q_linearized_features

February 9, 2025

1 [HW1 - Q5] Visualizing features from local linearization of neural nets

[1]:
```
!pip install ipympl torchviz --quiet
!pip install torch --quiet
```

[2]:
```
import torch
import torch.nn as nn
import matplotlib.pyplot as plt
import numpy as np
import copy
import time
from torchvision.models.feature_extraction import create_feature_extractor
from ipywidgets import fixed, interactive, widgets
%matplotlib inline
```

[3]:
```
def to_torch(x):
    return torch.from_numpy(x).float()


def to_numpy(x):
    return x.detach().cpu().numpy()


def plot_data(X, y, X_test, y_test):
    clip_bound = 2.5
    plt.xlim(0, 1)
    plt.ylim(-clip_bound, clip_bound)
    plt.scatter(X[:, 0], y, c='darkorange', s=40.0, label='training data␣
↪points')
    plt.plot(X_test, y_test, '--', color='royalblue', linewidth=2.0,␣
↪label='Ground truth')


def plot_relu(bias, slope):
    plt.scatter([-bias / slope], 0, c='darkgrey', s=40.0)
    if slope > 0 and bias < 0:
```

```
        plt.plot([0, -bias / slope, 1], [0, 0, slope * (1 - bias)], ':')
    elif slope < 0 and bias > 0:
        plt.plot([0, -bias / slope, 1], [-bias * slope, 0, 0], ':')


def plot_relus(params):
    slopes = to_numpy(params[0]).ravel()
    biases = to_numpy(params[1])
    for relu in range(biases.size):
        plot_relu(biases[relu], slopes[relu])


def plot_function(X_test, net):
    y_pred = net(to_torch(X_test))
    plt.plot(X_test, to_numpy(y_pred), '-', color='forestgreen',␣
 ↪label='prediction')


def plot_update(X, y, X_test, y_test, net, state=None):
    if state is not None:
        net.load_state_dict(state)
    plt.figure(figsize=(10, 7))
    plot_relus(list(net.parameters()))
    plot_function(X_test, net)
    plot_data(X, y, X_test, y_test)
    plt.legend()
    plt.show();


def train_network(X, y, X_test, y_test, net, optim, n_steps, save_every,␣
 ↪device="cpu", initial_weights=None, verbose=False):
    loss = torch.nn.MSELoss()
    y_train = to_torch(y.reshape(-1, 1)).to(device=device)
    X_train = to_torch(X).to(device=device)

    y_test = to_torch(y_test.reshape(-1, 1)).to(device=device)
    X_test = to_torch(X_test).to(device=device)
    if initial_weights is not None:
        net.load_state_dict(initial_weights)
    history = {}
    for s in range(n_steps):
        perm = torch.randperm(y.size, device=device)
        subsample = perm[:y.size // 5]
        step_loss = loss(y_train[subsample], net(X_train[subsample, :]))
        optim.zero_grad()
        step_loss.backward()
        optim.step()
```

```
        if (s + 1) % save_every == 0 or s == 0:
            history[s + 1] = {}
            history[s + 1]['state'] = copy.deepcopy(net.state_dict())
            with torch.no_grad():
                test_loss = loss(y_test, net(X_test))
            history[s + 1]['train_error'] = to_numpy(step_loss).item()
            history[s + 1]['test_error'] = to_numpy(test_loss).item()
            if verbose:
                print("SGD Iteration %d" % (s + 1))
                print("\tTrain Loss: %.3f" % to_numpy(step_loss).item())
                print("\tTest Loss: %.3f" % to_numpy(test_loss).item())
            else:
                # Print update every 10th save point
                if (s + 1) % (save_every * 10) == 0:
                    print("SGD Iteration %d" % (s + 1))

    return history


def plot_test_train_errors(history):
    sample_points = np.array(list(history.keys()))
    etrain = [history[s]['train_error'] for s in history]
    etest = [history[s]['test_error'] for s in history]
    plt.plot(sample_points / 1e3, etrain, label='Train Error')
    plt.plot(sample_points / 1e3, etest, label='Test Error')
    plt.xlabel("Iterations (1000's)")
    plt.ylabel("MSE")
    plt.yscale('log')
    plt.legend()
    plt.show();


def make_iter_slider(iters):
    return widgets.SelectionSlider(
        options=iters,
        value=1,
        description='SGD Iterations: ',
        disabled=False
    )


def history_interactive(history, idx, X, y, X_test, y_test, net):
    plot_update(X, y, X_test, y_test, net, state=history[idx]['state'])
    plt.show()
    print("Train Error: %.3f" % history[idx]['train_error'])
    print("Test Error: %.3f" % history[idx]['test_error'])
```

```
def make_history_interactive(history, X, y, X_test, y_test, net):
    sample_points = list(history.keys())
    return interactive(history_interactive,
                       history=fixed(history),
                       idx=make_iter_slider(sample_points),
                       X=fixed(X),
                       y=fixed(y),
                       X_test=fixed(X_test),
                       y_test=fixed(y_test),
                       net=fixed(net))


%matplotlib inline
```

2 Generate Training and Test Data

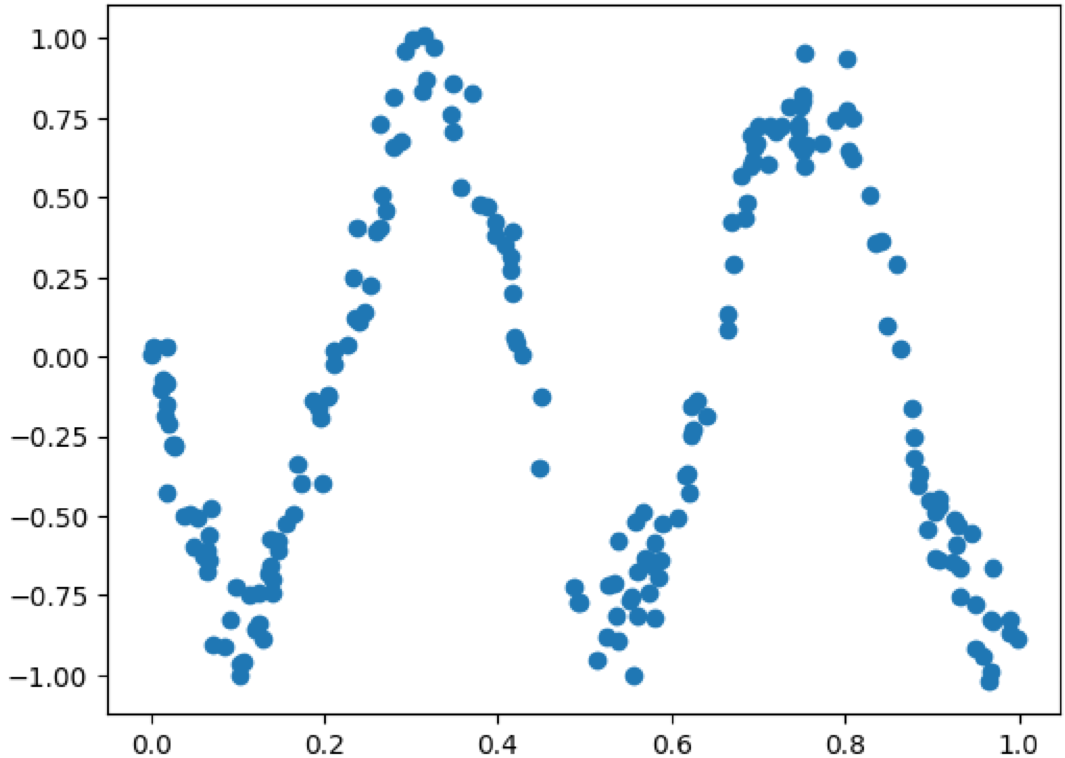
We are using piecewise linear function. Our training data has added noise $y = f(x)+\epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma^2)$. The test data is noise free.

Once you have gone through the discussion once you may wish to adjust the number of training samples and noise variance to see how gradient descent behaves under the new conditions.

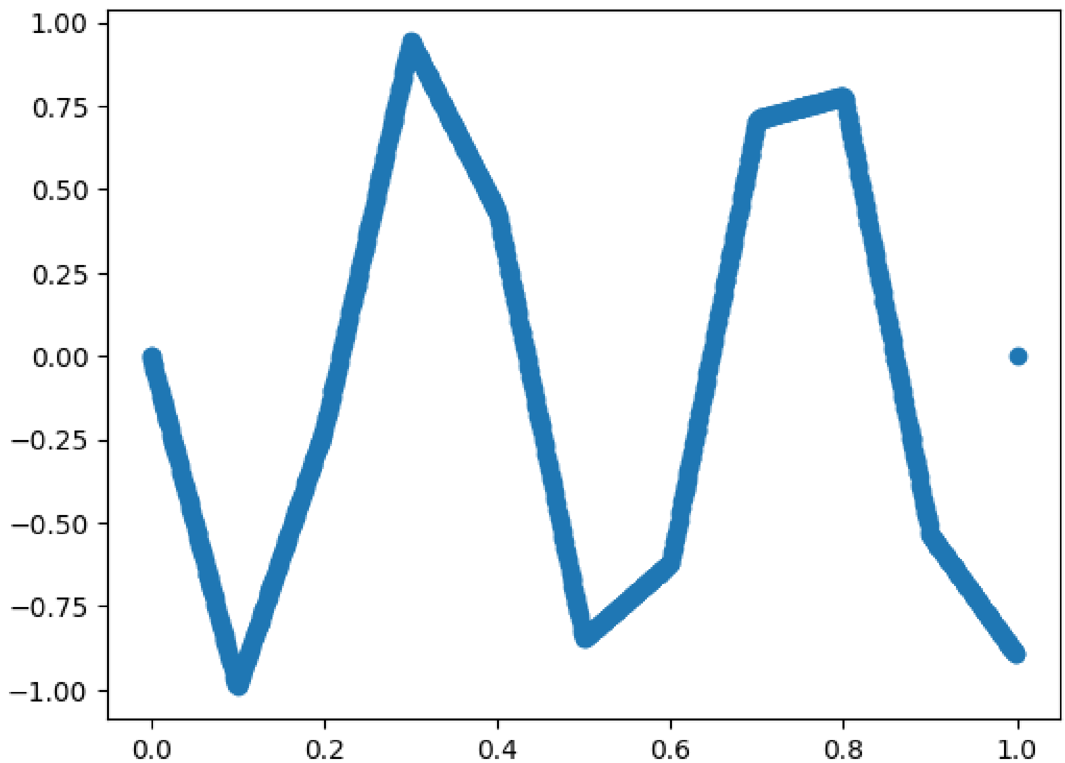
[4]:
```
f_type = 'piecewise_linear'

def f_true(X, f_type):
    if f_type == 'sin(20x)':
        return np.sin(20 * X[:,0])
    else:
        TenX = 10 * X[:,0]
        _ = 12345
        return (TenX - np.floor(TenX)) * np.sin(_ * np.ceil(TenX)) - (TenX - np.
 ↪ceil(TenX)) * np.sin(_ * np.floor(TenX))

n_features = 1
n_samples = 200
sigma = 0.1
rng = np.random.RandomState(1)

# Generate train data
X = np.sort(rng.rand(n_samples, n_features), axis=0)
y = f_true(X, f_type) + rng.randn(n_samples) * sigma

# Generate NOISELESS test data
X_test = np.concatenate([X.copy(), np.expand_dims(np.linspace(0., 1., 1000),␣
 ↪axis=1)])
X_test = np.sort(X_test, axis=0)
```

```python
y_test = f_true(X_test, f_type)
```

[5]:
```python
plt.scatter(X, y)
plt.show()
```



[6]:
```python
plt.scatter(X_test, y_test)
plt.show()
```



3 Define the Neural Networks

We will learn the piecewise linear target function using a simple 1-hidden layer neural network with ReLU non-linearity, defined by

$$\hat{y} = \mathbf{W}^{(2)}\Phi\left(\mathbf{W}^{(1)}x + \mathbf{b}^{(1)}\right) + \mathbf{b}^{(2)}$$

where $\Phi(x) = ReLU(x)$ and superscripts refer to indices, not the power operator.

