fit_sine_with_third_order_polynomial

March 2, 2021

1 Fit $y = sin(x)$ with a third order polynomial

In PyTorch, the nn package defines a set of Modules, which are roughly equivalent to neural network layers. A Module receives input Tensors and computes output Tensors, but may also hold internal state such as Tensors containing learnable parameters. The nn package also defines a set of useful loss functions that are commonly used when training neural networks.

1.1 nn package

[1]:
```
import torch
import math
```

[2]:
```
# Create Tensors to hold input and outputs.
x = torch.linspace(-math.pi, math.pi, 2000)
y = torch.sin(x)
print(f"x= {x}\n")
print(f"y= {y}\n")
print(x.shape, y.shape)
```

```
x= tensor([-3.1416, -3.1384, -3.1353,  …,  3.1353,  3.1384,  3.1416])

y= tensor([ 8.7423e-08, -3.1430e-03, -6.2863e-03,  …,  6.2863e-03,
         3.1432e-03, -8.7423e-08])

torch.Size([2000]) torch.Size([2000])
```

For this example, the output y is a linear function of (x, x^2, x^3), so we can consider it as a linear layer neural network. Let's prepare the tensor (x, x^2, x^3).

[3]:
```
p = torch.tensor([1, 2, 3])
xx = x.unsqueeze(-1).pow(p)
print(f"x.unsqueeze(-1) =\n {x.unsqueeze(-1)}\n")
print(f"x.unsqueeze(-1).shape = {x.unsqueeze(-1).shape}\n")
print(f"xx = {xx}\n")
print(f"xx.shape = {xx.shape}\n")
```

```
x.unsqueeze(-1) =
 tensor([[-3.1416],
        [-3.1384],
```

```
        [-3.1353],
        …,
        [ 3.1353],
        [ 3.1384],
        [ 3.1416]])

x.unsqueeze(-1).shape = torch.Size([2000, 1])

xx = tensor([[ -3.1416,   9.8696, -31.0063],
        [ -3.1384,   9.8499, -30.9133],
        [ -3.1353,   9.8301, -30.8205],
        …,
        [  3.1353,   9.8301,  30.8205],
        [  3.1384,   9.8499,  30.9133],
        [  3.1416,   9.8696,  31.0063]])

xx.shape = torch.Size([2000, 3])
```

Use the nn package to define our model as a sequence of layers.
`nn.Sequential` is a Module which contains other Modules, and applies them in sequence to produce its output. The Linear Module computes output from input using a linear function, and holds internal Tensors for its weight and bias.
The Flatten layer flatens the output of the linear layer to a 1D tensor, to match the shape of `y`.

[4]:
```python
model = torch.nn.Sequential(
    torch.nn.Linear(3, 1),
    torch.nn.Flatten(0, 1)# Flattens a contiguous range of dims into a tensor. ␣
 ↪                                    torch.nn.Flatten(start_dim: int = 1,␣
 ↪end_dim: int = -1)
)
```

The nn package also contains definitions of popular loss functions; in this case we will use Mean Squared Error (MSE) as our loss function.

