

Exercise 2

Due on: Thursday, 02.05.2024

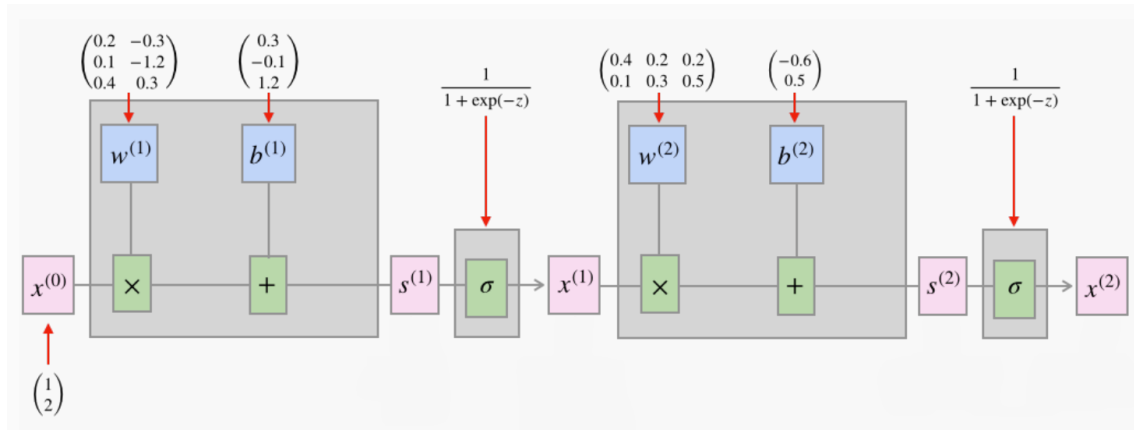


Figure 1: A simple neural network.

Task 5 A Simple Neural Network

Let $x^{(0)} = (1, 2)^\top \in \mathbb{R}^2$ be a data point and $y = (0, 1)^\top \in \mathbb{R}^2$ be the target. Consider the neural network with sigmoid activation functions depicted in Figure 1.

- Compute the forward pass of $x^{(0)}$ by hand. What is the value of $x^{(2)}$?
- Compute the gradients with respect to all parameters in the network using backpropagation. For simplicity, you can use the squared loss function.

Task 6 A Neural Network Implementation

We now want to implement a neural network as a class in Python. Check the template `code2.py`.

Part 1

- Implement the ReLU and sigmoid activation functions and their derivatives.

- (ii) The class `NeuralNetwork` already has two member functions `__init__` and `forward`. Fix the TODOs and
 - (a) initialize the weights via $w_{ij} \sim \mathcal{N}(0, \sigma^2)$, where $\sigma = \sqrt{\frac{2}{d_{\text{in}} + d_{\text{out}}}}$, d_{in} denotes the number of input neurons, and d_{out} denotes the number of output neurons of that layer
 - (b) initialize the biases as zeros
 - (c) implement the forward pass

Make sure to also save the intermediate results (e.g. $x^{(\ell)}$, $s^{(\ell)}$, see Figure 1) when computing the forward pass. We will need those later on.

Hint: You can test your implementation by overwriting the weights and biases with the values from Task 5 (i) and compare all intermediate results.

Part 2

- (i) Implement backpropagation as a member function `backprop(self, x, y)`. It should compute the gradients of all parameters.
- (ii) Implement a training function `train(self, x, y, eta=.01, iterations=100)` that implements (batch) gradient descent. You can use the squared loss if not stated otherwise.
- (iii) Test your training procedure by fitting a binary classification problem on toy data and visualize the prediction appropriately. Make sure to use a sigmoid activation and a single neuron in the output layer.

Hint: You can test your implementation by comparing the results with the values from Task 5 (ii).

Task 7 Approximating a Function Using ReLUs

In this task, we aim to approximate a function $f : [a, b] \rightarrow \mathbb{R}$ arbitrarily well using a neural network with a single hidden layer consisting of n neurons based on ReLU activations.

Consider a grid of n equidistant points $x_1, x_2, x_3, \dots, x_n$, with $a = x_1$ and $b = x_n$. Furthermore, the grid has a constant spacing of $h = x_{i+1} - x_i$ for $i = 1, 2, \dots, n-1$. We want to approximate f using a linear combination of ReLU functions given by

$$\text{NN}(x) = \sum_{i=1}^n \lambda_i \cdot \text{ReLU}(x - b_i),$$

where $\lambda_i \in \mathbb{R}$ are weights and the biases are given by $b_1 = a - h$, $b_2 = a$, $b_3 = a + h$, \dots , $b_n = b - h$.

Prior to b_1 , all ReLU functions $\max(0, x - b_i)$ are zero. Between $b_1 = a - h$ and $b_2 = a = x_1$, only the first ReLU function $\max(0, x - b_1)$ can be non-zero. The function $\lambda_1 \cdot \max(0, x - b_1)$ is supposed to approximate f at x_1 . If we subtract that function from f , we obtain a new function which the next ReLU function can approximate, and iterate to the end. Hence, we can approximate the function f on the interval $[a, b]$ using a sum of n ReLU functions.

To learn the parameters λ_i we can construct a linear system of equations

$$f(x_i) = \sum_{j=1}^n \lambda_j \cdot \text{ReLU}(x_i - b_j) \quad \text{for } i = 1, \dots, n.$$

By using $x_i = a + (i - 1)h$ and $b_j = a + (j - 2)h$, we obtain $x_i - b_j = (i - j + 1)h$. Considering i and j where the ReLU is positive,

$$f(x_i) = \sum_{j=1}^i \lambda_j (i - j + 1)h \quad \text{for } i = 1, \dots, n. \tag{1}$$

Write down the linear system determined by Equation (1). Then, implement this approximation method, solve for $\lambda_1, \lambda_2, \dots, \lambda_n$, and experiment with various values of n . Check `code2.py`.