We will also create two SGD optimizers to allow us to choose whether to train all parameters or only the linear output layer's parameters. Note that we use separate learning rates for the two version of training. There is too much variance in the gradients when training all layers to use a large learning rate, so we have to decrease it.

We will modify the default initialization of the biases so that the ReLU elbows are all inside the region we are interested in.

We create several versions of this network with varying widths to explore how hidden layer width impacts learning performance.

Once you have gone through the discussion once you may wish to train networks with even larger widths to see how they behave under the three different training paradigms in this notebook.

[7]:
```
# Don't rerun this cell after training or you will lose all your work
nets_by_size = {}
```

[8]:
```
widths = [10, 20, 40]
for width in widths:
    # Define a 1-hidden layer ReLU nonlinearity network
    net = nn.Sequential(nn.Linear(1, width),
                        nn.ReLU(),
                        nn.Linear(width, 1))
    loss = nn.MSELoss()
    # Get trainable parameters
    weights_all = list(net.parameters())
    # Get the output weights alone
    weights_out = weights_all[2:]
    # Adjust initial biases so elbows are in [0,1]
    elbows = np.sort(np.random.rand(width))
    new_biases = -elbows * to_numpy(weights_all[0]).ravel()
    weights_all[1].data = to_torch(new_biases)
    # Create SGD optimizers for outputs alone and for all weights
    lr_out = 0.2
    lr_all = 0.02
    opt_all = torch.optim.SGD(params=weights_all, lr=lr_all)
    opt_out = torch.optim.SGD(params=weights_out, lr=lr_out)
    # Save initial state for comparisons
    initial_weights = copy.deepcopy(net.state_dict())
    # print("Initial Weights", initial_weights)
    nets_by_size[width] = {'net': net, 'opt_all': opt_all,
                           'opt_out': opt_out, 'init': initial_weights}
```

[9]:
```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
for width, net in nets_by_size.items():
  net['net'].to(device=device)
```

[10]:
```
print(device)
```

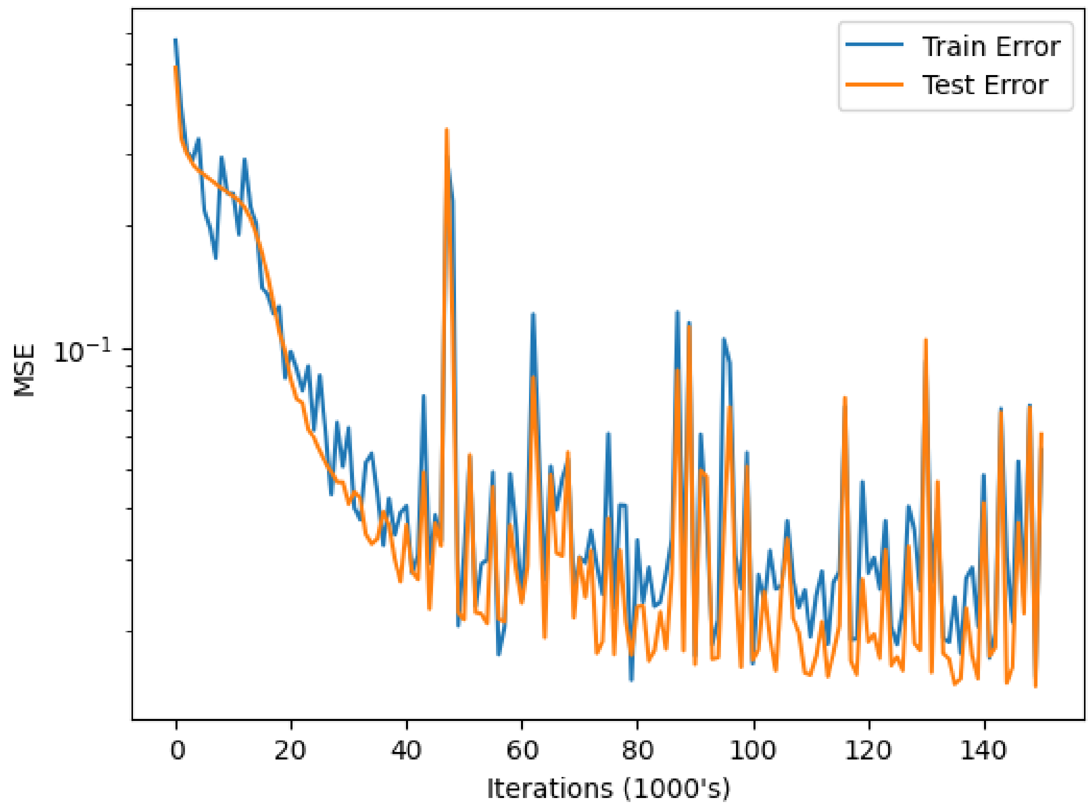
```
cuda
```

4 Train the neural networks

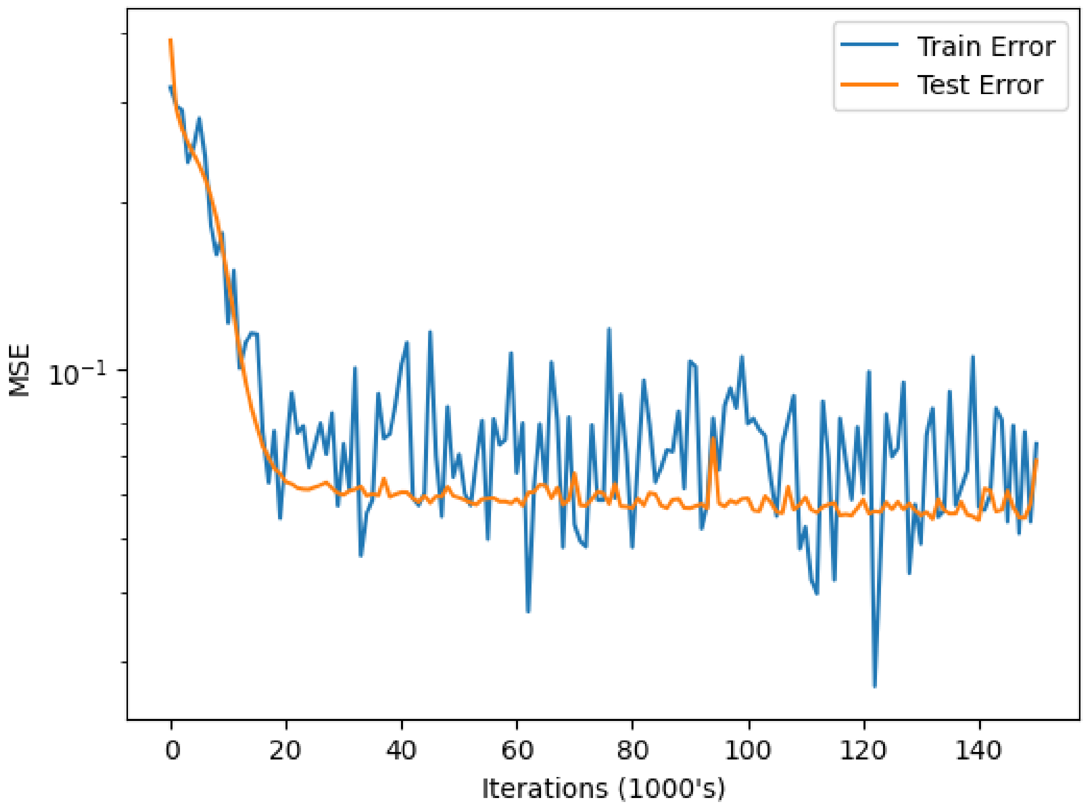
[11]:
```
n_steps = 150000
save_every = 1000
t0 = time.time()
for w in widths:
    print("-"*40)
    print("Width", w)
    new_net = nn.Sequential(nn.Linear(1, w),
                            nn.ReLU(),
                            nn.Linear(w, 1))
    new_net.load_state_dict(nets_by_size[w]['net'].state_dict().copy())
    new_net.to(device=device)
```

```python
    opt_all = torch.optim.SGD(params=new_net.parameters(), lr=lr_all)
    initial_weights = nets_by_size[w]['init']
    history_all = train_network(X, y, X_test, y_test,
                                new_net, optim=opt_all,
                                n_steps=n_steps, save_every=save_every,
                                initial_weights=initial_weights,
                                verbose=False, device=device)
    nets_by_size[w]['trained_net'] = new_net
    nets_by_size[w]['hist_all'] = history_all
    print("Width", w)
    plot_test_train_errors(history_all)
t1 = time.time()
print("-"*40)
print("Trained all layers in %.1f minutes" % ((t1 - t0) / 60))
```

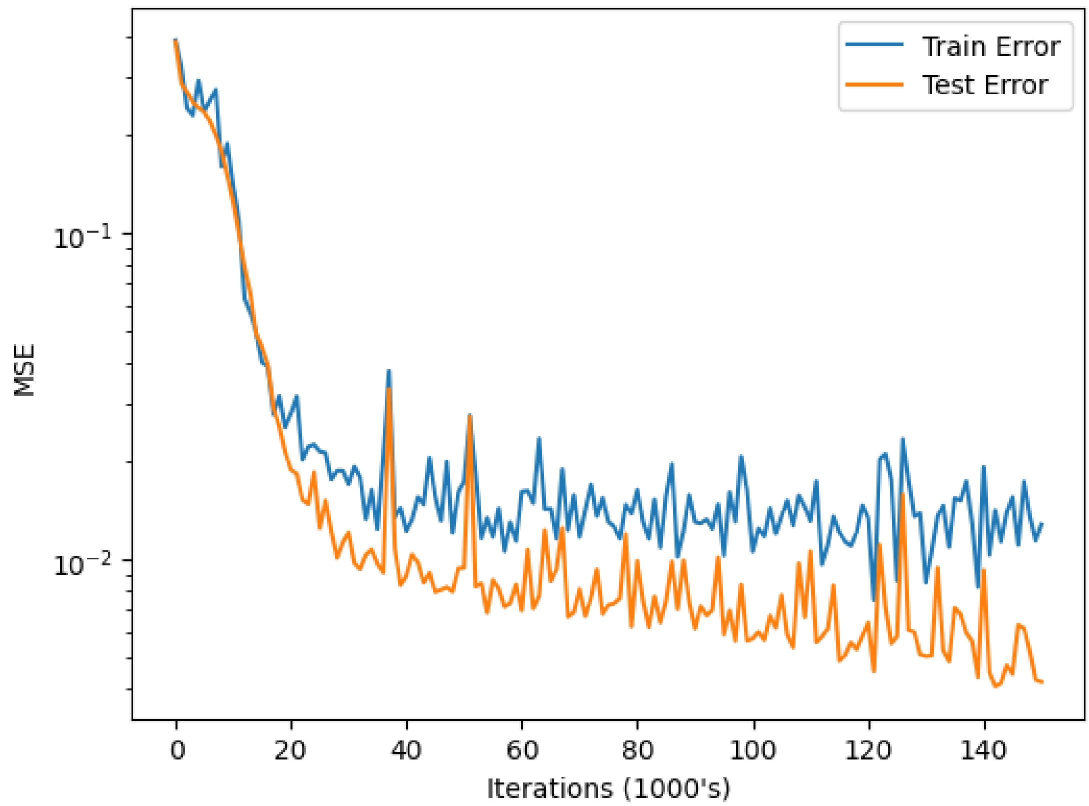
```
----------------------------------------
Width 10
SGD Iteration 10000
SGD Iteration 20000
SGD Iteration 30000
SGD Iteration 40000
SGD Iteration 50000
SGD Iteration 60000
SGD Iteration 70000
SGD Iteration 80000
SGD Iteration 90000
SGD Iteration 100000
SGD Iteration 110000
SGD Iteration 120000
SGD Iteration 130000
SGD Iteration 140000
SGD Iteration 150000
Width 10
```




```
----------------------------------------
Width 20
SGD Iteration 10000
SGD Iteration 20000
SGD Iteration 30000
SGD Iteration 40000
SGD Iteration 50000
SGD Iteration 60000
SGD Iteration 70000
SGD Iteration 80000
SGD Iteration 90000
SGD Iteration 100000
SGD Iteration 110000
SGD Iteration 120000
SGD Iteration 130000
SGD Iteration 140000
SGD Iteration 150000
Width 20
```




```
----------------------------------------
Width 40
SGD Iteration 10000
SGD Iteration 20000
SGD Iteration 30000
SGD Iteration 40000
SGD Iteration 50000
SGD Iteration 60000
SGD Iteration 70000
SGD Iteration 80000
SGD Iteration 90000
SGD Iteration 100000
SGD Iteration 110000
SGD Iteration 120000
SGD Iteration 130000
SGD Iteration 140000
SGD Iteration 150000
Width 40
```