[5]:
```python
loss_fn = torch.nn.MSELoss(reduction='sum')
```

[6]:
```python
learning_rate = 1e-6
```

[7]:
```python
for t in range(3000):

    # Forward pass: compute predicted y by passing x to the model. Module␣
 ↪objects
    # override the __call__ operator so you can call them like functions. When
    # doing so you pass a Tensor of input data to the Module and it produces
    # a Tensor of output data.
    y_pred = model(xx)
```

```python
    # Compute and print loss. We pass Tensors containing the predicted and true
    # values of y, and the loss function returns a Tensor containing the
    # loss.
    loss = loss_fn(y_pred, y)
    if t % 200 == 199:
        print(f"{t+1}-th epoch: MSE = {loss.item()}") # '.item()' is to obtain␣
↪its value

    # Zero the gradients before running the backward pass.
    model.zero_grad()

    # Backward pass: compute gradient of the loss with respect to all the␣
↪learnable
    # parameters of the model. Internally, the parameters of each Module are␣
↪stored
    # in Tensors with requires_grad=True, so this call will compute gradients␣
↪for
    # all learnable parameters in the model.
    loss.backward()

    # Update the weights using gradient descent. Each parameter is a Tensor, so
    # we can access its gradients like we did before.
    with torch.no_grad():
        for param in model.parameters():
            param -= learning_rate * param.grad
```

```
200-th epoch: MSE = 905.8662719726562
400-th epoch: MSE = 402.9305114746094
600-th epoch: MSE = 182.0838165283203
800-th epoch: MSE = 85.04901123046875
1000-th epoch: MSE = 42.38545227050781
1200-th epoch: MSE = 23.612943649291992
1400-th epoch: MSE = 15.345804214477539
1600-th epoch: MSE = 11.701425552368164
1800-th epoch: MSE = 10.093147277832031
2000-th epoch: MSE = 9.382526397705078
2200-th epoch: MSE = 9.06808853149414
2400-th epoch: MSE = 8.928747177124023
2600-th epoch: MSE = 8.866888999938965
2800-th epoch: MSE = 8.839372634887695
3000-th epoch: MSE = 8.827112197875977
```

[8]:
```python
# You can access the first layer of `model` like accessing the first item of a␣
↪list
linear_layer = model[0]
print(linear_layer)
print(linear_layer.bias)
```

```python
print(linear_layer.weight)
```

```
Linear(in_features=3, out_features=1, bias=True)
Parameter containing:
tensor([0.0014], requires_grad=True)
Parameter containing:
tensor([[ 8.5397e-01, -2.4788e-04, -9.2937e-02]], requires_grad=True)
```

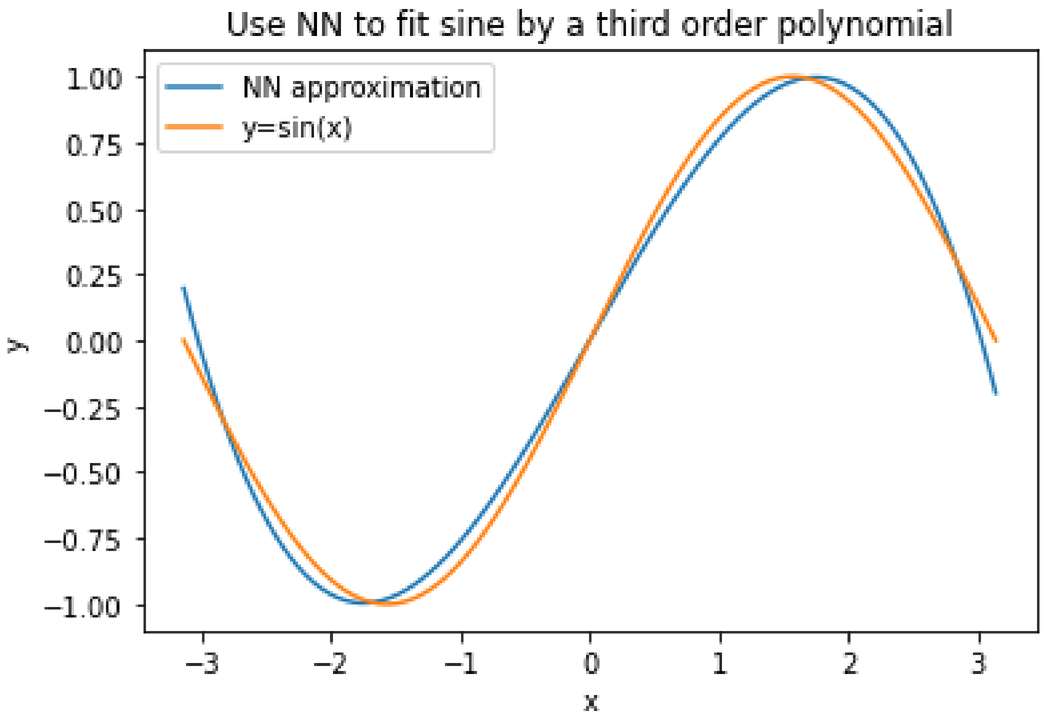
[9]:
```python
# For linear layer, its parameters are stored as `weight` and `bias`.
print(f'The third order polynomial aproximation of sine function is :\n\ty =␣
↪{linear_layer.bias.item()} + {linear_layer.weight[:, 0].item()} x +␣
↪{linear_layer.weight[:, 1].item()} x^2 + {linear_layer.weight[:, 2].item()}␣
↪x^3')
```

```
The third order polynomial aproximation of sine function is :
        y = 0.0014368174597620964 + 0.8539739847183228 x +
-0.0002478751994203776 x^2 + -0.09293682873249054 x^3
```

