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15./16.05.2024

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

Summer Term 2024

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.

   a) The dataset: We need a training and a test dataset (often, also a validation dataset to find the best hyperpameters) to let the model learn from.

   b) The model: We need a model to train, which can be simple or complex but is wrapped in a PyTorch Module.

   c) The optimiser: We need an optimiser to update the model parameters.

   d) The loss function: We need a loss function to calculate the error of the model.

   e) The training loop: We need a training loop to iteratively calculate the loss for the current state of the model and update its parameters.

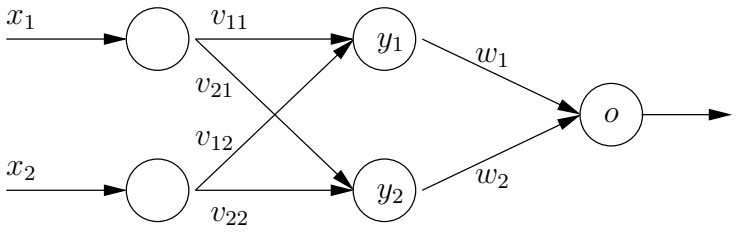
2. Suppose we build a neural network that is able to generate text. We need to find a loss function that is used to optimise the model. A friend suggests: "From the lecture, we know that a loss function must give a number that indicates how bad the model is, such that we can minimize this during gradient descent. Why don't we ask people to rate the quality of generated texts and use them as the loss function?" Assuming we want to optimize our model via backpropagation, what is the problem of this approach?

   The loss function indeed outputs a number given the output of the network. However, the loss function must be differentiable, in order to propagate the gradients to the model parameters. Humans are not differentiable, since we cannot calculate a derivative of their decision/rating process. There are meth-

ods in machine/deep learning that work with non-differentiable feedback (e.g. human feedback), for example reinforcement learning. However, in the general learning setting, we cannot directly use humans as loss functions.

2 Neural Networks and Circuit Diagrams

Given the following neural network with `sigmoid` as activation function:

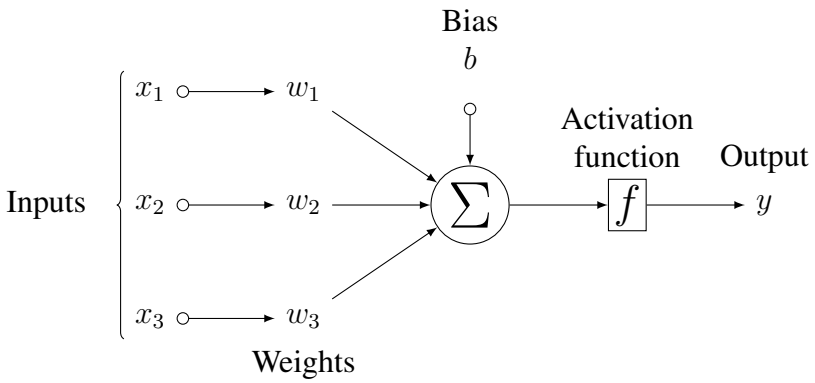


1. Represent the network as three equations (one each for y_1, y_2 and o)! We do not use any bias in this network.

$$
\begin{aligned}
y_1 &= \sigma(x_1 v_{11} + x_2 v_{12}) \\
y_2 &= \sigma(x_1 v_{21} + x_2 v_{22}) \\
o &= \sigma(y_1 w_1 + y_2 w_2)
\end{aligned}
$$

2. Convert the network to a circuit diagram as the one shown in the lecture!
   Hint: Draw the diagram as large as possible. You will need space for the back-propagation.