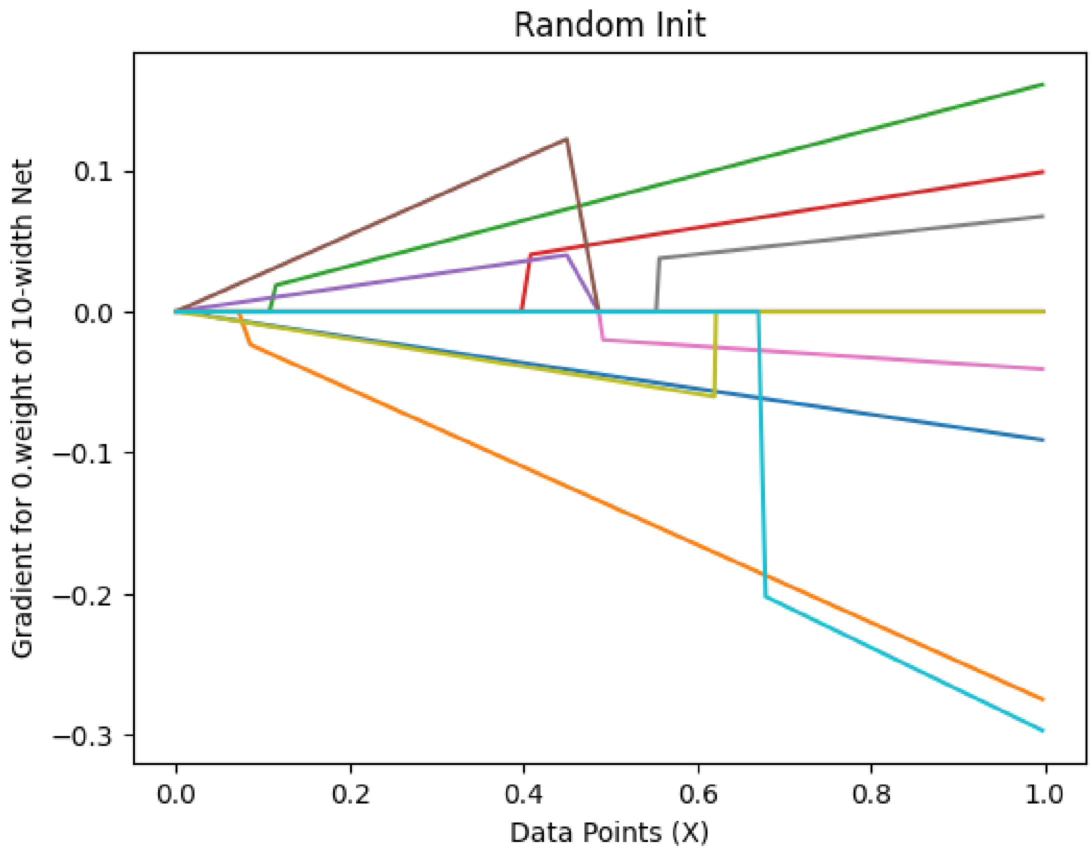

```
----------------------------------------
Trained all layers in 20.1 minutes
```

5 (a) Visualize Gradients

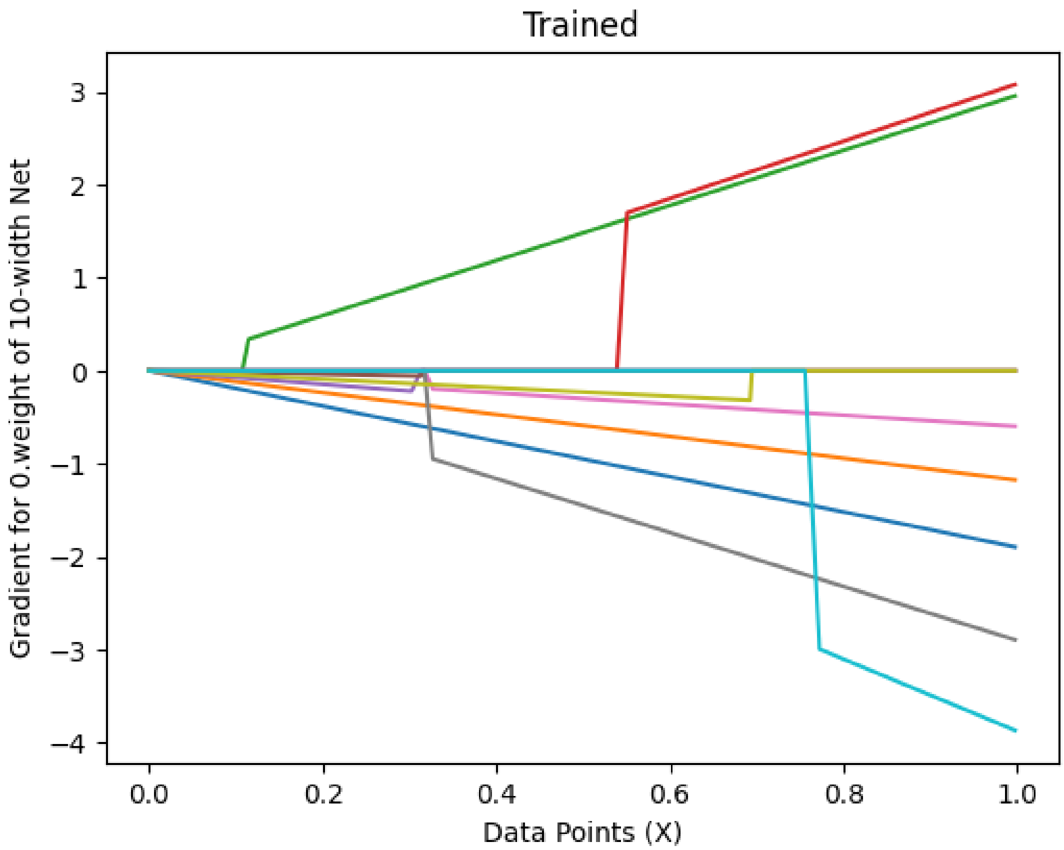
Visualize the features corresponding to $\frac{\partial}{\partial w_i^{(1)}} y(x)$ and $\frac{\partial}{\partial b_i^{(1)}} y(x)$ where $w_i^{(1)}$ are the first hidden layer's weights and the $b_i^{(1)}$ are the first hidden layer's biases. These derivatives should be evaluated at at least both the random initialization and the final trained network. When visualizing these features, plot them as a function of the scalar input x, the same way that the notebook plots the constituent "elbow" features that are the outputs of the penultimate layer.

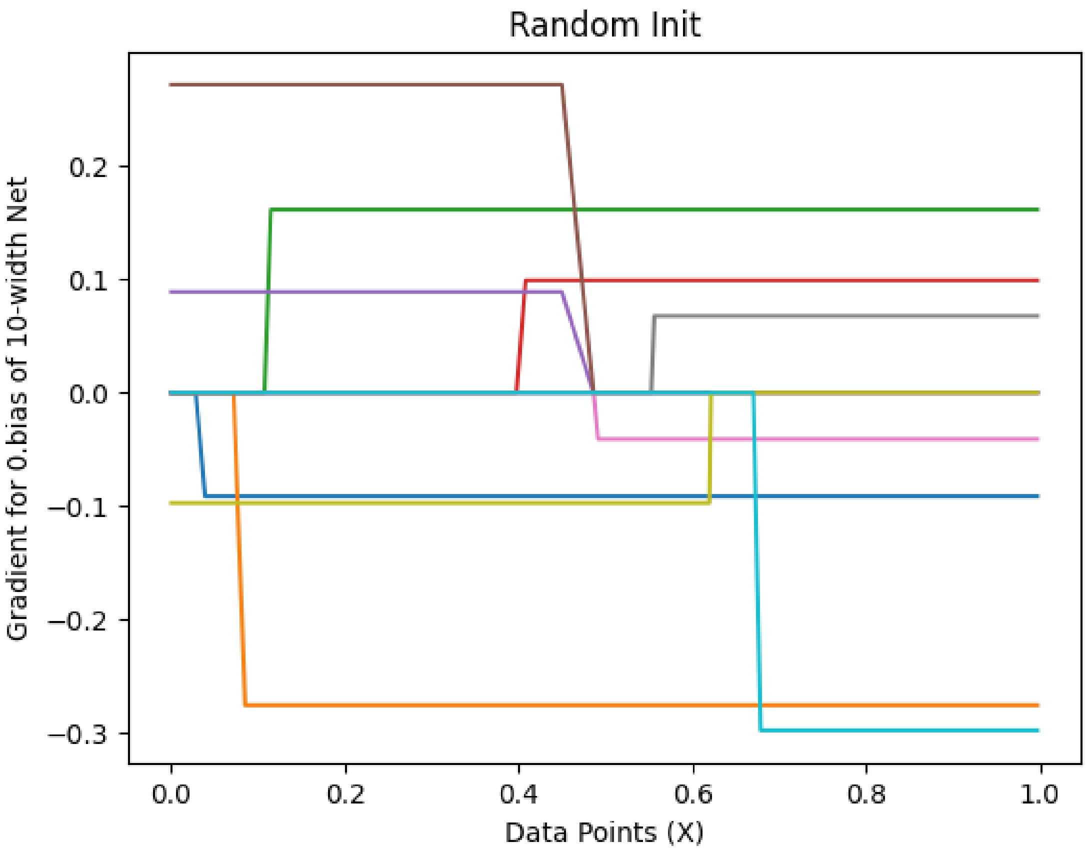
[12]:
```
def backward_and_plot_grad(X, model, vis_name='all', title='', legend=False):
    """
    Run backpropagation on `model` using `X` as the input
    to compute the gradient w.r.t. parameters of `y`,
    and then visualize collected gradients according to `vis_name`
    """
    width = model[0].out_features  # the width is the number of hidden units.
    gradients = np.zeros((width, X.shape[0]))
    num_pts = 0
```

```python
    gradient_collect, vis_collect = { }, { }
    for x in X:
        y = model(to_torch(x).to(device=device))

        ########################################################################
        # TODO: Complete the following part to run backpropagation. (2 lines)
        # Hint: Remember to set grad to zero before backpropagation
        ########################################################################
        # (YOUR CODE HERE)

        model.zero_grad()
        y.backward()

        ########################################################################

        # collect gradients from `p.grad.data`
        for n, p in model.named_parameters():
            for w_idx, w_grad in enumerate( p.grad.data.reshape(-1) ):
                if f'{n}.{w_idx}' not in gradient_collect:
                    gradient_collect[ f'{n}.{w_idx}' ] = {'x':[], 'y': []}
                if vis_name == 'all' or vis_name == n:
                    if f'{n}.{w_idx}' not in vis_collect:
                        vis_collect[f'{n}.{w_idx}'] = True
                gradient_collect[ f'{n}.{w_idx}' ]['y'].append( w_grad.item() )
                gradient_collect[ f'{n}.{w_idx}' ]['x'].append( x )

    for w_n in vis_collect:
        # we assume that X is sorted, so we use line plot
        plt.plot( X, gradient_collect[w_n]['y'], label=w_n )

    plt.xlabel('Data Points (X)')
    plt.ylabel(f'Gradient for {vis_name} of {width}-width Net')
    if legend:
        plt.legend()
    plt.title(title)
    plt.show()


for width in nets_by_size:
    backward_and_plot_grad(X, nets_by_size[width]['net'], '0.weight', 'Random␣
 ↪Init')
    backward_and_plot_grad(X, nets_by_size[width]['trained_net'], '0.weight',␣
 ↪'Trained')
    backward_and_plot_grad(X, nets_by_size[width]['net'], '0.bias', 'Random␣
 ↪Init')
    backward_and_plot_grad(X, nets_by_size[width]['trained_net'], '0.bias',␣
 ↪'Trained')
```