[10]:
```python
import matplotlib.pyplot as plt
import numpy as np
import math

x_np = x.detach().numpy()
y_pred_np = y_pred.detach().numpy()
```

[11]:
```python
plt.figure()
plt.plot(x_np, y_pred_np, label='NN approximation')
plt.plot(x_np, np.sin(x_np), label='y=sin(x)')
plt.xlabel("x")
plt.ylabel("y")
plt.legend()
plt.title("Use NN to fit sine by a third order polynomial")
plt.show()
```



1.2 Optim package

Up to this point we have updated the weights of our models by manually mutating the Tensors holding learnable parameters with `torch.no_grad()`. This is not a huge burden for simple optimization algorithms like stochastic gradient descent, but in practice we often train neural networks using more sophisticated optimizers like **Adagrad, RMSProp, Adam**, etc.

The optim package in PyTorch abstracts the idea of an optimization algorithm and provides implementations of commonly used optimization algorithms.

In this example we will use the nn package to define our model as before, but we will optimize the model using the RMSprop algorithm provided by the optim package:

[12]:
```
import torch
import math


# Create Tensors to hold input and outputs.
x = torch.linspace(-math.pi, math.pi, 2000)
y = torch.sin(x)

# Prepare the input tensor (x, x^2, x^3).
p = torch.tensor([1, 2, 3])
```

```
xx = x.unsqueeze(-1).pow(p)

# Use the nn package to define our model and loss function.
model = torch.nn.Sequential(
    torch.nn.Linear(3, 1),
    torch.nn.Flatten(0, 1)
)
loss_fn = torch.nn.MSELoss(reduction='sum')
```

[13]:
```
# Use the optim package to define an Optimizer that will update the weights of
# the model for us. Here we will use RMSprop; the optim package contains many␣
↪other
# optimization algorithms. The first argument to the RMSprop constructor tells␣
↪the
# optimizer which Tensors it should update.
learning_rate = 1e-3
optimizer = torch.optim.RMSprop(model.parameters(), lr=learning_rate)
# optimizer = torch.optim.Adagrad(model.parameters(), lr=learning_rate)
# optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

[14]:
```
for t in range(3000):
    # Forward pass: compute predicted y by passing x to the model.
    y_pred = model(xx)

    # Compute and print loss.
    loss = loss_fn(y_pred, y)
    if t % 200 == 199:
        print(f"{t+1}-th epoch: MSE = {loss.item()}")

    # Before the backward pass, use the optimizer object to zero all of the
    # gradients for the variables it will update (which are the learnable
    # weights of the model). This is because by default, gradients are
    # accumulated in buffers( i.e, not overwritten) whenever .backward()
    # is called. Checkout docs of torch.autograd.backward for more details.
    optimizer.zero_grad()

