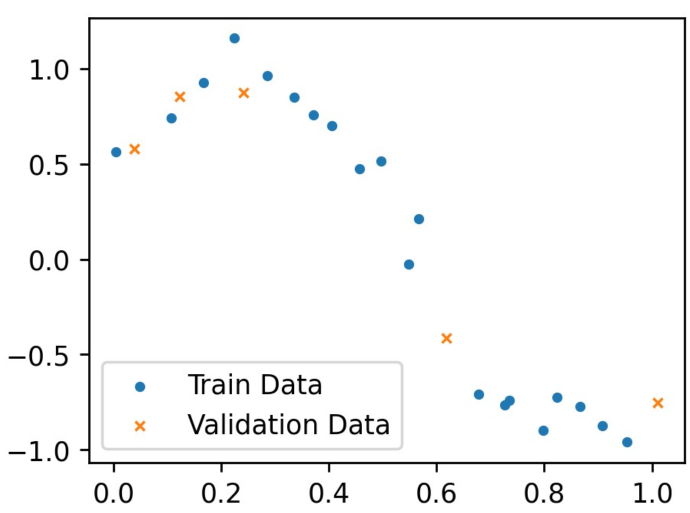
M8-L2 Problem 1

In this problem, you will create 3 regression networks with different complexities in PyTorch. By looking at the validation loss curves superimposed on the training loss curves, you should determine which model is optimal.

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

def generate_data():
    np.random.seed(5)
    N = 25
    x = np.random.normal(np.linspace(0,1,N),0.01).reshape(-1,1)
    y = np.random.normal(np.sin(5*(x+0.082)),0.2)
    train_mask = np.zeros(N,dtype=np.bool_)
    train_mask[np.random.permutation(N)[:int(N*0.8)]] = True
    train_x, val_x = torch.Tensor(x[train_mask]),
torch.Tensor(x[np.logical_not(train_mask)])
    train_y, val_y = torch.Tensor(y[train_mask]),
torch.Tensor(y[np.logical_not(train_mask)])

    return train_x, val_x, train_y, val_y

def train(model, lr=0.0001, epochs=10000):
    train_x, val_x, train_y, val_y = generate_data()
    opt = optim.Adam(model.parameters(),lr=lr)
    lossfun = nn.MSELoss()
    train_hist = []
    val_hist = []

    for _ in range(epochs):
        model.train()
        loss_train = lossfun(train_y, model(train_x))
        train_hist.append(loss_train.item())

        model.eval()
        loss_val = lossfun(val_y, model(val_x))
        val_hist.append(loss_val.item())

        opt.zero_grad()
        loss_train.backward()
        opt.step()

    train_hist, val_hist = np.array(train_hist), np.array(val_hist)
    return train_hist, val_hist
```

```
def plot_loss(train_loss, val_loss):
    plt.plot(train_loss,label="Training")
    plt.plot(val_loss,label="Validation",linewidth=1)
    plt.legend()
    plt.xlabel("Epoch")
    plt.ylabel("MSE Loss")

def plot_data(model = None):
    train_x, val_x, train_y, val_y = generate_data()
    plt.scatter(train_x, train_y,s=8,label="Train Data")
    plt.scatter(val_x, val_y,s=12,marker="x",label="Validation
Data",linewidths=1)

    if model is not None:
        xvals = torch.linspace(0,1,1000).reshape(-1,1)

plt.plot(xvals.detach().numpy(),model(xvals).detach().numpy(),label="M
odel",color="black")

    plt.legend(loc="lower left")

def get_loss(model):
    lossfun = nn.MSELoss()
    train_x, val_x, train_y, val_y = generate_data()
    loss_train = lossfun(train_y, model(train_x))
    loss_val = lossfun(val_y, model(val_x))
    return loss_train.item(), loss_val.item()


plt.figure(figsize=(4,3),dpi=250)
plot_data()
plt.show()
```



Coding neural networks for regression

Here, create 3 neural networks from scratch. You can use `nn.Sequential()` to simplify things. Each network should have 1 input and 1 output. After each hidden layer, apply ReLU activation. Name the models `model1`, `model2`, and `model3`, with architectures as follows:

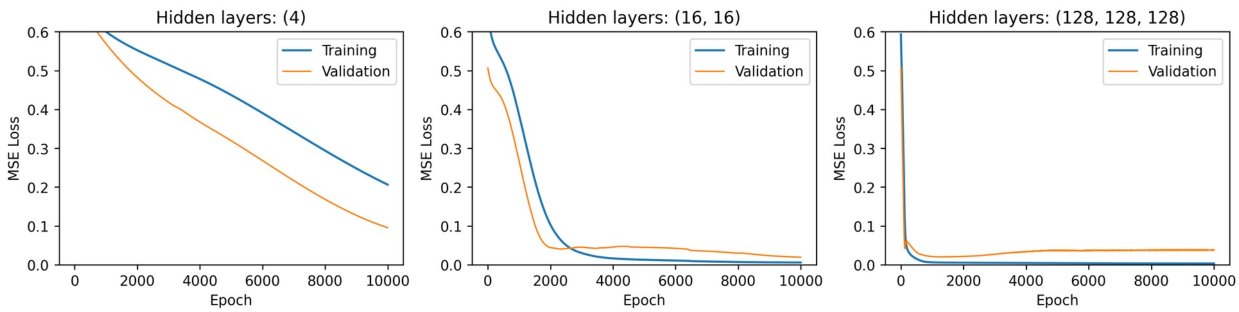
- `model1`: 1 hidden layer with 4 neurons. That is, the network should have a linear transformation from size 1 to size 4. Then a ReLU activation should be applied. Finally, a linear transformation from size 4 to size 1 gives the network output. (Note: Your regression network should not have an activation after the last layer!)
- `model2`: Hidden sizes (16, 16). (Two hidden layers, each with 16 neurons)
- `model3`: Hidden sizes (128, 128, 128). (3 hidden layers, each with 128 neurons)

