test_loss /= len(test_loader)
    # print('Test Loss: %.6f' % test_loss)

    return torch.cat(all_outputs), test_loss
```

[ ]:
```
def dataset_pinn(x, y, test_size=0.2):
    x_train, x_test, y_train, y_test = train_test_split(x, y,␣
 ↪test_size=test_size, random_state=42)
    train_dataset = TensorDataset(x_train.float(), y_train.float())
    test_dataset = TensorDataset(x_test.float(), y_test.float())
```

```
    return train_dataset, test_dataset
```

[ ]:
```
def plot_pinn(test_dataset, train_losses, outputs):
    # plt.plot(test_dataset.tensors[0][1].detach().numpy(), test_dataset.
 ↪tensors[1][1].detach().numpy(), 'o' ,label='True values')
    # plt.plot(test_dataset.tensors[0][1].detach().numpy(), outputs.numpy(),␣
 ↪'o' ,label='Predictions')
    # plt.legend()
    # plt.show()

    plt.figure()
    plt.plot(train_losses)
    plt.xlabel('Epoch')
    plt.ylabel('Training Loss')
    plt.show()
```

[ ]:
```
train_dataset_q11, test_dataset_q11 = dataset_pinn(X_star, u_star, test_size=0.
 ↪2)

train_loader_q11 = DataLoader(train_dataset_q11, batch_size=1000)
test_loader_q11 = DataLoader(test_dataset_q11, batch_size=1000)

net_q11 = Net_general(2, 20, 4, activation_function=torch.tanh)
criterion_q11 = nn.MSELoss()
optimizer_q11 = optim.Adam(net_q11.parameters(), lr=0.001)

