

Introduction to neural networks II

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Objectives

- Recall the feedforward of a neural network
- The binary classification problem
- How to build a neural network that can classify a binary labeled data?
- How can we build a neural network that can classify a multi-labeled data?
- Introduction of the sigmoid function
- Introduction of the softmax function
- Computational Graphs
- Backprop and automatic differentiation
- The approximation power of neural networks (universal approximation theorem)

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Lets recall the feedforward algorithm before first.

Feedforward Neural Network

How do we compute a feedforward neural network on an input x ?

Feedforward Neural Network

Start with an input $x = a^{(0)}$. In the picture, this is represented by the first layer of nodes. We will call this layer 0.

$$x = a^{(0)}$$

Feedforward Neural Network

We apply the weight $W^{(1)}$ coming from the edges between layer 0 and layer 1 and add the biases and then apply the Activation function on the resulting vector coordinate-wise.

$$x = a^{(0)} \longrightarrow \sigma(W^{(1)}a^{(0)} + b^{(1)})$$

$W^{(1)}$: Edges between
layer 0 and layer 1

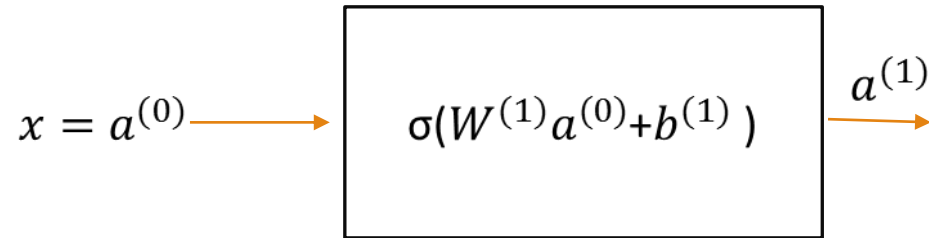
$a^{(0)}$: input

$b^{(1)}$: biases applied to layer 1

σ : activation function

Feedforward Neural Network

We will call the output of this computation $a^{(1)}$. This is now represented by the nodes in layer 1.



$W^{(1)}$: Edges between
layer 0 and layer 1

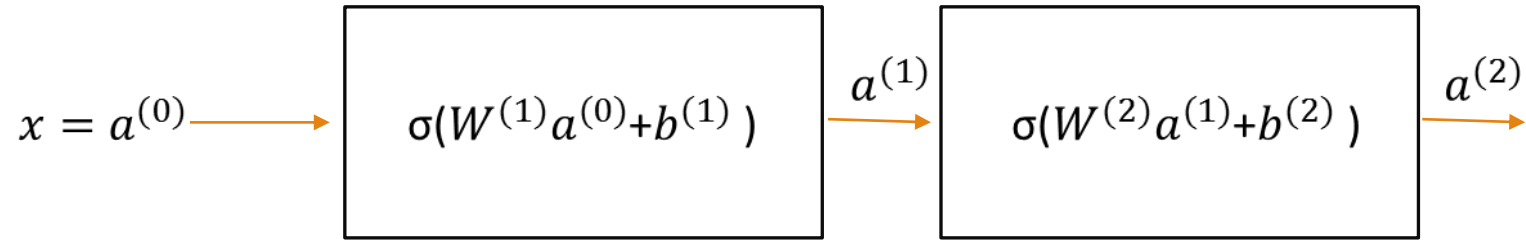
$a^{(0)}$: input

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σ : activation function

Feedforward Neural Network

Repeat.