    # Backward pass: compute gradient of the loss with respect to model
    # parameters
    loss.backward()

    # Calling the step function on an Optimizer makes an update to its
    # parameters
    optimizer.step()


linear_layer = model[0]
```

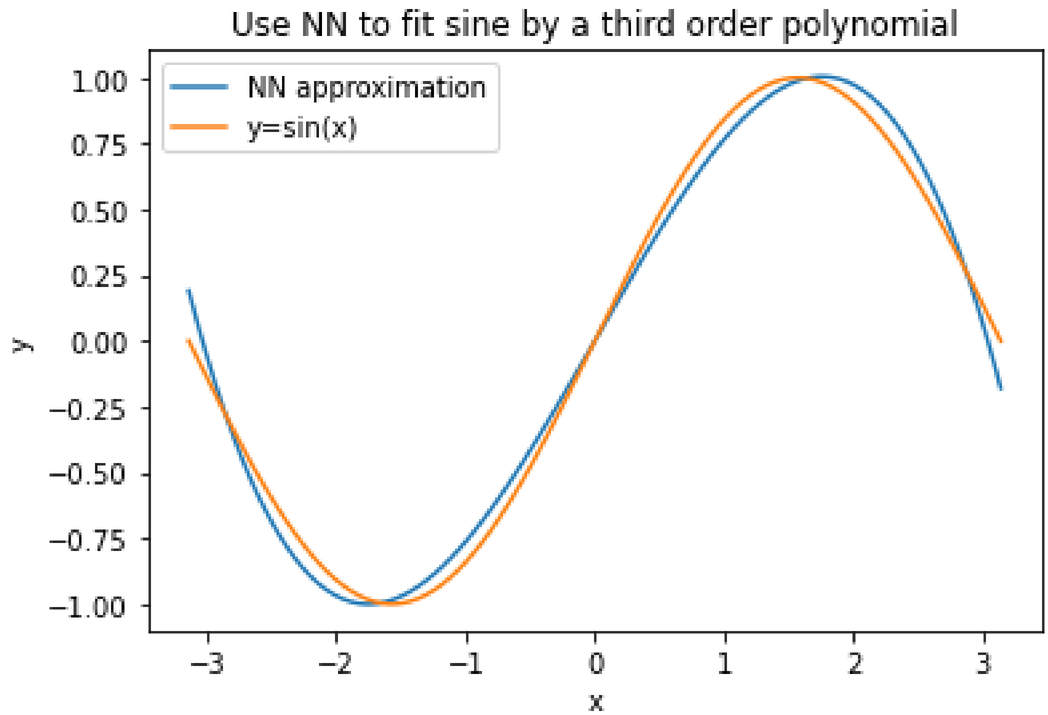
```
print(f'The third order polynomial aproximation of sine function is :\n\ty =␣
↪{linear_layer.bias.item()} + {linear_layer.weight[:, 0].item()} x +␣
↪{linear_layer.weight[:, 1].item()} x^2 + {linear_layer.weight[:, 2].item()}␣
↪x^3')
```

```
200-th epoch: MSE = 11084.0458984375
400-th epoch: MSE = 2702.912841796875
600-th epoch: MSE = 1795.74365234375
800-th epoch: MSE = 1300.1849365234375
1000-th epoch: MSE = 884.49853515625
1200-th epoch: MSE = 567.79638671875
1400-th epoch: MSE = 330.41302490234375
1600-th epoch: MSE = 164.8553924560547
1800-th epoch: MSE = 64.73673248291016
2000-th epoch: MSE = 19.500205993652344
2200-th epoch: MSE = 9.276893615722656
2400-th epoch: MSE = 8.919900894165039
2600-th epoch: MSE = 8.91881275177002
2800-th epoch: MSE = 8.921417236328125
3000-th epoch: MSE = 8.920509338378906
The third order polynomial aproximation of sine function is :
        y = -0.0005010199965909123 + 0.8562425971031189 x +
-0.0005010294844396412 x^2 + -0.09382958710193634 x^3
```

[15]:
```
import matplotlib.pyplot as plt
import numpy as np
import math