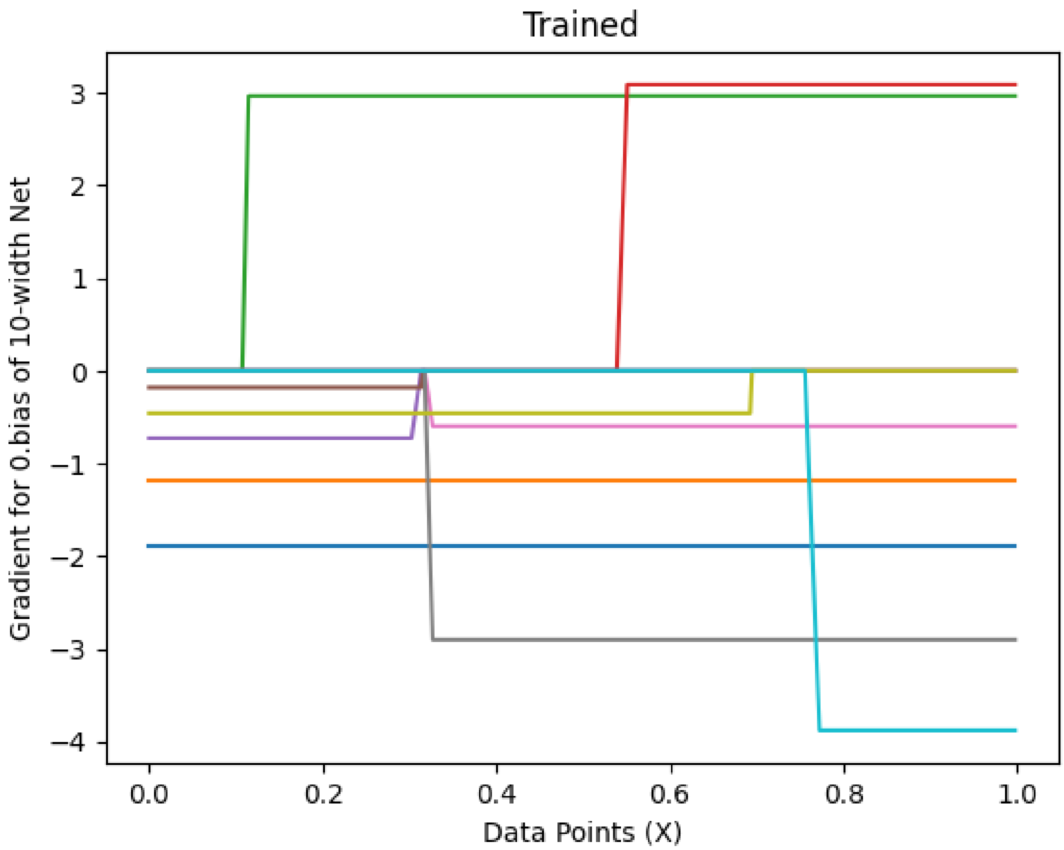


Random Init
Gradient for 0.weight of 10-width Net
0.1
0.0
−0.1
−0.2
−0.3
0.0
0.2
0.4
0.6
0.8
1.0
Data Points (X)

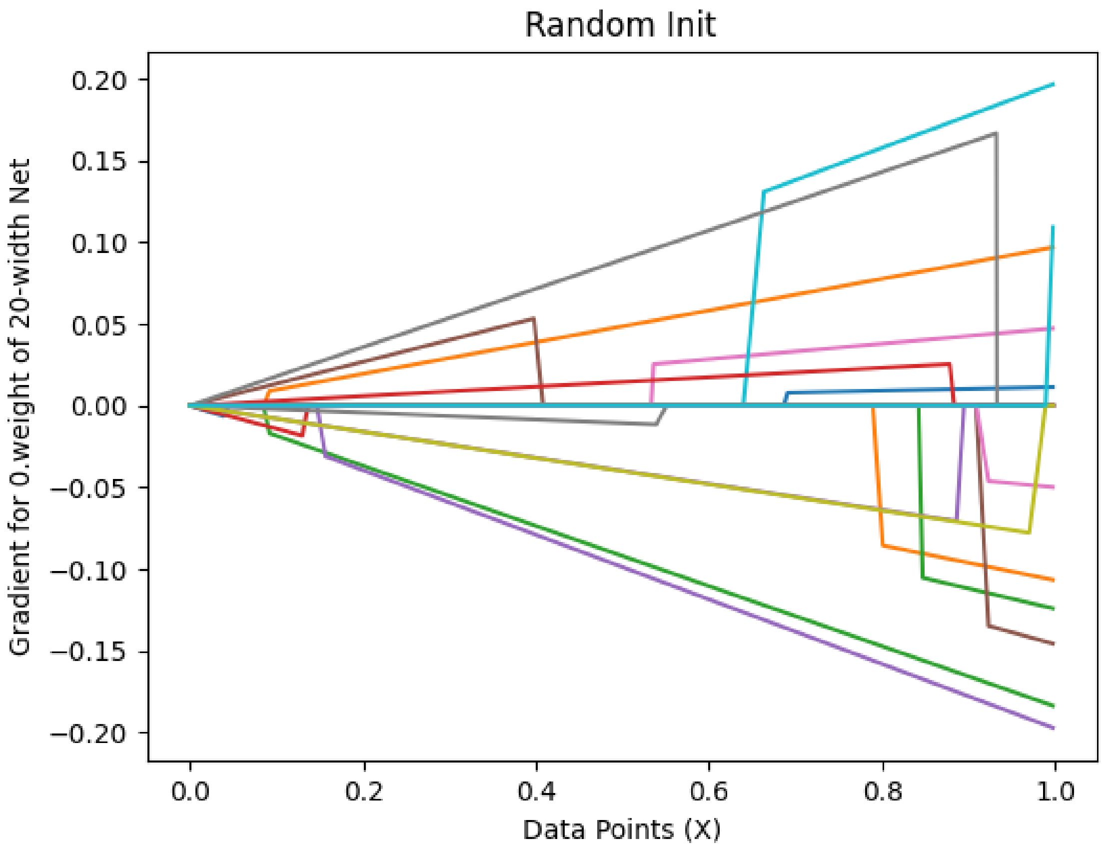

Trained
Gradient for 0.weight of 10-width Net
Data Points (X)
3
2
1
0
−1
−2
−3
−4
0.0
0.2
0.4
0.6
0.8
1.0

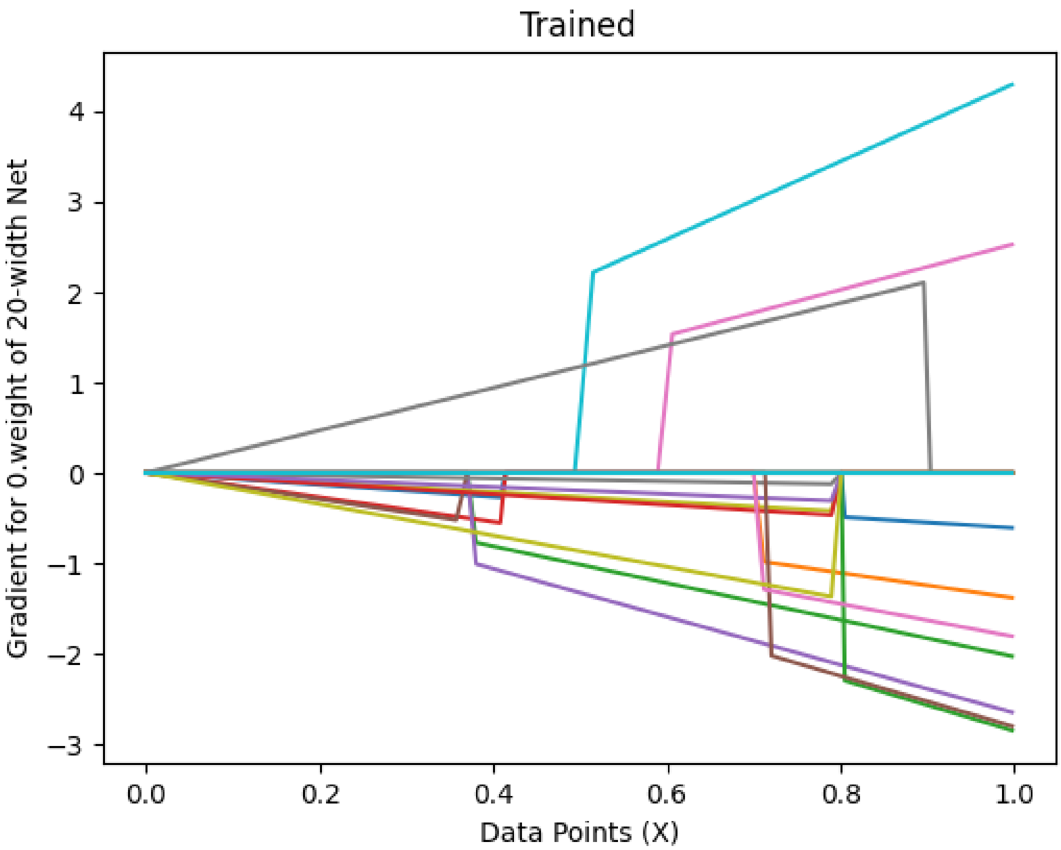


Random Init
Gradient for 0.bias of 10-width Net
0.2
0.1
0.0
−0.1
−0.2
−0.3
0.0
0.2
0.4
0.6
0.8
1.0
Data Points (X)