train_losses_q11 = train_pinn(net_q11, criterion_q11, optimizer_q11,␣
 ↪train_loader_q11)
```

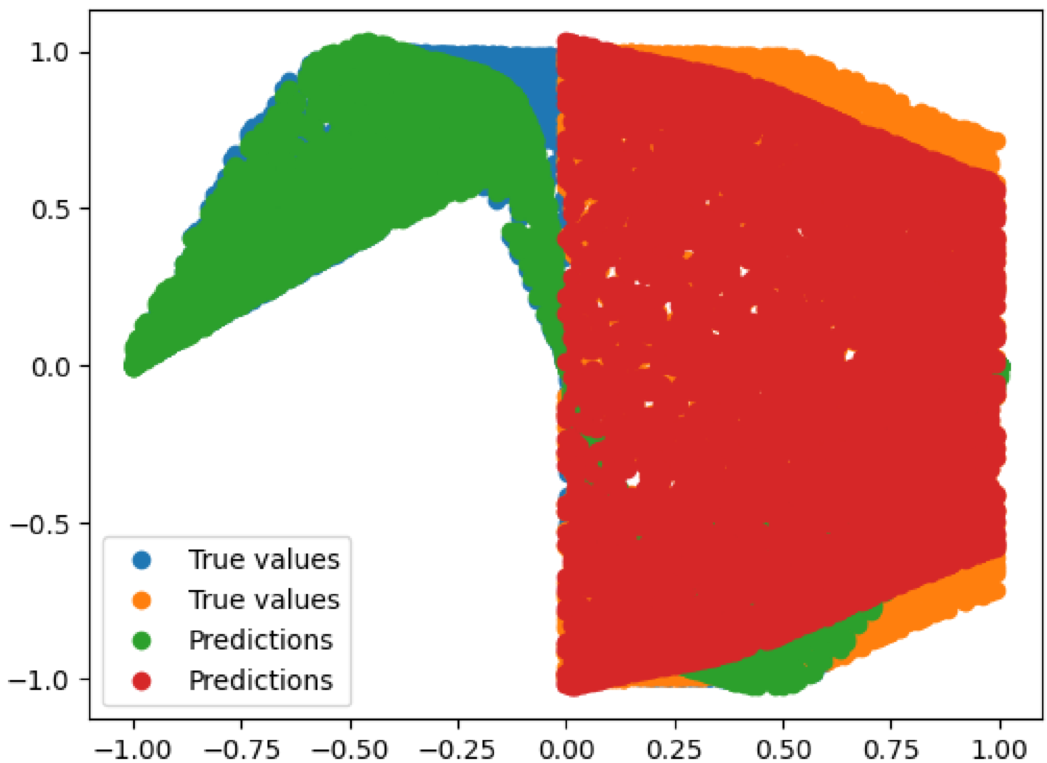
```
Epoch 0 Loss: 17.516550302505493
Epoch 10 Loss: 3.776117727160454
Epoch 20 Loss: 1.7877108454704285
Epoch 30 Loss: 1.1737946048378944
Epoch 40 Loss: 0.7277551665902138
Epoch 50 Loss: 0.5748756993561983
Epoch 60 Loss: 0.508511470630765
Epoch 70 Loss: 0.473147626966238
Epoch 80 Loss: 0.4463872164487839
Epoch 90 Loss: 0.42470825649797916
```

[ ]:
```
outputs_q11, test_loss_q11 = test_pinn(net_q11, criterion_q11, test_loader_q11)
```

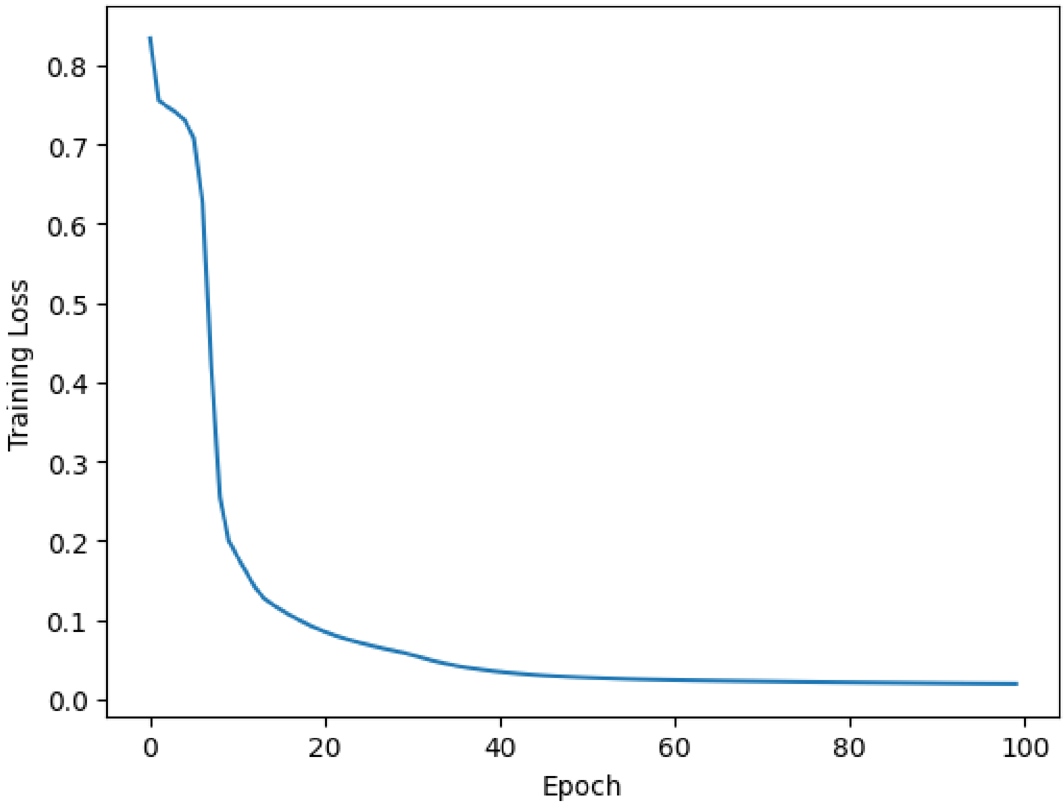
```
Test Loss: 0.014295
```

[ ]:
```
print('Test loss: %.6f' % test_loss_q11)
plot_pinn(test_dataset_q11, train_losses_q11, outputs_q11)
```