x_np = x.detach().numpy()
y_pred_np = y_pred.detach().numpy()
```

[16]:
```
plt.figure()
plt.plot(x_np, y_pred_np, label='NN approximation')
plt.plot(x_np, np.sin(x_np), label='y=sin(x)')
plt.xlabel("x")
plt.ylabel("y")
plt.legend()
plt.title("Use NN to fit sine by a third order polynomial")
plt.show()
```



1.3 Consider a multi-layer network

Next, we don't use the third order polynomial approximation, instead, we only want to see how multi-layer NN can approximate the sine function.

[17]:
```
import torch
import math


# Create Tensors to hold input and outputs.
x = torch.linspace(-math.pi, math.pi, 2000)
y = torch.sin(x)

xx = x.unsqueeze(-1)

# Use the nn package to define our model and loss function.
model = torch.nn.Sequential( # Have one hidden layer
    torch.nn.Linear(1, 3),
    torch.nn.ReLU(), # Use ELU activation function
    torch.nn.Linear(3, 1),
    torch.nn.Flatten(0, 1)
)
```

```python
loss_fn = torch.nn.MSELoss(reduction='sum')

# Use the optim package to define an Optimizer that will update the weights of
# the model for us. Here we will use RMSprop; the optim package contains many␣
 ↪other
# optimization algorithms. The first argument to the RMSprop constructor tells␣
 ↪the
# optimizer which Tensors it should update.
learning_rate = 1e-3
optimizer = torch.optim.RMSprop(model.parameters(), lr=learning_rate)
# optimizer = torch.optim.Adagrad(model.parameters(), lr=learning_rate)
# optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

for t in range(20000):
    # Forward pass: compute predicted y by passing x to the model.
    y_pred = model(xx)

    # Compute and print loss.
    loss = loss_fn(y_pred, y)
    if t % 200 == 199:
        print(f"{t+1}-th epoch: MSE = {loss.item()}")

    # Before the backward pass, use the optimizer object to zero all of the
    # gradients for the variables it will update (which are the learnable
    # weights of the model). This is because by default, gradients are
    # accumulated in buffers( i.e, not overwritten) whenever .backward()
    # is called. Checkout docs of torch.autograd.backward for more details.
    optimizer.zero_grad()

    # Backward pass: compute gradient of the loss with respect to model
    # parameters
    loss.backward()

    # Calling the step function on an Optimizer makes an update to its
    # parameters
    optimizer.step()


linear_layer_0 = model[0]
print(linear_layer_0)
print(linear_layer_0.bias)
print(linear_layer_0.weight)
# 'model[1]' is the ELU function
linear_layer_1 = model[2]
print(linear_layer_1)
print(linear_layer_1.bias)
print(linear_layer_1.weight)
```