Remember that a neuron's internal structure looks like this:



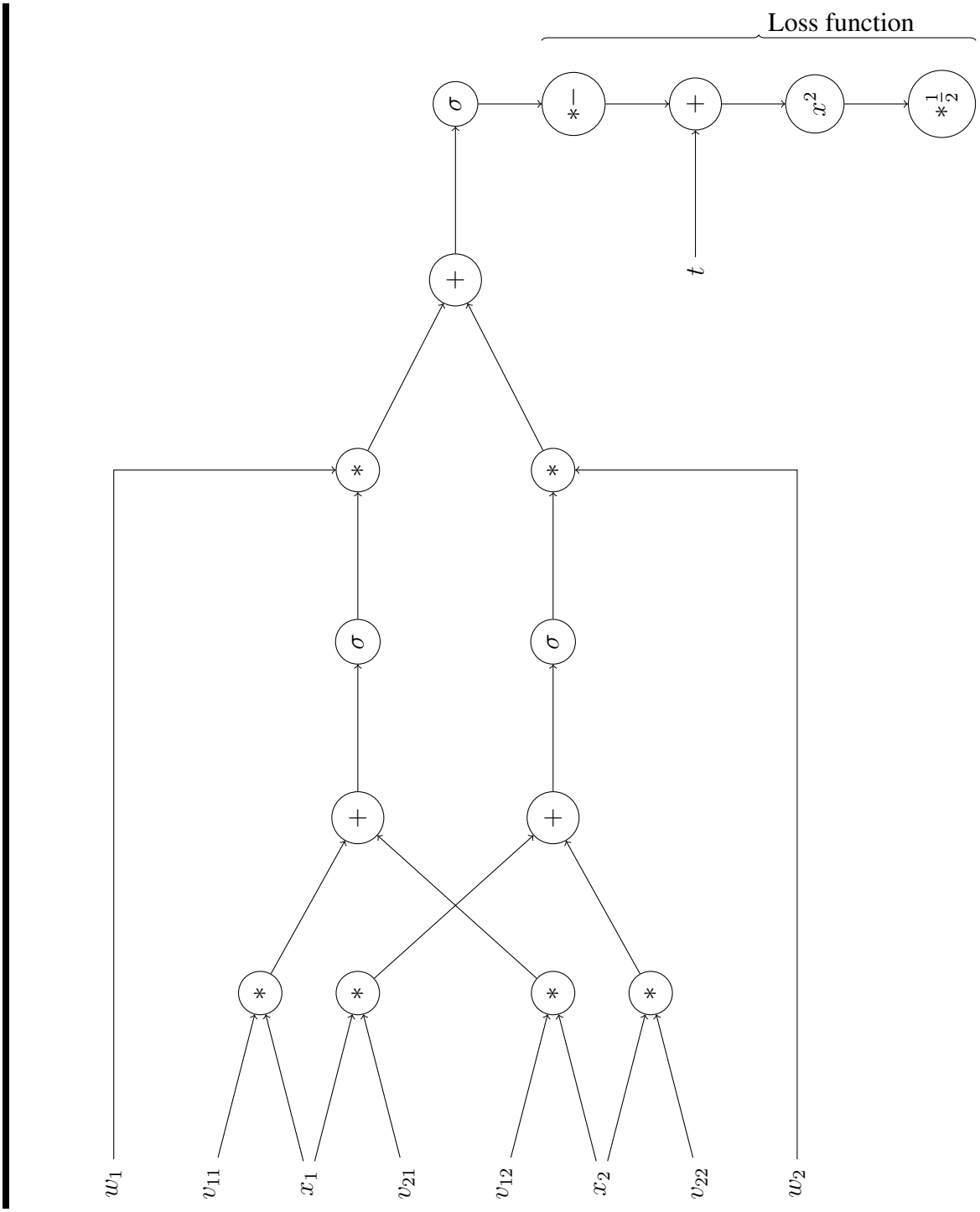
For the circuit diagram, see the next solution.

3. To measure the quality of our weights, we will use the following loss function:

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

where o is the output of the network and t is the target (correct) label.

Add the loss function to the circuit diagram from the last subtask!



4. Now that we have a circuit diagram, we can rather easily do backpropagation.

Determine the partial derivatives for all *weights* ($v_{11}, v_{12}, v_{21}, v_{22}, w_1$ and w_2) in the network!

Assume the following initial values: $v = \begin{pmatrix} 0.5 & 0.75 \\ 0.25 & 0.25 \end{pmatrix}$, $w = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$.