$W^{(2)}$: Edges between
layer 1 and layer 2

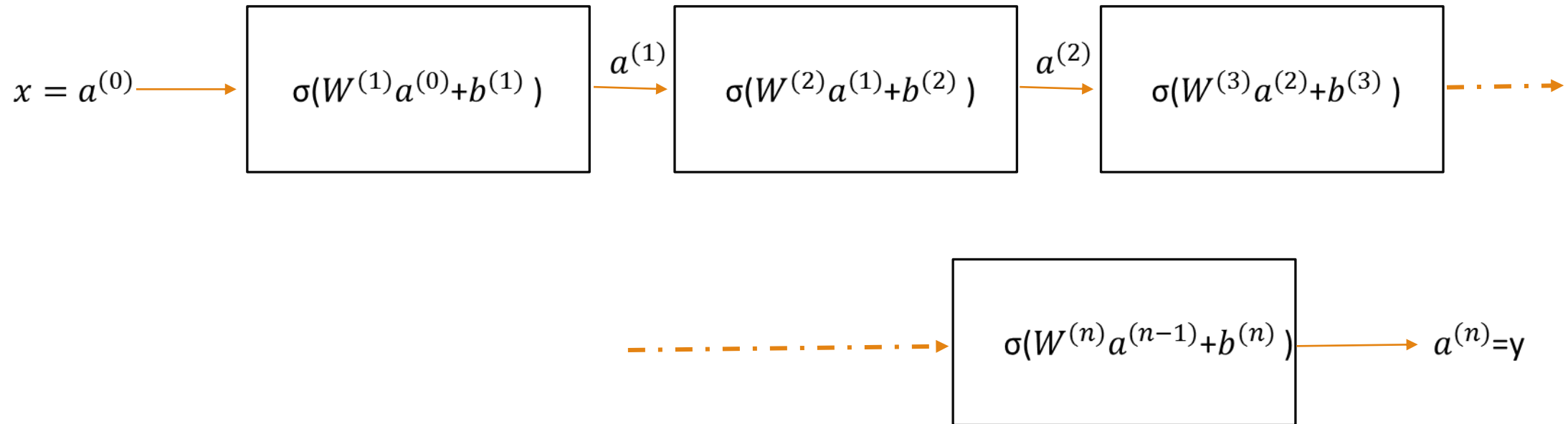
$a^{(1)}$: input from layer 1

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Feedforward Neural Network

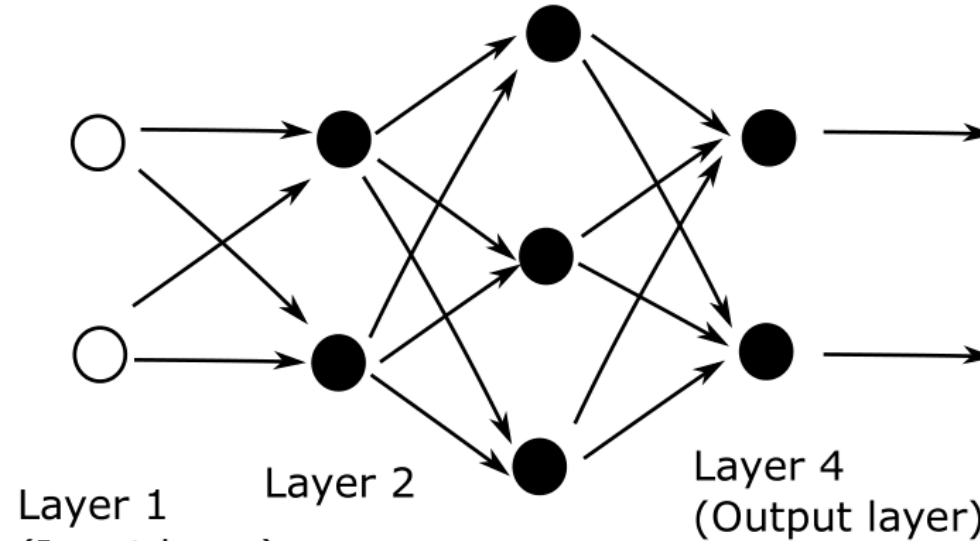
Until you finish the neural network and get the final output.



Example

We will use an example from [this](#) paper.