```
200-th epoch: MSE = 222.1185302734375
400-th epoch: MSE = 163.39878845214844
600-th epoch: MSE = 114.3281478881836
800-th epoch: MSE = 82.08216857910156
1000-th epoch: MSE = 66.6541976928711
1200-th epoch: MSE = 51.417076110839844
1400-th epoch: MSE = 38.91912078857422
1600-th epoch: MSE = 29.173322677612305
1800-th epoch: MSE = 22.206064224243164
2000-th epoch: MSE = 16.30120277404785
2200-th epoch: MSE = 10.724164009094238
2400-th epoch: MSE = 7.6106367111206055
2600-th epoch: MSE = 6.814985752105713
2800-th epoch: MSE = 6.6911115646362305
3000-th epoch: MSE = 6.647377967834473
3200-th epoch: MSE = 6.6219401359558105
3400-th epoch: MSE = 6.610921859741211
3600-th epoch: MSE = 6.602062702178955
3800-th epoch: MSE = 6.596940517425537
4000-th epoch: MSE = 6.596714019775391
4200-th epoch: MSE = 6.592458724975586
4400-th epoch: MSE = 6.591907501220703
4600-th epoch: MSE = 6.593267440795898
4800-th epoch: MSE = 6.591717720031738
5000-th epoch: MSE = 6.592395305633545
5200-th epoch: MSE = 6.590991497039795
5400-th epoch: MSE = 6.5931549072265625
5600-th epoch: MSE = 6.590023040771484
5800-th epoch: MSE = 6.593349456787109
6000-th epoch: MSE = 6.589641094207764
6200-th epoch: MSE = 6.594057083129883
6400-th epoch: MSE = 6.588294982910156
6600-th epoch: MSE = 6.593108177185059
6800-th epoch: MSE = 6.589034557342529
7000-th epoch: MSE = 6.583995342254639
7200-th epoch: MSE = 6.6082258224487305
7400-th epoch: MSE = 6.5732645988464355
7600-th epoch: MSE = 6.606942176818848
7800-th epoch: MSE = 6.595523834228516
8000-th epoch: MSE = 6.571382999420166
8200-th epoch: MSE = 6.61057186126709
8400-th epoch: MSE = 6.584150791168213
8600-th epoch: MSE = 6.573294162750244
8800-th epoch: MSE = 6.62542200088501
9000-th epoch: MSE = 6.577882766723633
9200-th epoch: MSE = 6.577963352203369
9400-th epoch: MSE = 6.636216640472412
9600-th epoch: MSE = 6.574609279632568
```