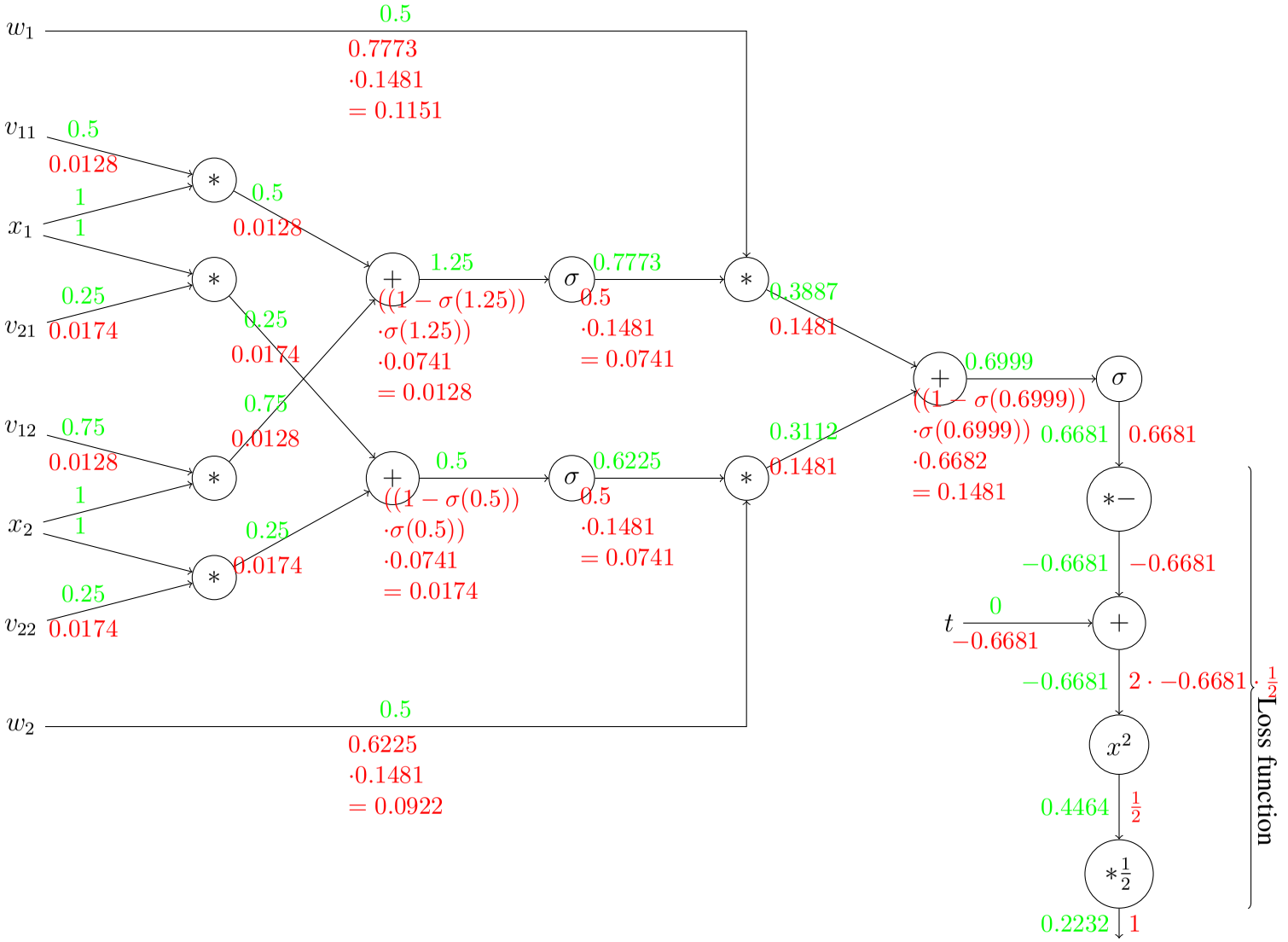
The inputs are $(x_1, x_2) = (1, 1)$ and the target label is $t = 0$.

