Prof. Dr. Andreas Hotho, Albin Zehe, Konstantin Kobs
Lehrstuhl für Data Science

24./25.5.2022

3. Assignment in "Machine Learning for Natural Language Processing"

Summer Term 2022

1 General Questions

1. What are the main components needed to train a neural network in PyTorch? Explain what each of these components is good for.
2. Suppose we build a neural network that is able to generate text. We need to find a loss function that is used to optimise the model. A friend suggests: "From the lecture, we know that a loss function must give a number that indicates how bad the model is, such that we can minimize this during gradient descent. Why don't we ask people to rate the quality of the quality of generated texts and use them as the loss function?" Why does this not work?

2 Neural Networks

Softmax and Categorical Cross Entropy

In the lecture, you learned that PyTorch's Categorical Cross Entropy Loss function implementation takes the unnormalised outputs of the network (called logits) and implicitly applies Softmax function to obtain a probability distribution that is required in the mathematical definition of Cross Entropy.

Cross Entropy is defined as $L_{CE}(p) = -\sum_{i=1}^{n} y_i \log(p_i)$, where p is the predicted probability distribution, y is the desired output probability distribution, and n is the length of both of these vectors. Assuming that only one class is correct, i.e. y is a one-hot encoded vector, this leads to Categorical Cross Entropy: $L_{CCE}(p) = -\log(p_c)$, where c is the index of the correct output class.

On the other hand, Softmax is defined as $p_i = Softmax(o_i) = \frac{e^{o_i}}{\sum_{k=1}^{n} e^{o_k}}$ for an element of the unnormalised output vector o.

To optimise the gradient calculation of the combination of Softmax and Categorical Cross Entropy, PyTorch combines them in one single Module.

In order to understand why implicitly applying the Softmax function is more efficient, calculate the derivatives for the combination of both functions w.r.t. the output of the neural network o (you should do this by hand). Compare this to the derivatives of each step individually (you are encouraged to do this by hand; you will need the quotient rule).

3 Python

3.1 Implementing Neural Networks Part 1 — The Forward Pass

In this assignment, you will implement a neural network "library" yourself, using `Python` and `Numpy` (`import numpy as np`). The tool is inspired by PyTorch's implementation. This week, you will implement the forward pass. Next week, the backward pass and backpropagation will follow.

Modules We will follow PyTorch's code structure when building single parts of our library, such as neural network layers, loss functions, or optimizers. Parts are called "Modules" in PyTorch, so we will use this terminology. Each of the following modules should have the same structure: A module is a Python class with a `forward` and a `backward` function. The `forward` function calculates the results for the module based on the previous results. The `backward` function calculates the gradients of the module. Today, you only have to code the `forward` functions of the following modules.

Sigmoid Implement the `forward` function that takes as parameter a Numpy array of numbers and applies an element-wise sigmoid on this array!

```
class Sigmoid:
    def __init__(self):
        #...
        pass

    def forward(self, x: np.array) -> np.array:
        #...
        pass
```

```
def backward(self, x: np.array, grad: np.array =
↪  np.array([[1]])) -> np.array:
    # don't mind me this week
    pass
```

Mean Squared Error Implement the `forward` function that takes as parameter two Numpy arrays of numbers and returns the mean squared error between these arrays! The mean squared error is defined as follows:

$$se = \frac{1}{2}(t - o)^2,$$

$$mse = \frac{1}{n}\sum_{i=1}^{n} se_i,$$

where n is the size of the vectors, o is the predicted output of the neural network and t is the true label.

```
class MeanSquaredError:
def __init__(self):
    #...
    pass

def forward(self, y_pred: np.array, y_true:
↪  np.array) -> float:
    #...
    pass

def backward(self, y_pred: np.array, y_true:
↪  np.array, grad: np.array = np.array([[1]])) ->
↪  np.array:
    # don't mind me this week
    pass
```

Fully Connected Layer A neural network layer is also a module. If we define one layer as a module, we can create multiple instances of it and send the output of one layer into another layer. This way, we are very flexible in terms of how the data flows through our program. To be very flexible when it comes to the layer input and output sizes, we specify two parameters in this module.

Implement the following class such that we can create a fully connected layer with any input or output size (larger than zero). `self.weights` and `self.bias` are attributes of this class. They store the weights and bias matrix, respectively. For initialization, the weights should be standard-normally distributed. The initial bias values are zero. The `forward` function gets the input and calculates the output of the layer. The input is a 2d array, where each **row** is a data point. This is the same as PyTorch handles data points.

```
class FullyConnectedLayer:
def __init__(self, input_size: int, output_size:
 ↪  int):
    #...
    pass

def forward(self, x: np.array) -> np.array:
    #...
    pass

def backward(self, x: np.array, grad: np.array =
 ↪  np.array([[1]])) -> np.array:
    # don't mind me this week
    pass
```

Neural Network We now have all of the required building blocks to create our first neural network! We will implement a neural network also as a module, i.e. as a class.

In the constructor of the class, we can create all layers and activation functions that we need for the network. In the `forward` function the flow of an input `x` through the network is then implemented. The return value of this function should be the output of the network.

To make the network more flexible, implement the class such that we can specify the following parameters during initialization:

input_size The number of input neurons

output_size The number of output neurons

hidden_sizes The number of neurons in the hidden layers as a list

activation A class reference of the activation function used for the hidden layers

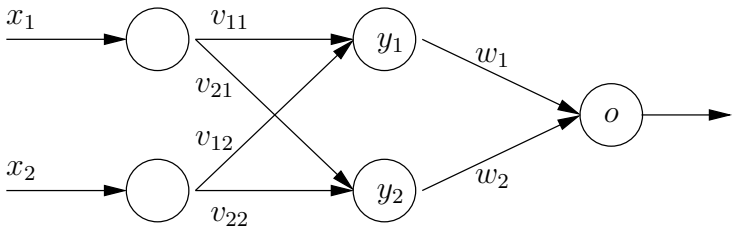
```
class NeuralNetwork:
def __init__(self,
```

```
                input_size: int,
                output_size: int,
                hidden_sizes: List[int],
                activation=Sigmoid):
        #...
        pass

    def forward(self, x: np.array) -> None:
        #...
        pass

    def backward(self, x: np.array, grad: np.array =
    ↪  np.array([[1]])) -> Tuple[np.array]:
        # don't mind me this week
        pass
```

Testing the Implementation We now have a (hopefully working) Neural Network class. To test this, we will model the network from last week. The network looks like this:



We compute the output and the loss function of the network for input $x = (1, 1)$ and target label $t = 0$. Assume the same initial values as last week:

$$v = \begin{pmatrix} 0.5 & 0.75 \\ 0.25 & 0.25 \end{pmatrix}, w = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$$

One very convenient thing in Python is that we can just change values of object attributes.

```
if __name__ == "__main__":
    # Network Initialization
    net = NeuralNetwork(2, 1, [2], Sigmoid)
```

```
# Setting the layer weights
net.layers[0].weights = np.array([[0.5, 0.75], [0.25,
↪  0.25]])
net.layers[1].weights = np.array([[0.5], [0.5]])

# Loss
loss_function = MeanSquaredError()

# Input
x = np.array([[1, 1]])
y = np.array([[0]])

# Forward Pass
pred = net.forward(x)

# Loss Calculation
loss = loss_function.forward(pred, y)

print(f"Prediction: {pred}")
print(f"Loss: {loss}")
```