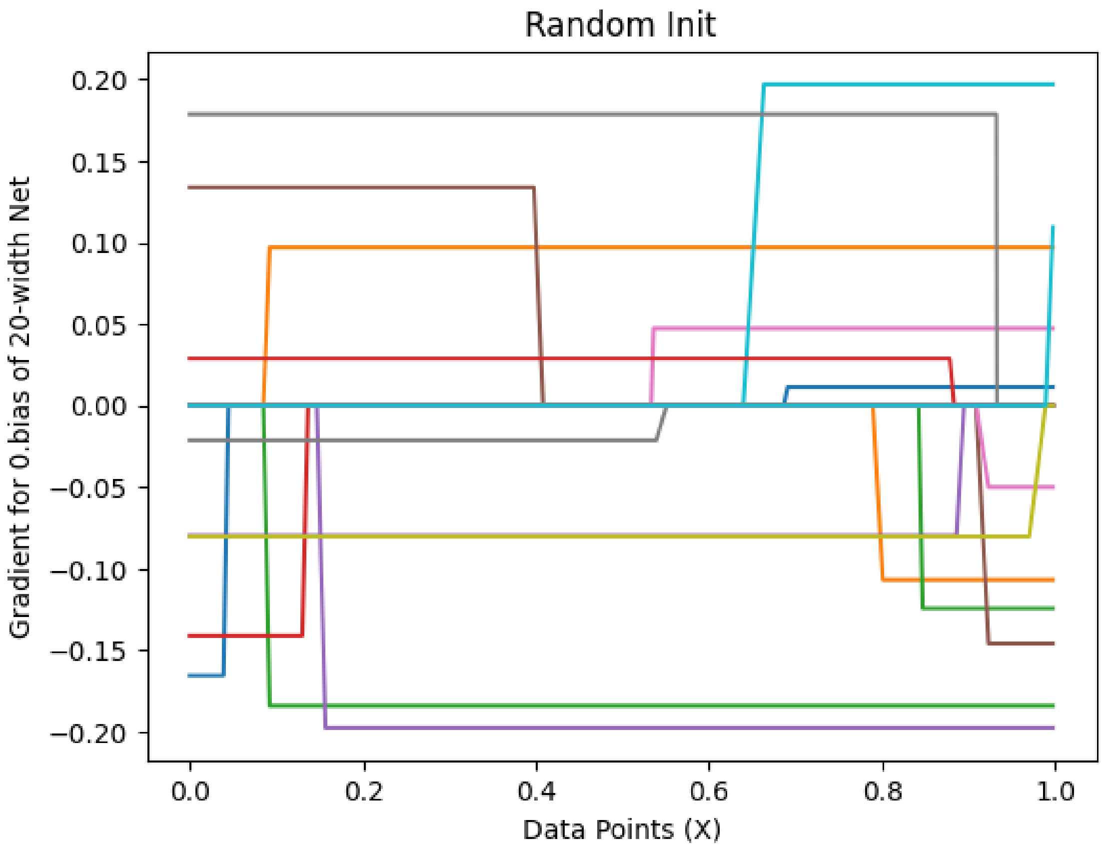


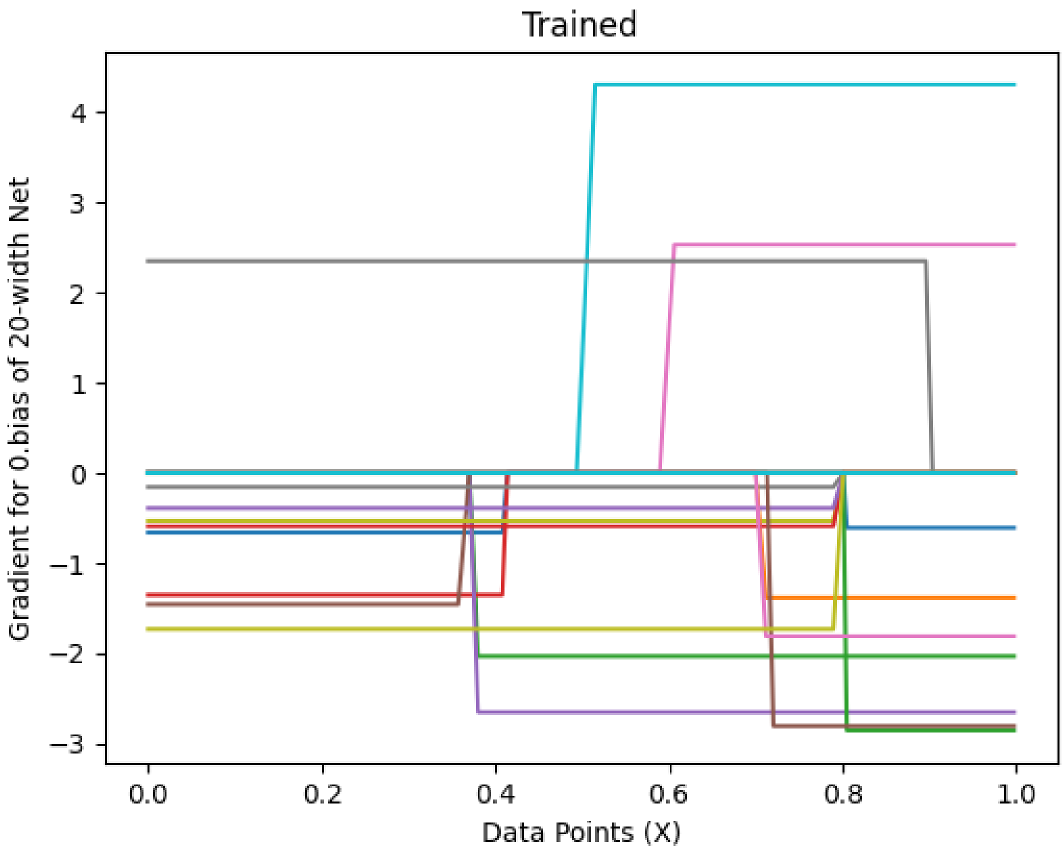
Trained
Gradient for 0.bias of 10-width Net
Data Points (X)
3
2
1
0
−1
−2
−3
−4
0.0
0.2
0.4
0.6
0.8
1.0

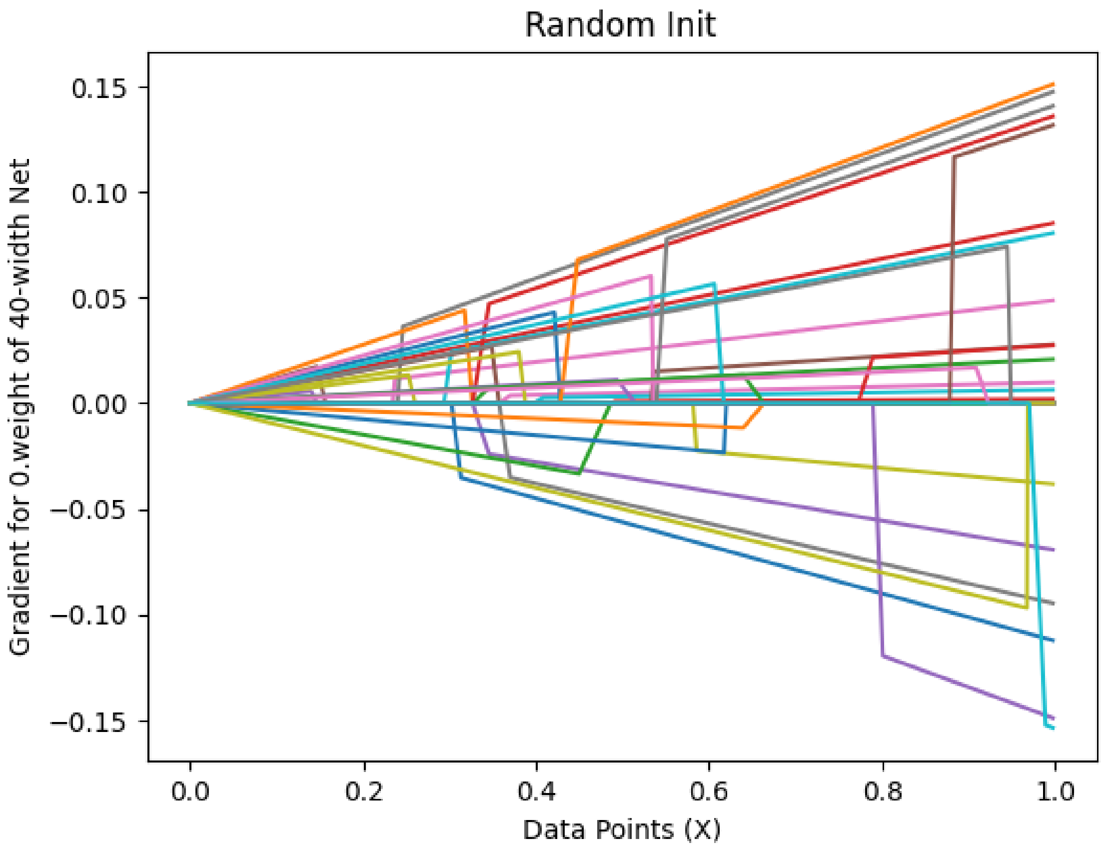

Random Init
Gradient for 0.weight of 20-width Net
Data Points (X)
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0.0
0.2
0.4
0.6
0.8
1.0

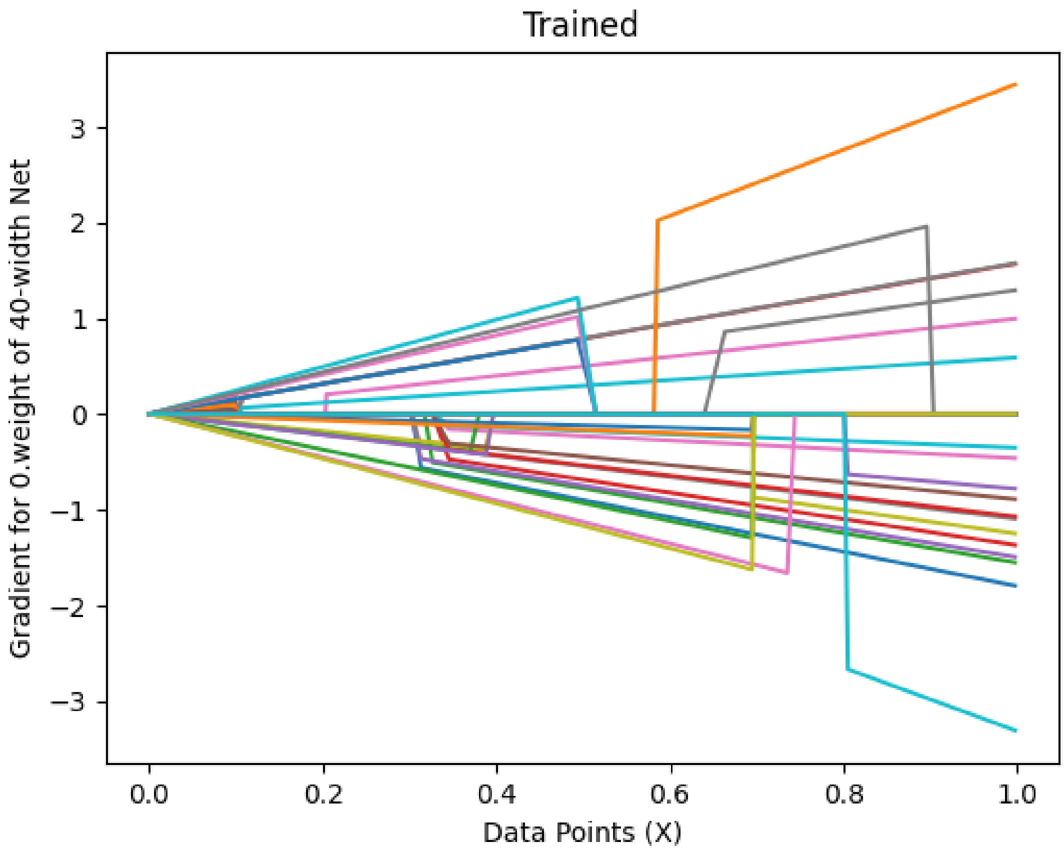


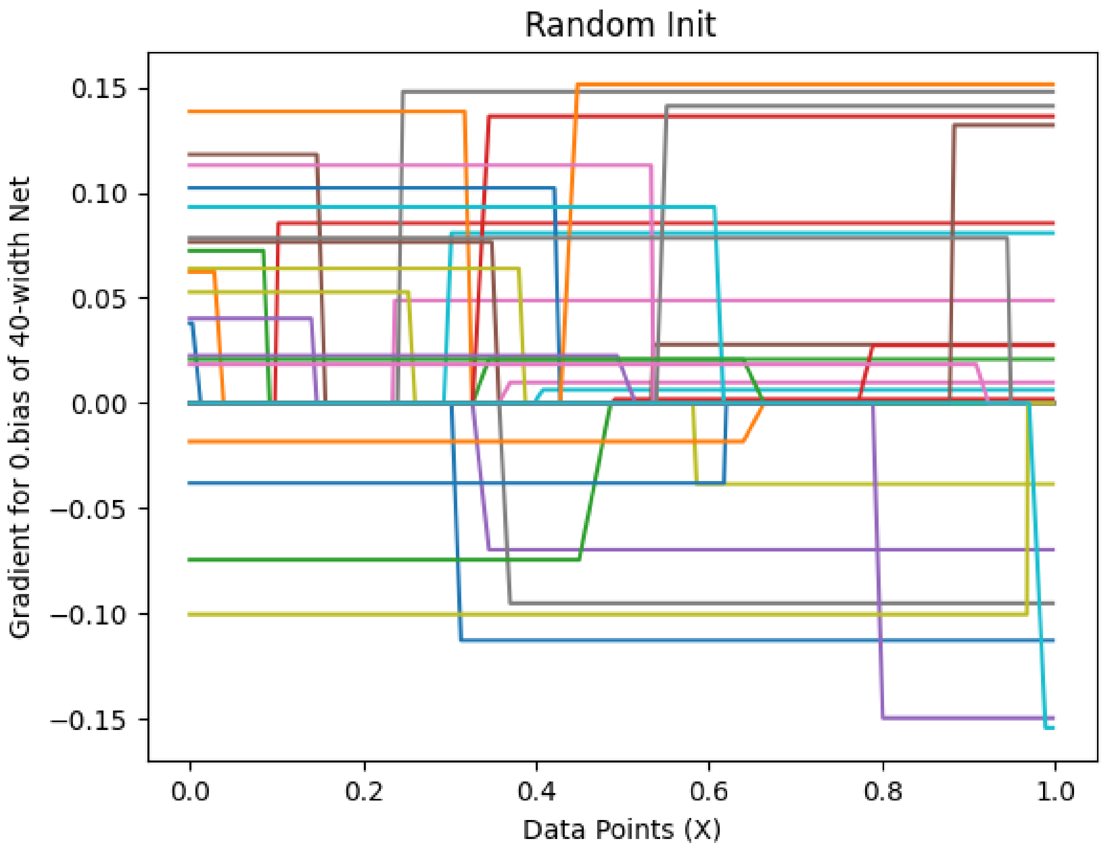
Trained
Gradient for 0.weight of 20-width Net
4
3
2
1
0
−1
−2
−3
0.0
0.2
0.4
0.6
0.8
1.0
Data Points (X)