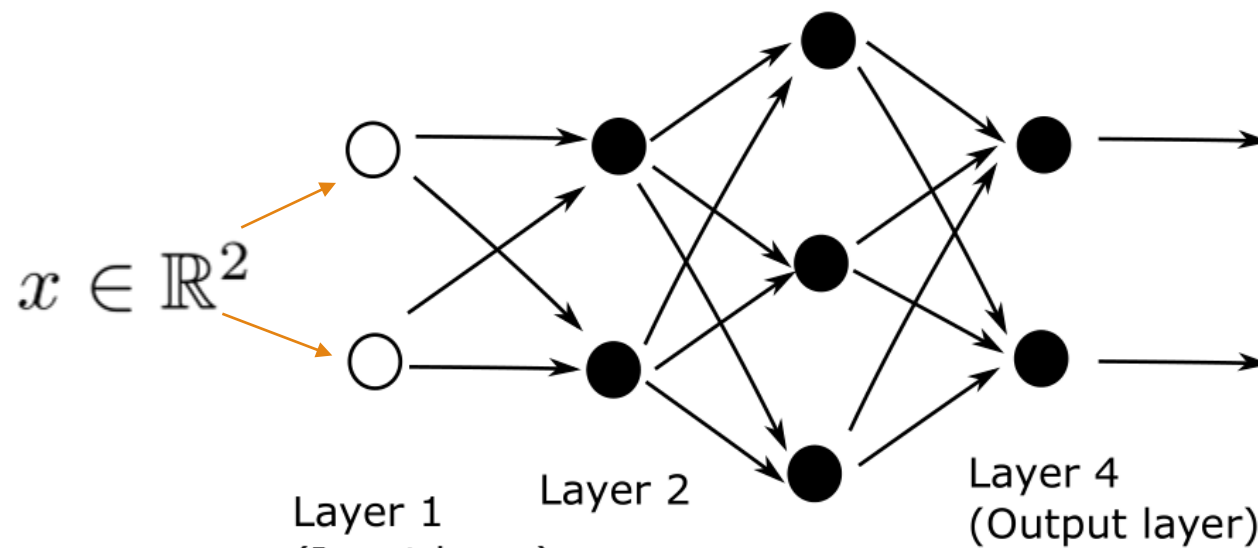
(note that the convention of the index is a little different here)