```
Test loss: 0.014295
```

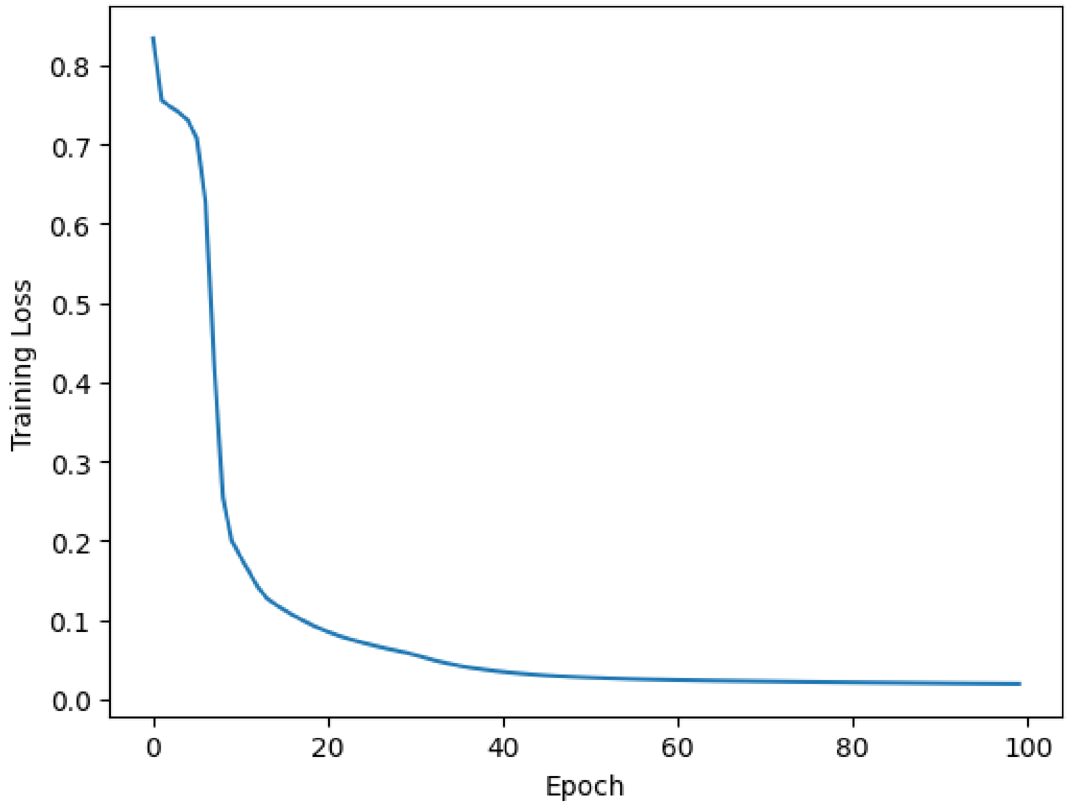


1.0
0.5
0.0
−0.5
−1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
True values
True values
Predictions
Predictions