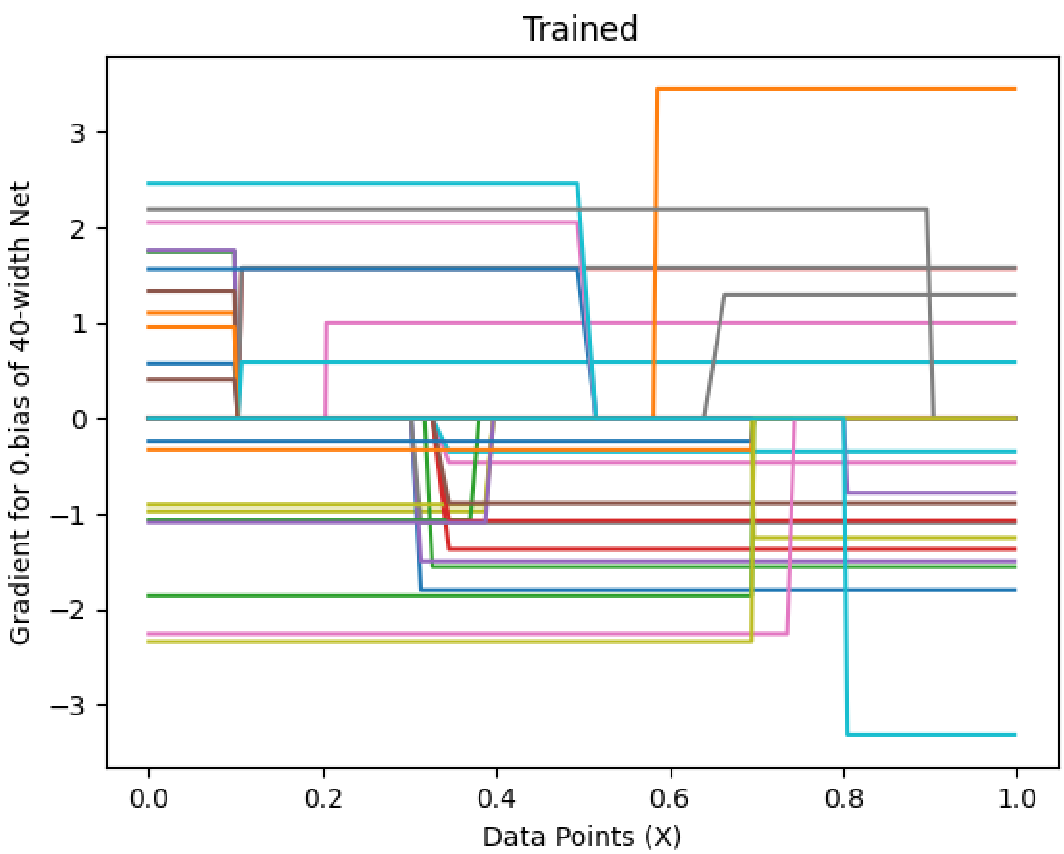

Random Init
Gradient for 0.bias of 20-width Net
Data Points (X)
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0.0
0.2
0.4
0.6
0.8
1.0


Trained
Gradient for 0.bias of 20-width Net
Data Points (X)
4
3
2
1
0
−1
−2
−3
0.0
0.2
0.4
0.6
0.8
1.0


Random Init
Gradient for 0.weight of 40-width Net
Data Points (X)
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
0.0
0.2
0.4
0.6
0.8
1.0


Trained
Gradient for 0.weight of 40-width Net
Data Points (X)
3
2
1
0
−1
−2
−3
0.0
0.2
0.4
0.6
0.8
1.0


Random Init
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
Gradient for 0.bias of 40-width Net
0.0
0.2
0.4
0.6
0.8
1.0
Data Points (X)



6 (b) SVD for feature matrix

During training, we can imagine that we have a generalized linear model with a feature matrix corresponding to the linearized features corresponding to each learnable parameter. We know from our analysis of gradient descent, that the singular values and singular vectors corresponding to this feature matrix are important.

Use the SVD of this feature matrix to plot both the singular values and visualize the "principle features" that correspond to the d-dimensional singular vectors multiplied by all the features corresponding to the parameters

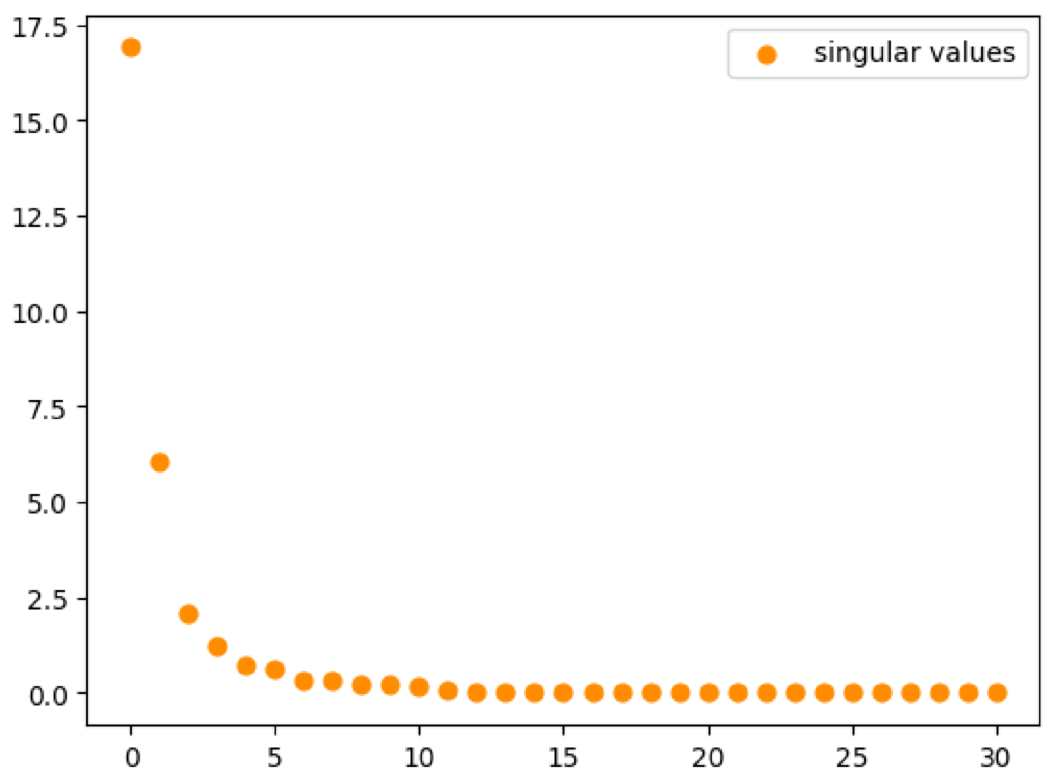
(HINT: Remember that the feature matrix whose SVD you are taking has n rows where each row corresponds to one training point and d columns where each column corresponds to each of the learnable features. Meanwhile, you are going to be plotting/visualizing the "principle features" as functions of x even at places where you don't have training points.)

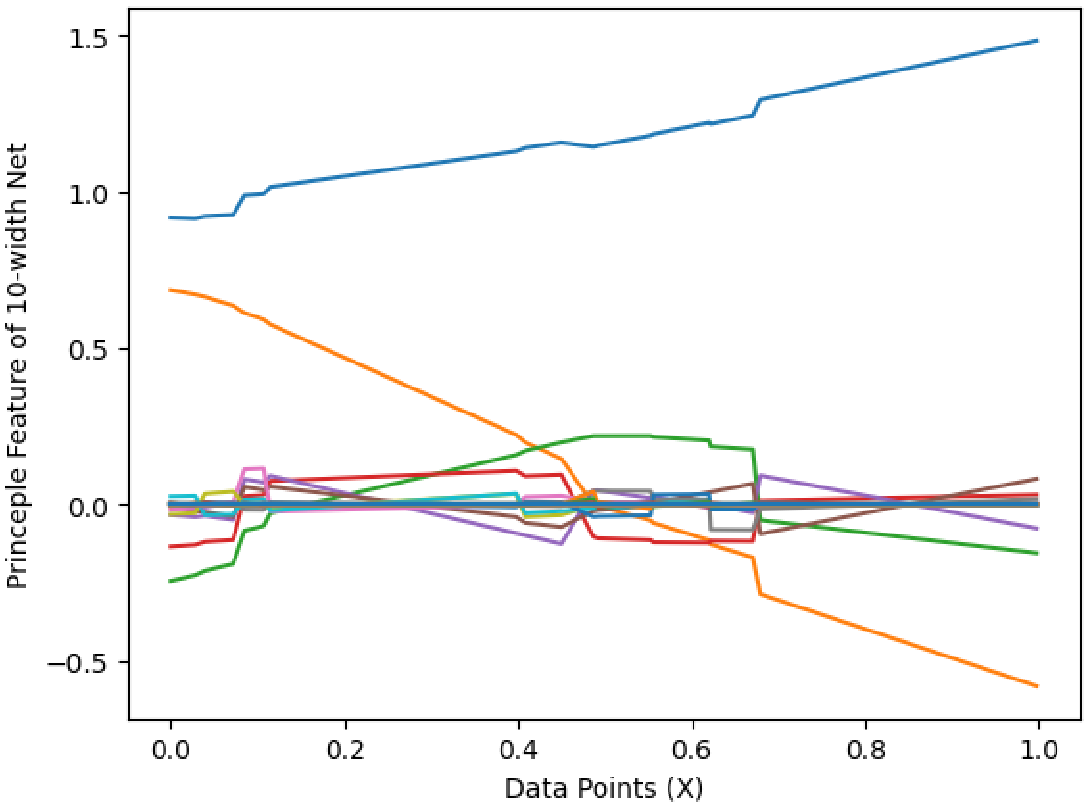
[13]:
```
def compute_svd_plot_features(X, y, X_test, y_test, model):
    width = model[0].out_features  # the width is the number of hidden units.
    gradients = np.zeros((width, X.shape[0]))
    num_pts = 0
```

```python
    gradient_collect, vis_collect = { }, { }
    for x in X:
        y = model(to_torch(x).to(device=device))

        #########################################################################
        # TODO: Complete the following part to run backpropagation. (2 lines)
        # Hint: The same as part (a)
        #########################################################################
        # (YOUR CODE HERE)

        model.zero_grad()
        y.backward()

        #########################################################################

        for n, p in model.named_parameters():
            for w_idx, w_grad in enumerate( p.grad.view(-1).data ):
                if f'{n}.{w_idx}' not in gradient_collect:
                    gradient_collect[ f'{n}.{w_idx}' ] = {'x':[], 'y': []}
                gradient_collect[ f'{n}.{w_idx}' ]['y'].append( w_grad.item() )
                gradient_collect[ f'{n}.{w_idx}' ]['x'].append( x )

    feature_matrix = []
    for w_n in gradient_collect:
        feature_matrix.append( gradient_collect[w_n]['y'] )
    feature_matrix = np.array( feature_matrix ).T

    #############################################################################
    # TODO: Complete the following part to SVD-decompose the feature matrix.
    #       (1 line)
    # Hint: the shape of u, s, vh should be [n, d], [d], and [d, d]
    #       respectively
    #############################################################################
    # (YOUR CODE HERE)

    u, s, vh = np.linalg.svd(feature_matrix, full_matrices=False)

    #############################################################################

    plt.scatter(np.arange(s.shape[0]), s, c='darkorange', s=40.0,␣
↪label='singular values')
    plt.legend()
    plt.show()

    # Construct more training matrix
    #############################################################################
    # TODO: Complete the following part to compute the pricipal feature
```

```
    #       (1 line)
    ############################################################################
    # (YOUR CODE HERE)

    princple_feature = np.dot(u, np.diag(s))

    ############################################################################


    for w_idx in range(feature_matrix.shape[1]):
        plt.plot( X, princple_feature.T[w_idx] )

    plt.xlabel('Data Points (X)')
    plt.ylabel(f'Princeple Feature of {width}-width Net')
    plt.show()

for w in widths:
    net = nets_by_size[w]['net']
    print("Width", w)
    compute_svd_plot_features(X, y, X_test, y_test, net)
```