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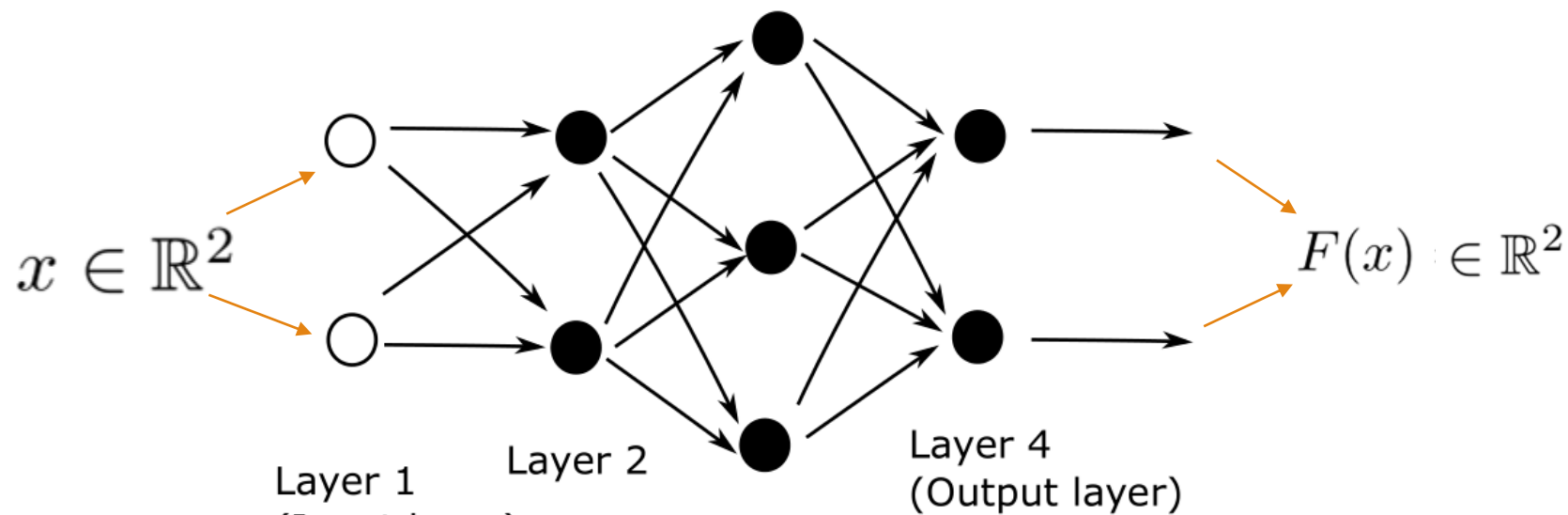
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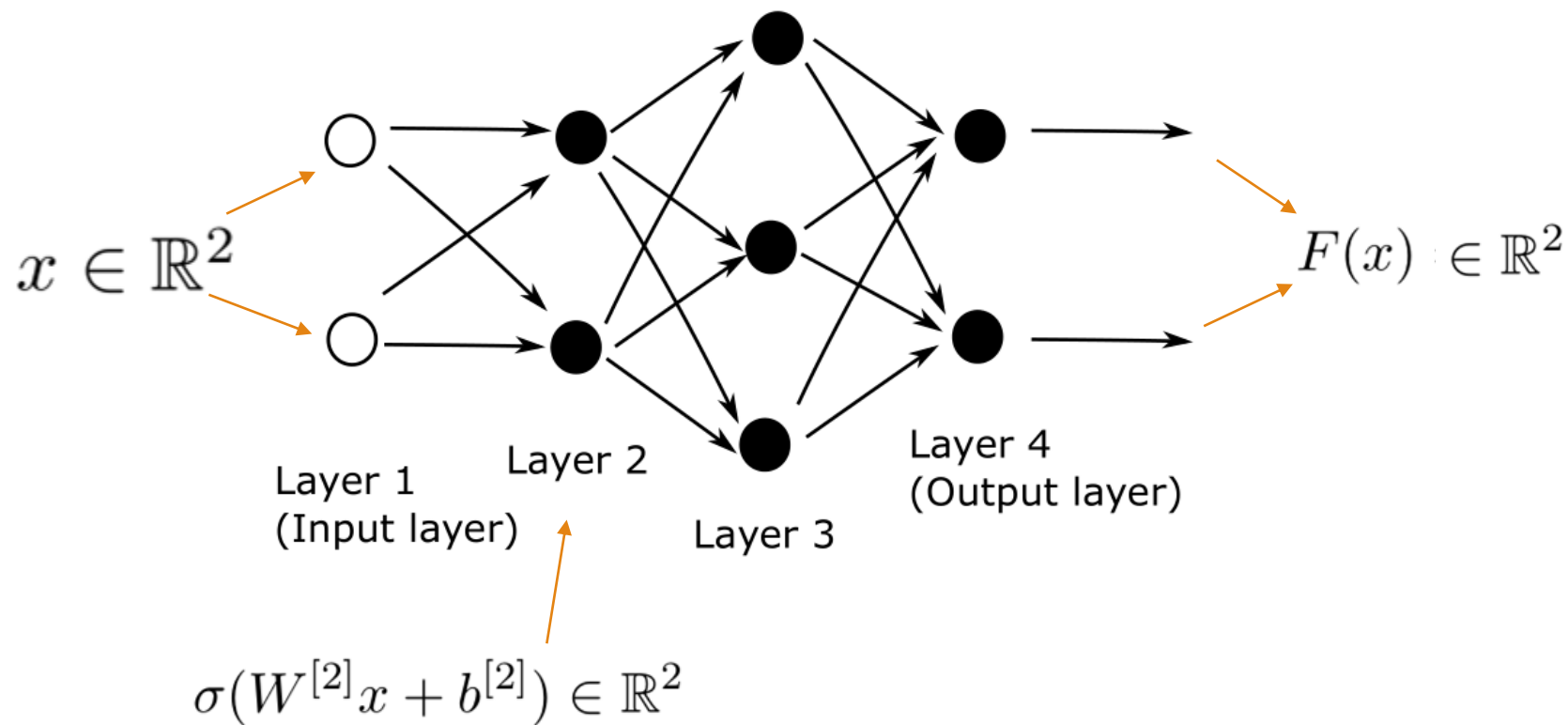