Remember the intuitive properties of $+$ and $*$ from the slides:

- $+$ just passes the gradient through, both inputs have the same partial derivative as the output
- $*$ "switches" the input, that is: if the gradient after the $*$ is 2 and the inputs are 1 and 3, then first input gets the partial derivative $3 \cdot 2 = 6$ and the second input gets $1 \cdot 2 = 2$.

Here are some gradients that you will need:

- $f_a(x) = ax \rightarrow \frac{df}{dx} = a$
- $f(x) = x^2 \rightarrow \frac{df}{dx} = 2x$


w_1
0.5
0.7773
·0.1481
= 0.1151
v_{11}
0.5
0.0128
x_1
1
1
v_{21}
0.25
0.0174
v_{12}
0.75
0.0128
x_2
1
1
v_{22}
0.25
0.0174
w_2
0.5
0.6225
·0.1481
= 0.0922
0.5
0.0128
0.25
0.0174
0.75
0.0128
0.25
0.0174
1.25
((1 − σ(1.25))
·σ(1.25))
·0.0741
= 0.0128
0.5
((1 − σ(0.5))
·σ(0.5))
·0.0741
= 0.0174
0.7773
0.5
·0.1481
= 0.0741
0.6225
0.5
·0.1481
= 0.0741
0.3887
0.1481
0.3112
0.1481
0.6999
((1 − σ(0.6999))
·σ(0.6999))
·0.6682
= 0.1481
0.6681
0.6681
−0.6681
−0.6681
0
−0.6681
−0.6681
2 · −0.6681 · $\frac{1}{2}$
0.4464
$\frac{1}{2}$
0.2232
1
Loss function

❓ Something to think about

5. Backpropagation would enable us to compute a gradient for the *input values* (x_1, x_2), too. What could we do with the information about the input's gradient?

> The gradient of inputs is used, for example, in the creation of *adversarial examples*. These inputs are specifically crafted to confuse a network, for example to achieve a misclassification.
>
> For more details, see `https://arxiv.org/abs/1412.6572`.

3 Python

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

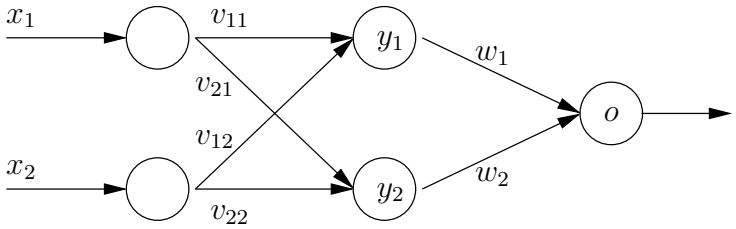
activation A class reference of the activation function used for the hidden layers

```
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}")
```

```
import numpy as np
from typing import List, Tuple


class Sigmoid:
    def __init__(self):
        pass

    def forward(self, x: np.array) -> np.array:
        return 1 / (1 + np.exp(-x))

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

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

    def forward(self, y_pred: np.array, y_true:
    ↪  np.array) -> float:
        return np.mean(0.5 * (y_true - y_pred) ** 2)

    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


class FullyConnectedLayer:
    def __init__(self, input_size: int, output_size:
    ↪  int):
        self.input_size = input_size
        self.output_size = output_size

        self.weights = np.random.randn(self.input_size,
        ↪  self.output_size)
        self.bias = np.zeros((1, self.output_size))

    def forward(self, x: np.array) -> np.array:
        return np.matmul(x, self.weights) + self.bias

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


class NeuralNetwork:
    def __init__(self,
                 input_size: int,
                 output_size: int,
                 hidden_sizes: List[int],
```

```
                activation=Sigmoid):
        s = [input_size] + hidden_sizes + [output_size]

        self.layers = [FullyConnectedLayer(
            s[i], s[i+1]) for i in range(len(s) - 1)]
        self.activation = activation()

    def forward(self, x: np.array) -> None:
        for layer in self.layers[:-1]:
            x = layer.forward(x)
            x = self.activation.forward(x)

        # The last layer should not be using an
        ↪  activation function
        x = self.layers[-1].forward(x)

        return x

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


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}")
```