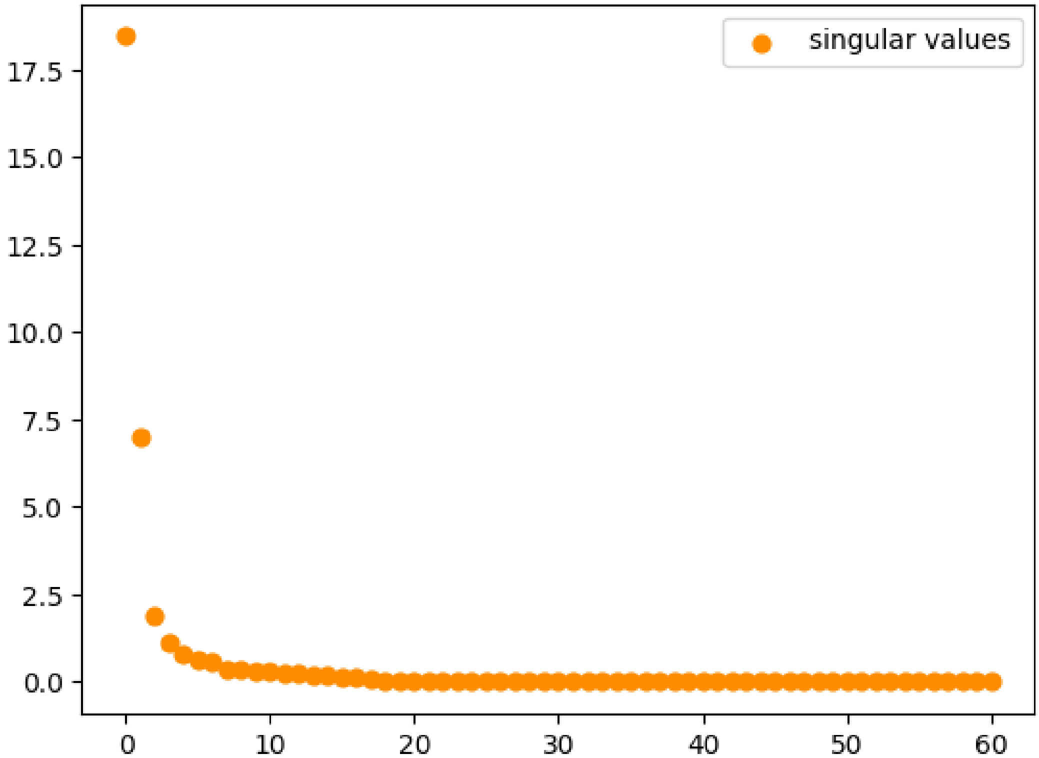
```
Width 10
```

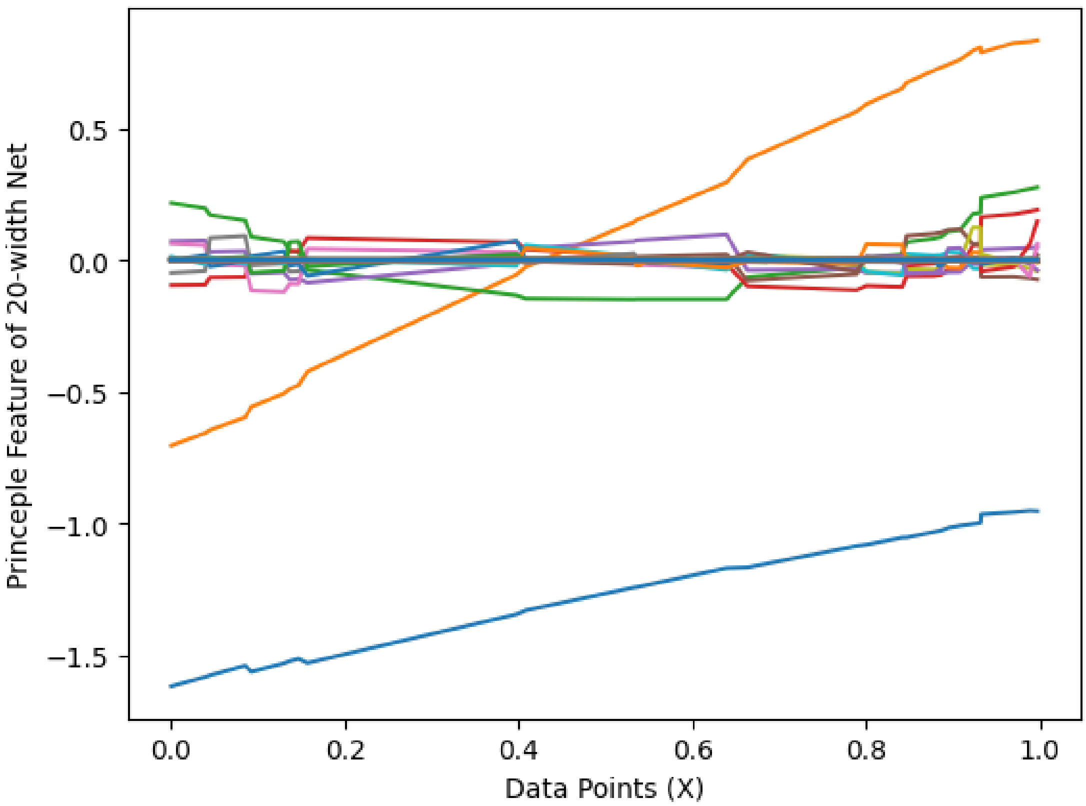




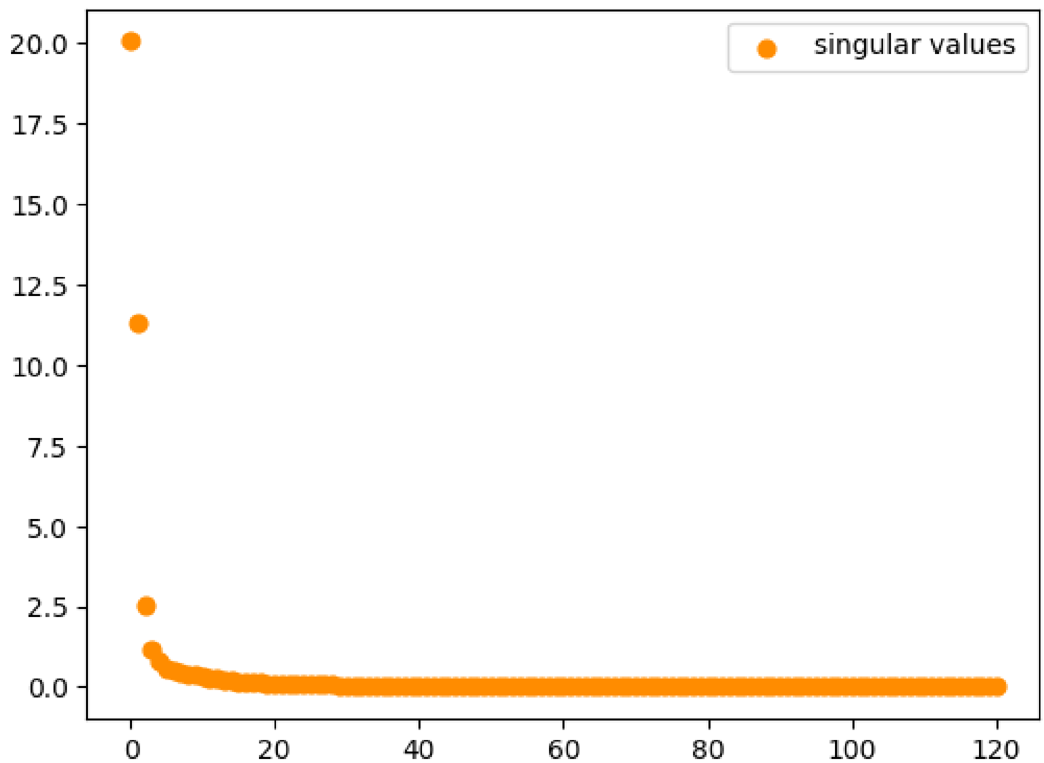
Principle Feature of 10-width Net
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
Data Points (X)

Width 20

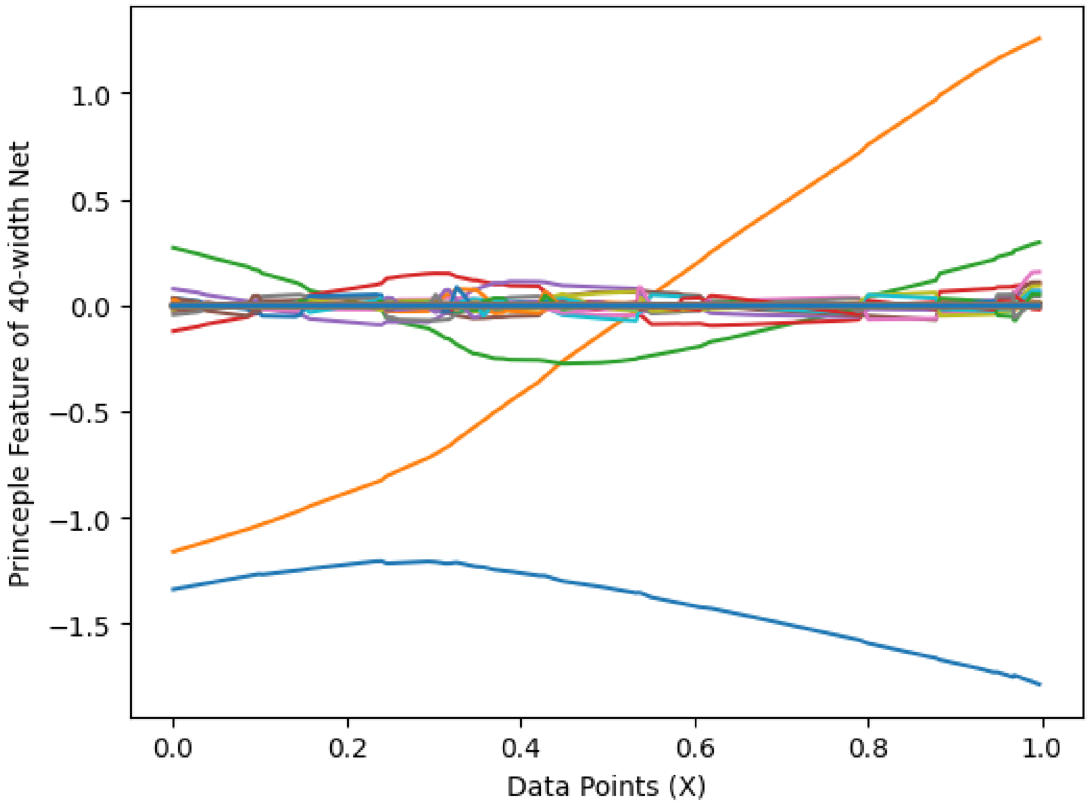

singular values
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
10
20
30
40
50
60


0.5
0.0
−0.5
−1.0
−1.5
Principle Feature of 20-width Net
0.0
0.2
0.4
0.6
0.8
1.0
Data Points (X)

Width 40



singular values
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
20
40
60
80
100
120



7 (c) Two-layer Network

Augment the jupyter notebook to add a second hidden layer of the same size as the first hidden layer, fully connected to the first hidden layer.

Allow the visualization of the features corresponding to the parameters in both hidden layers, as well as the "principle features" and the singular values.

