

ML Theory Week 1

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1 A tutorial on PyTorch

```
>>> import torch
>>> import torch.nn as nn
>>> import torch.optim as optim
>>>
```

The goal is to approximate the XOR gate defined as follows:

```
>>> def xor(a,b):
...     return a ^ b
>>> inputs = [(0, 0), (0, 1), (1, 0), (1, 1)]
...     outputs = [xor(x[0], x[1]) for x in inputs]
>>>
```

The XOR gate is approximated by a single layer neural net defined as:

```
>>> class XORNet(nn.Module):
...     def __init__(self):
...         super(XORNet, self).__init__()
...         self.layer1 = nn.Linear(2,4)
...         self.layer2 = nn.Linear(4,1)
...     def forward(self, x):
...         x = torch.relu(self.layer1(x))
...         x = self.layer2(x)
...         return x
>>> model = XORNet()
>>> # Define the loss function and optimizer
...     loss_func = nn.MSELoss() # Mean Squared Error Loss
...     optimizer = optim.SGD(model.parameters(), lr=0.01) # Stochastic Gradient Descent
>>> def weights_init(model):
...     for m in model.modules():
...         if isinstance(m, nn.Linear):
...             # initialize the weight tensor, here we use a normal distribution
...             m.weight.data.normal_(0, 1)
...
...     weights_init(model)
>>>
```

Convert inputs and outputs data to torch tensors for training

```
>>> X = torch.tensor(inputs, dtype=torch.float32)
>>> Y = torch.tensor([y for y in outputs], dtype=torch.float32).view(-1,1)
print("Inputs:", X)
print("Outputs:", Y)
#print(model(X))

Inputs: tensor([[0., 0.],
               [0., 1.],
               [1., 0.],
               [1., 1.]])
Outputs: tensor([[0.],
                [1.],
                [1.],
                [0.]])
```

```

>>> epochs = 2000 # Increased epochs
for epoch in range(epochs):
    Y_pred = model(X)
    loss = loss_func(Y_pred, Y)
    if epoch % 500 == 0:
        print(f'Epoch [{epoch}] Loss: {loss.item()}')

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

Epoch 0 Loss: 3.7070677280426025
Epoch 500 Loss: 0.014563385397195816
Epoch 1000 Loss: 0.001690817647613585
Epoch 1500 Loss: 0.00018612013082019985

>>> # Test the model
with torch.no_grad():
    test_pred = model(X)
    print("Predicted outputs:")
    print(test_pred.round())

Predicted outputs:
tensor([[0.],
       [1.],
       [1.],
       [0.]])

```

>>>

However, if we only use a single layer network defined below, it cannot approximate the XOR gate:

```

>>> class XORNetSingleLayer(nn.Module):
    def __init__(self):
        super(XORNetSingleLayer, self).__init__()
        self.layer1 = nn.Linear(2,1)
    def forward(self, x):
        x = torch.relu(self.layer1(x))
        return x

>>> model_single_layer = XORNetSingleLayer()
>>> # Define the loss function and optimizer
    loss_func = nn.MSELoss() # Mean Squared Error Loss
    optimizer = optim.SGD(model.parameters(), lr=0.01) # Stochastic Gradient Descent
>>> weights_init(model)
>>> epochs = 2000 # Increased epochs
for epoch in range(epochs):
    Y_pred = model_single_layer(X)
    loss = loss_func(Y_pred, Y)
    if epoch % 500 == 0:
        print(f'Epoch [{epoch}] Loss: {loss.item()}')

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

Epoch 0 Loss: 0.2725851237773895
Epoch 500 Loss: 0.2725851237773895
Epoch 1000 Loss: 0.2725851237773895
Epoch 1500 Loss: 0.2725851237773895

>>> # Test the model
with torch.no_grad():
    test_pred = model_single_layer(X)
    print("Predicted outputs:")
    print(test_pred.round())

Predicted outputs:
tensor([[0.],
       [0.],
       [1.],
       [1.]])

```

[0.]])

>>>

2 Homework

Problem 1. Formally state and prove that a single layer neural network (also known as perceptron) cannot approximate the **XOR** gate. Verify your result empirically. *Hint: derive a lower bound of the approximation error. Verify your bound by drawing the approximation error w.r.t. number of iterations.*

Problem 2. Formally state and prove that a two-layer neural network with more than 2 neurons in the hidden layer can approximate the **XOR** gate. *Hint: Manually construct a neural network that gives the same outputs as XOR gate and computes its parameters by hand.*