```python
# YOUR CODE GOES HERE
# model1 (1 hidden layer with 4 neurons)
model1 = nn.Sequential(
    nn.Linear(1, 4),
    nn.ReLU(),
    nn.Linear(4, 1)
)

# model2 (2 hidden layers each with 16 neurons)
model2 = nn.Sequential(
    nn.Linear(1, 16),
    nn.ReLU(),
    nn.Linear(16, 16),
    nn.ReLU(),
    nn.Linear(16, 1)
)

# model3 (3 hidden layers each with 128 neurons)
model3 = nn.Sequential(
    nn.Linear(1, 128),
    nn.ReLU(),
    nn.Linear(128, 128),
    nn.ReLU(),
    nn.Linear(128, 128),
    nn.ReLU(),
    nn.Linear(128, 1)
)
```

Training and Loss curves

The following cell calls the provided function `train` to train each of your neural network models. The training and validation curves are then displayed.

```
hidden_layers=["(4)","(16, 16)","(128, 128, 128)"]

plt.figure(figsize=(15,3),dpi=250)
for i,model in enumerate([model1, model2, model3]):
    loss_train, loss_val = train(model)
    plt.subplot(1,3,i+1)
    plot_loss(loss_train, loss_val)
    plt.ylim(0,0.6)
    plt.title(f"Hidden layers: {hidden_layers[i]}")
plt.show()
```



Model performance

Let's print the values of MSE on the training and testing/validation data after training. Make note of which model is "best" (has lowest testing error).

```
for i, model in enumerate([model1, model2, model3]):
    train_loss, val_loss = get_loss(model)
    print(f"Model {i+1}, hidden layers {hidden_layers[i]:>15}:   Train
MSE: {train_loss:.4f}    Test MSE: {val_loss:.4f}")
```

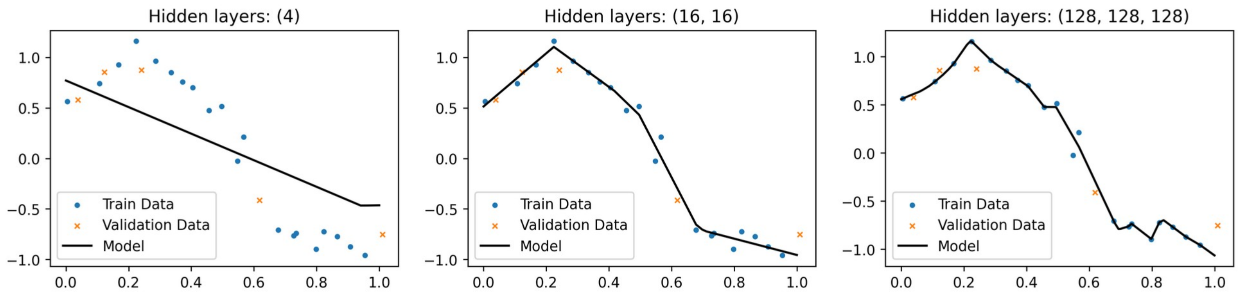
```
Model 1, hidden layers             (4):   Train MSE: 0.2061    Test
MSE: 0.0954
Model 2, hidden layers        (16, 16):   Train MSE: 0.0057    Test
MSE: 0.0192
Model 3, hidden layers (128, 128, 128):   Train MSE: 0.0031    Test
MSE: 0.0375
```

Visualization

Now we can look at how good each model's predictions are. Run the following cell to generate a visualization plot, then answer the questions.

```
plt.figure(figsize=(15,3),dpi=250)
for i,model in enumerate([model1, model2, model3]):
    plt.subplot(1,3,i+1)
    plot_data(model)
```

```
    plt.title(f"Hidden layers: {hidden_layers[i]}")
plt.show()
```



Questions

1. For the model that overfits the most, describe what happens to the loss curves while training.

   Model 3 (3 hidden layers each with 128 neurons) is the model that overfits the most. We can observe that its loss curves converge the fastest during training. The loss curve for train data also converges to a lower MSE compared to the loss curve for validation data. The loss curve for the train data is also very close to zero.

2. For the model that underfits the most, describe what happens to the loss curves while training.

   Model 1 (1 hidden layer with 4 neurons) is the model that underfits the most. We can observe that its loss curves converge the slowest during training. The loss curve for train data never converges to a smaller MSE compared to the loss curve for validation data. Furthermore, both MSE loss for training and validation data are relatively large.

3. For the "best" model, what happens to the loss curves while training?

   Model 2 (2 hidden layers each with 16 neurons) is the "best" model in our use case. The loss curves converge around the 2000 epoch, which is between Model 1 and Model 3. The loss curve for train data also converges to a lower MSE compared to the loss curve for validation data.