[14]:
```
################################################################################
# (YOUR CODE HERE)
# Hint: You can reuse most of the code from above. You should change the network
# definition and visualization function 'backward_and_plot_grad' such that an
# additional hidden layer is added.
################################################################################

widths = [10, 20, 40]
for width in widths:
    net = nn.Sequential(nn.Linear(1, width),
                        nn.ReLU(),
                        nn.Linear(width, width),
                        nn.ReLU(),
```

```
                        nn.Linear(width, 1))
    loss = nn.MSELoss()

    weights_all = list(net.parameters())
    weights_out = weights_all[4:]

    elbows = np.sort(np.random.rand(width))
    new_biases = -elbows * to_numpy(weights_all[0]).ravel()
    weights_all[1].data = to_torch(new_biases)


    lr_out = 0.2
    lr_all = 0.02
    opt_all = torch.optim.SGD(params=weights_all, lr=lr_all)
    opt_out = torch.optim.SGD(params=weights_out, lr=lr_out)

    initial_weights = copy.deepcopy(net.state_dict())
    nets_by_size[width] = {'net': net, 'opt_all': opt_all,
                            'opt_out': opt_out, 'init': initial_weights}
```

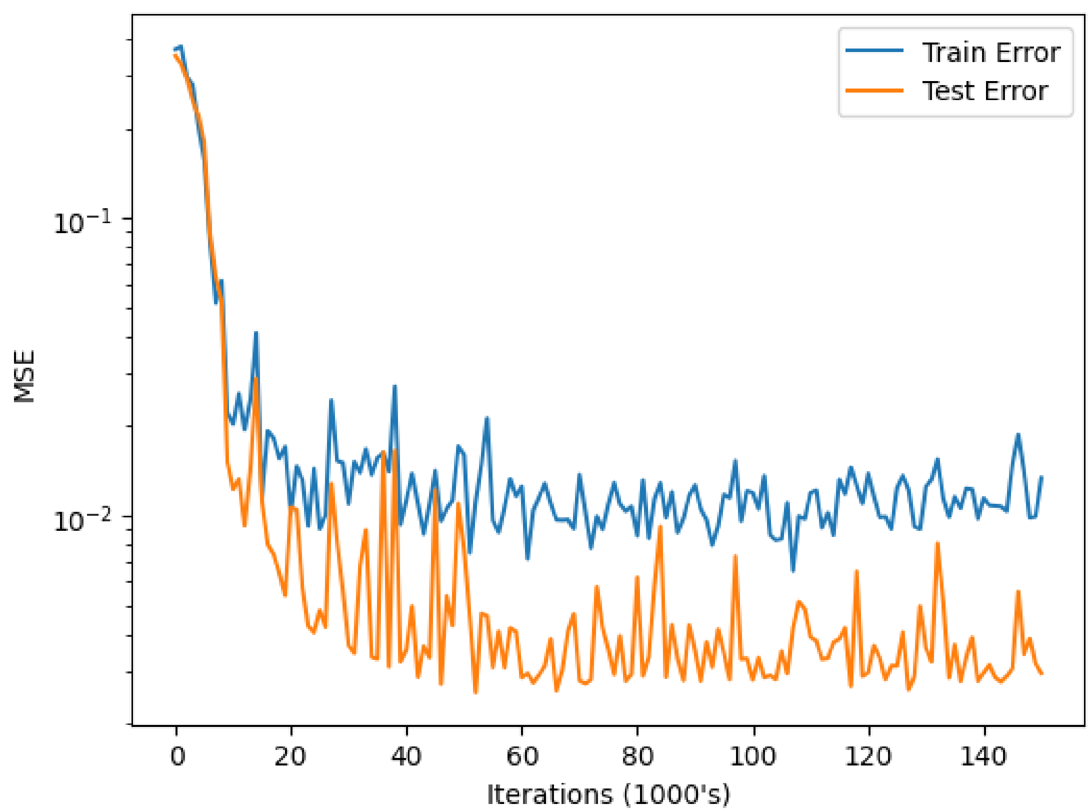
[15]:
```
print(device)
```

cuda

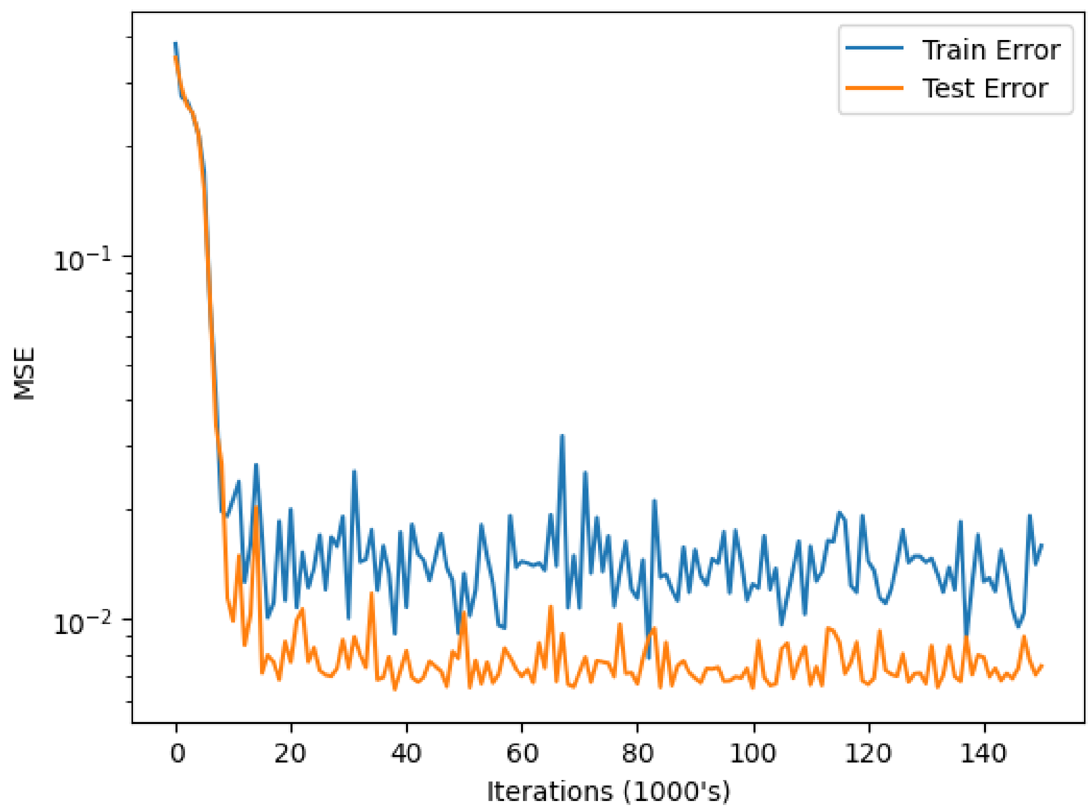
[16]:
```
n_steps = 150000
save_every = 1000
t0 = time.time()

for w in widths:
    print("-"*40)
    print("Width", w)
    new_net = nn.Sequential(nn.Linear(1, w),
                        nn.ReLU(),
                        nn.Linear(w, w),
                        nn.ReLU(),
                        nn.Linear(w, 1))
    new_net.load_state_dict(nets_by_size[w]['net'].state_dict().copy())
    new_net.to(device=device)
    opt_all = torch.optim.SGD(params=new_net.parameters(), lr=lr_all)
    initial_weights = nets_by_size[w]['init']
    history_all = train_network(X, y, X_test, y_test,
                            new_net, optim=opt_all,
                            n_steps=n_steps, save_every=save_every,
                            initial_weights=initial_weights,
                            verbose=False, device=device)
    nets_by_size[w]['trained_net'] = new_net
    nets_by_size[w]['hist_all'] = history_all
    print("Width", w)
```

```python
    plot_test_train_errors(history_all)

t1 = time.time()
print("-"*40)
print("Trained all layers in %.1f minutes" % ((t1 - t0) / 60))
```

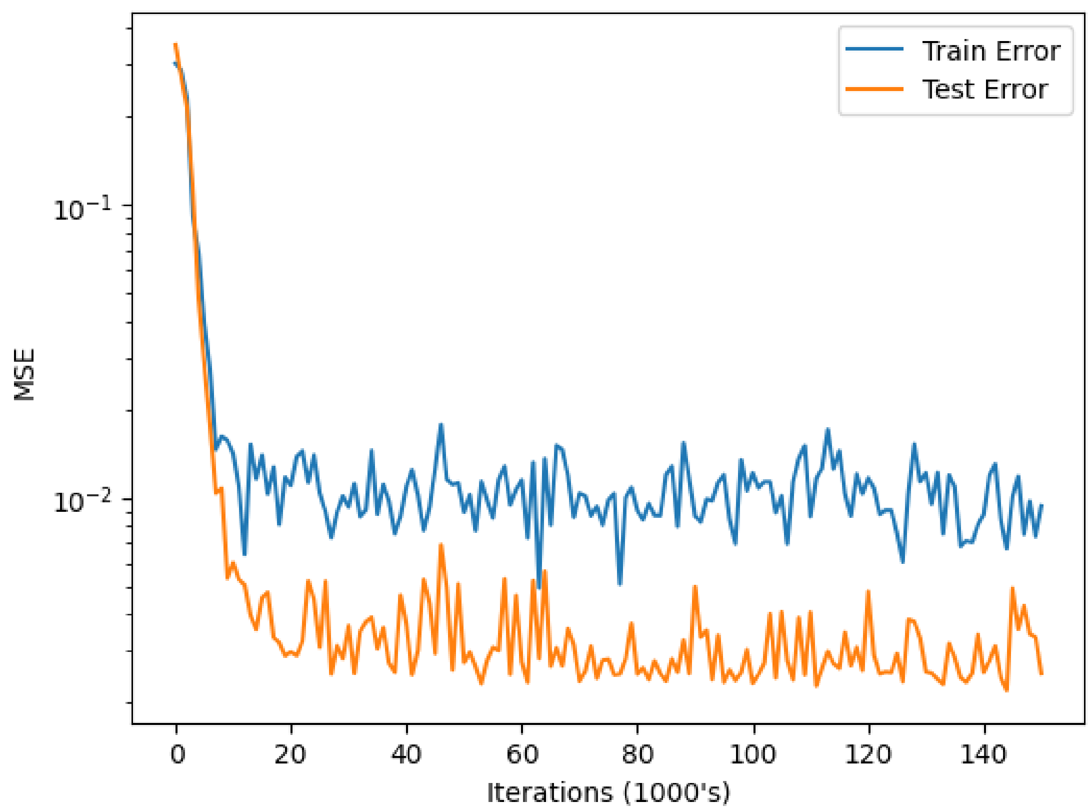
```
----------------------------------------
Width 10
SGD Iteration 10000
SGD Iteration 20000
SGD Iteration 30000
SGD Iteration 40000
SGD Iteration 50000
SGD Iteration 60000
SGD Iteration 70000
SGD Iteration 80000
SGD Iteration 90000
SGD Iteration 100000
SGD Iteration 110000
SGD Iteration 120000
SGD Iteration 130000
SGD Iteration 140000
SGD Iteration 150000
Width 10
```



```
----------------------------------------
Width 20
SGD Iteration 10000
SGD Iteration 20000
SGD Iteration 30000
SGD Iteration 40000
SGD Iteration 50000
SGD Iteration 60000
SGD Iteration 70000
SGD Iteration 80000
SGD Iteration 90000
SGD Iteration 100000
SGD Iteration 110000
SGD Iteration 120000
SGD Iteration 130000
SGD Iteration 140000
SGD Iteration 150000
Width 20
```



```
----------------------------------------
Width 40
SGD Iteration 10000
SGD Iteration 20000
SGD Iteration 30000
SGD Iteration 40000
SGD Iteration 50000
SGD Iteration 60000
SGD Iteration 70000
SGD Iteration 80000
SGD Iteration 90000
SGD Iteration 100000
SGD Iteration 110000
SGD Iteration 120000
SGD Iteration 130000
SGD Iteration 140000
SGD Iteration 150000
Width 40
```




```
----------------------------------------
Trained all layers in 12.0 minutes
```