```
9800-th epoch: MSE = 6.583264350891113
10000-th epoch: MSE = 6.6101250648498535
10200-th epoch: MSE = 6.570481300354004
10400-th epoch: MSE = 6.598320007324219
10600-th epoch: MSE = 6.593918800354004
10800-th epoch: MSE = 6.572445869445801
11000-th epoch: MSE = 6.616657733917236
11200-th epoch: MSE = 6.581990718841553
11400-th epoch: MSE = 6.57521915435791
11600-th epoch: MSE = 6.632552623748779
11800-th epoch: MSE = 6.577923774719238
12000-th epoch: MSE = 6.58056116104126
12200-th epoch: MSE = 6.624825954437256
12400-th epoch: MSE = 6.57264518737793
12600-th epoch: MSE = 6.584895133972168
12800-th epoch: MSE = 6.602884769439697
13000-th epoch: MSE = 6.5698771476745605
13200-th epoch: MSE = 6.604027271270752
13400-th epoch: MSE = 6.587477684020996
13600-th epoch: MSE = 6.5723958015441895
13800-th epoch: MSE = 6.621740341186523
14000-th epoch: MSE = 6.582928657531738
14200-th epoch: MSE = 6.572546005249023
14400-th epoch: MSE = 6.625034332275391
14600-th epoch: MSE = 6.576754093170166
14800-th epoch: MSE = 6.5805182456970215
15000-th epoch: MSE = 6.621831893920898
15200-th epoch: MSE = 6.5715789794921875
15400-th epoch: MSE = 6.589380741119385
15600-th epoch: MSE = 6.6073317527771
15800-th epoch: MSE = 6.573606967926025
16000-th epoch: MSE = 6.60157585144043
16200-th epoch: MSE = 6.593780040740967
16400-th epoch: MSE = 6.570576190948486
16600-th epoch: MSE = 6.612955093383789
16800-th epoch: MSE = 6.580706596374512
17000-th epoch: MSE = 6.572243690490723
17200-th epoch: MSE = 6.6237359046936035
17400-th epoch: MSE = 6.573812961578369
17600-th epoch: MSE = 6.5848541259765625
17800-th epoch: MSE = 6.609924793243408
18000-th epoch: MSE = 6.570241928100586
18200-th epoch: MSE = 6.597469329833984
18400-th epoch: MSE = 6.60195255279541
18600-th epoch: MSE = 6.572937965393066
18800-th epoch: MSE = 6.611828327178955
19000-th epoch: MSE = 6.585078239440918
19200-th epoch: MSE = 6.573753356933594
```

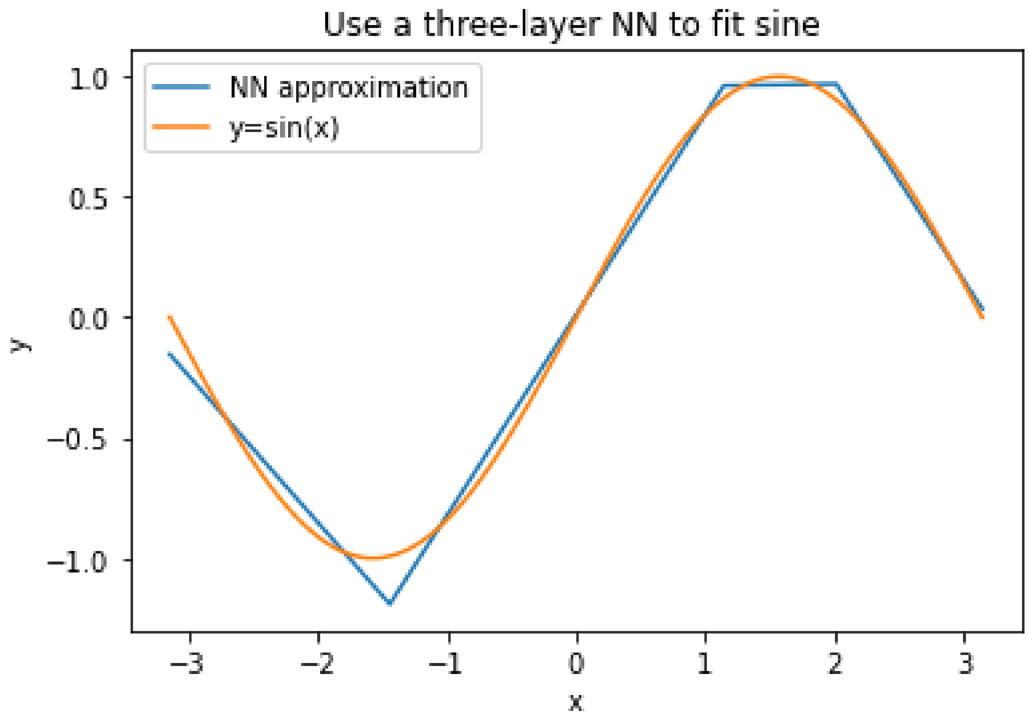
```
19400-th epoch: MSE = 6.625244140625
19600-th epoch: MSE = 6.576791286468506
19800-th epoch: MSE = 6.577754974365234
20000-th epoch: MSE = 6.619273662567139
Linear(in_features=1, out_features=3, bias=True)
Parameter containing:
tensor([-0.8312,  1.4884, -1.8790], requires_grad=True)
Parameter containing:
tensor([[ 0.7259],
        [-0.7384],
        [-1.3054]], requires_grad=True)
Linear(in_features=3, out_features=1, bias=True)
Parameter containing:
tensor([1.6921], requires_grad=True)
Parameter containing:
tensor([[-1.1360, -1.1261,  1.1094]], requires_grad=True)
```

[19]:

```
import matplotlib.pyplot as plt
import numpy as np
import math

x_np = x.detach().numpy()
y_pred_np = y_pred.detach().numpy()

plt.figure()
plt.plot(x_np, y_pred_np, label='NN approximation')
plt.plot(x_np, np.sin(x_np), label='y=sin(x)')
plt.xlabel("x")
plt.ylabel("y")
plt.legend()
plt.title("Use a three-layer NN to fit sine ")
plt.show()
```


Use a three-layer NN to fit sine
NN approximation
y=sin(x)
1.0
0.5
0.0
−0.5
−1.0
y
−3
−2
−1
0
1
2
3
x