```
[ ]: print('Test loss: %.6f' % test_loss_q11)
     plot_pinn(test_dataset_q11, train_losses_q11, outputs_q11)
```

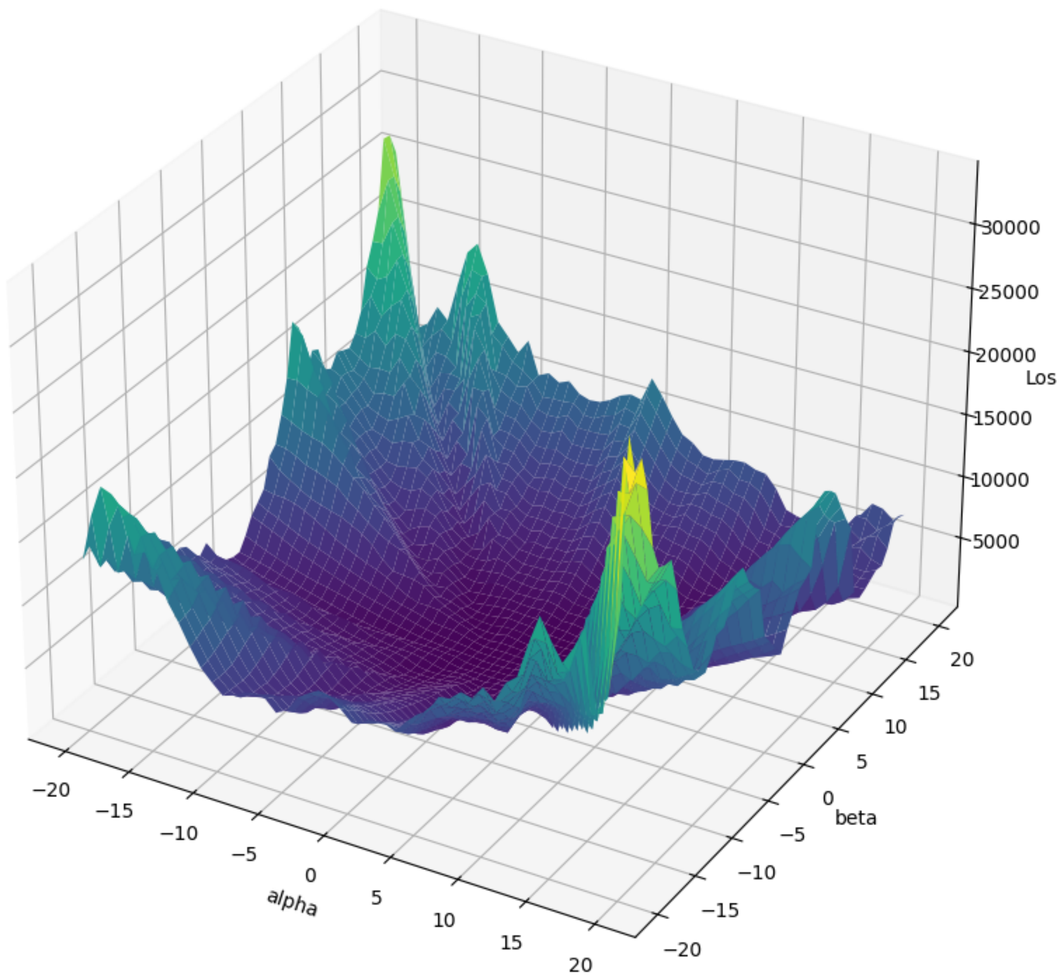
```
Test loss: 2341.047852
```




```
[ ]: params_learnt_q11 = Params2Vec(net_q11.parameters())
     directions_vec_1_q11 = get_direction_vector(net_q11)
     directions_vec_2_q11 = get_direction_vector(net_q11)

     range_q11 = torch.linspace(-20, 20, 50)
     alpha, beta = torch.meshgrid(range_q11, range_q11)

     eval_net_q11 = Net_general(2, 20, 4, activation_function=torch.tanh)
     criterion_q11 = nn.MSELoss()
     test_loss = 0.0
     lls_q11 = []
     for i,a in enumerate(alpha.flatten()):
             test_loss = 0.0
             with torch.no_grad():
               for inputs, targets in test_loader_q10:
                 Vec2Params(  params_learnt_q11 + a * directions_vec_1_q11 + beta.
      ↪flatten()[i] * directions_vec_2_q11,  eval_net_q11.parameters())
                 preds_q11, loss = test_pinn( eval_net_q11 , criterion_q11,␣
      ↪test_loader_q11)
                 test_loss += loss
               lls_q11.append(test_loss)
```

[ ]:

```
fig = plt.figure(figsize=(20, 10))
ax = fig.add_subplot(111, projection='3d')
ax.plot_surface(alpha, beta, np.array(lls_q11).reshape( alpha.shape ),␣
 ↪cmap='viridis')
ax.set_xlabel('alpha')
ax.set_ylabel('beta')
ax.set_zlabel('Loss')
plt.show()
```



q3_tensorflow-2

February 27, 2024

[ ]:
```
import tensorflow as tf
from tensorflow.keras import layers
from sklearn.model_selection import train_test_split
import numpy as np
import matplotlib.pyplot as plt
```

[ ]:
```
# define the model
model = tf.keras.Sequential([
    layers.Dense(50, activation='relu', input_shape=(1,)),
    layers.Dense(50, activation='relu'),
    layers.Dense(1)
])

model.compile(optimizer=tf.keras.optimizers.Adam(0.01),
              loss=tf.keras.losses.MeanSquaredError())
```

[ ]:
```
# generate data for uniform sampling
num_samples = 1000
x = np.linspace(-1, 1, num_samples).reshape(-1, 1)
y = 1 / (1 + 25 * x**2)

x_train, x_test, y_train, y_test = train_test_split(x, y, test_size=0.2,␣
 ↪random_state=42)
```

[ ]:
```
# train the model
history = model.fit(x_train, y_train, epochs=1000, batch_size=32, verbose=1)
```

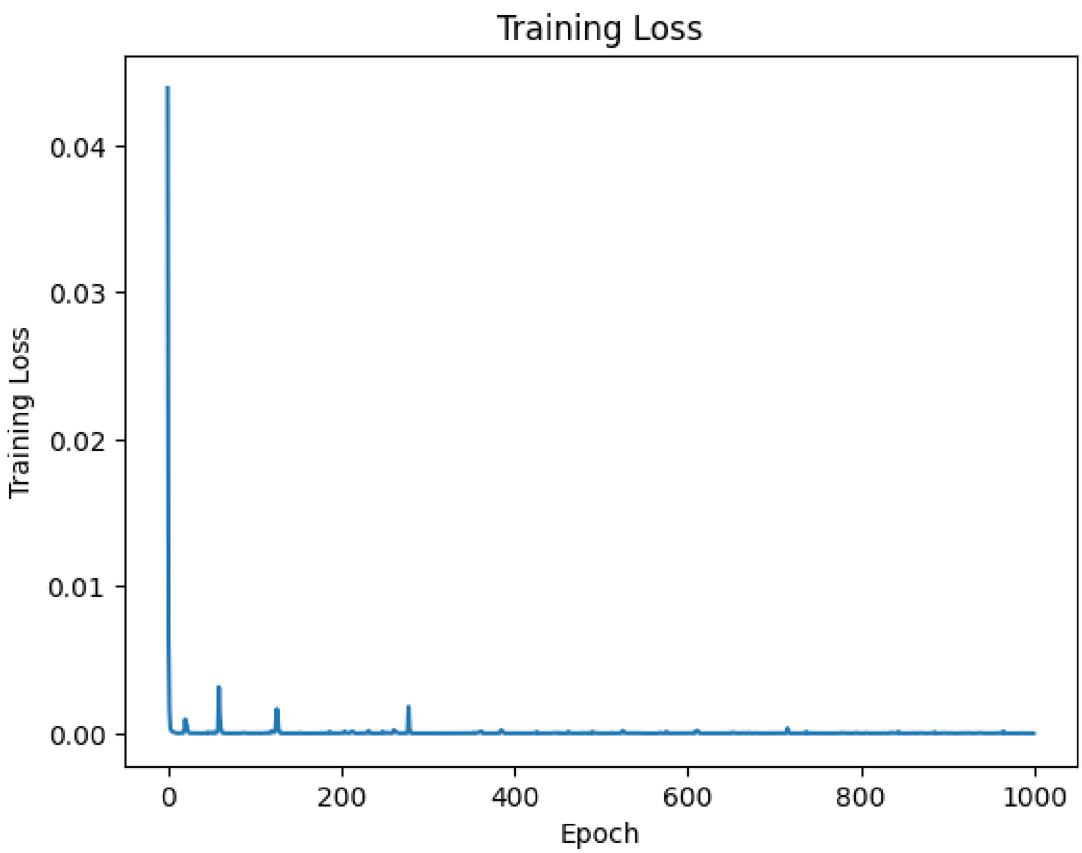
[ ]:
```
# evaluate the model
test_loss = model.evaluate(x_test, y_test, verbose=0)
print('Test Loss: %.6f' % test_loss)
```

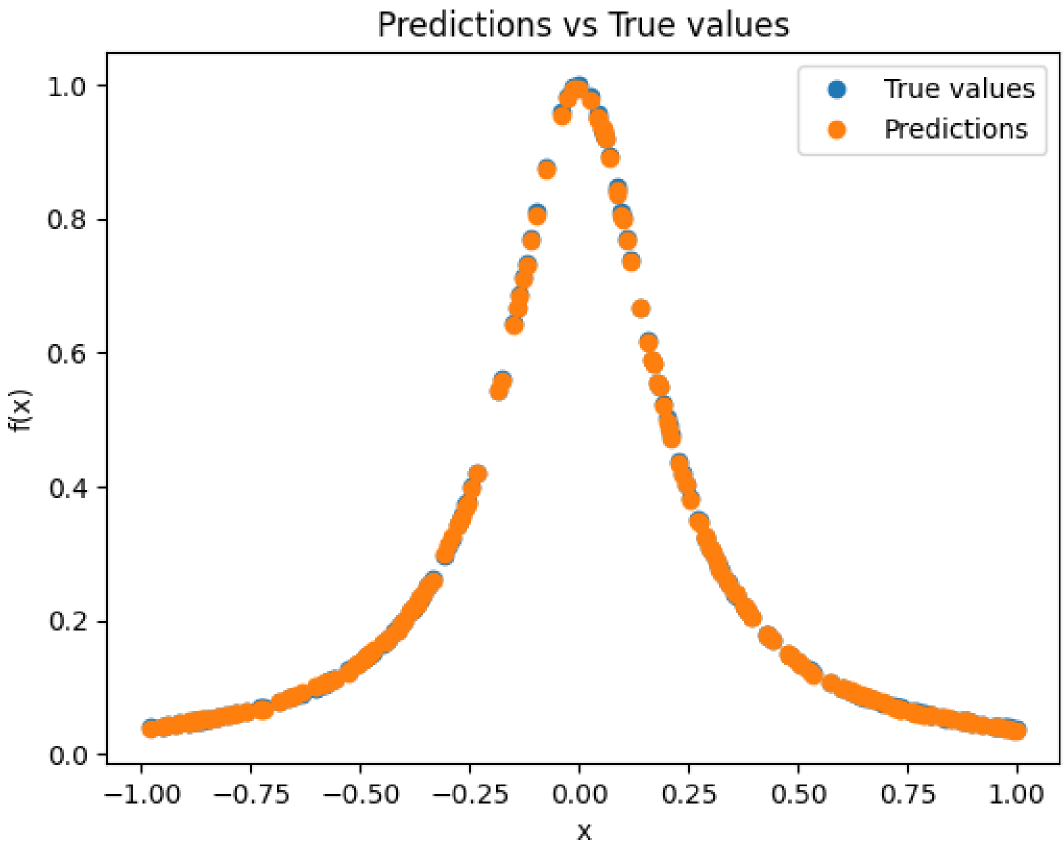
```
Test Loss: 0.000004
```

[ ]:
```
# predictions
outputs = model.predict(x_test)
```

```
7/7 [==============================] - 0s 1ms/step
```

[ ]:
```
plt.figure()
plt.plot(history.history['loss'])
plt.xlabel('Epoch')
plt.ylabel('Training Loss')
plt.title('Training Loss')
plt.show()

plt.figure()
plt.plot(x_test, y_test, 'o' ,label='True values')
plt.plot(x_test, outputs, 'o' ,label='Predictions')
plt.xlabel('x')
plt.ylabel('f(x)')
plt.title('Predictions vs True values')
plt.legend()
plt.show()
```




Predictions vs True values
True values
Predictions
f(x)
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
1.00