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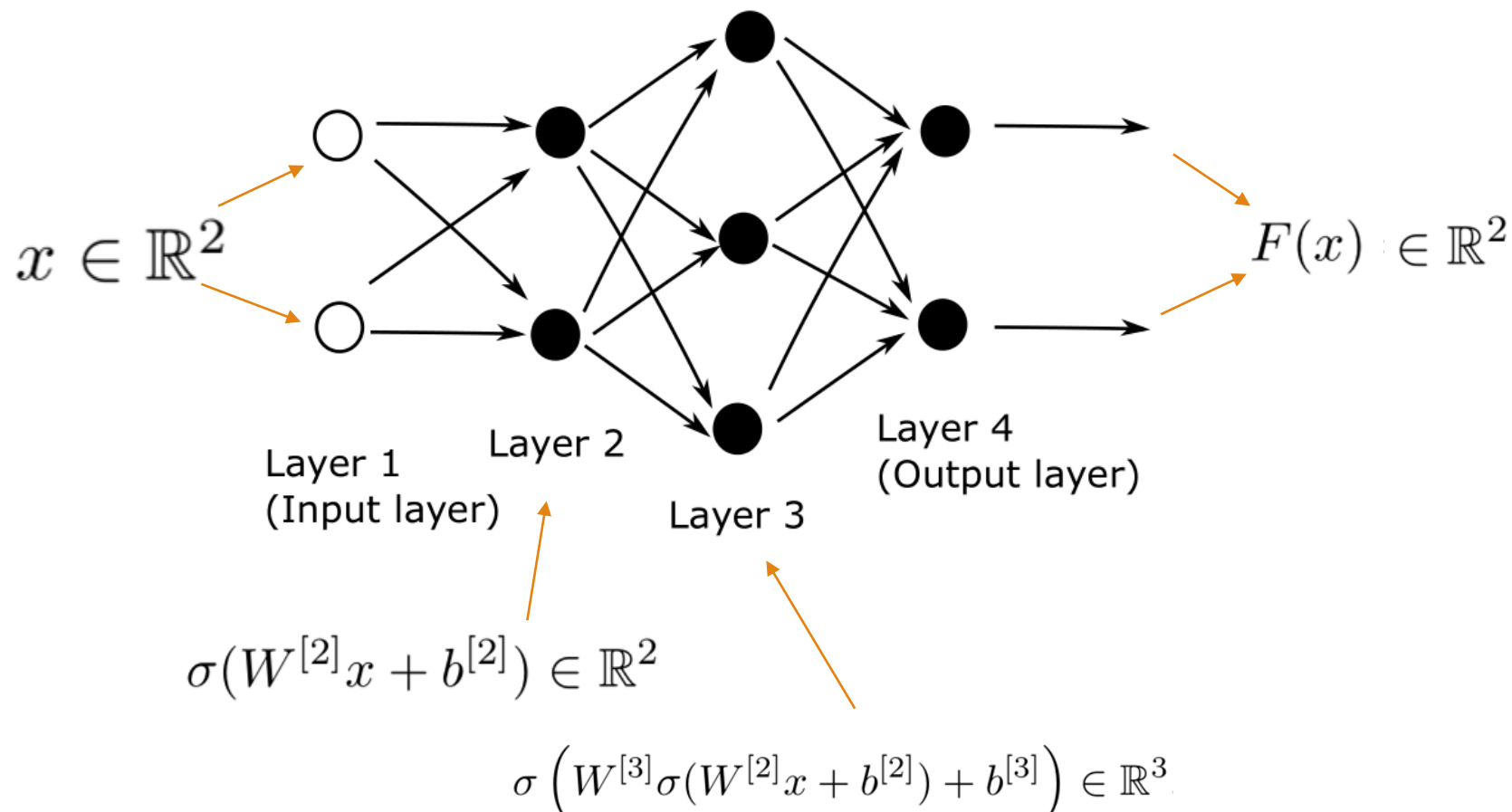
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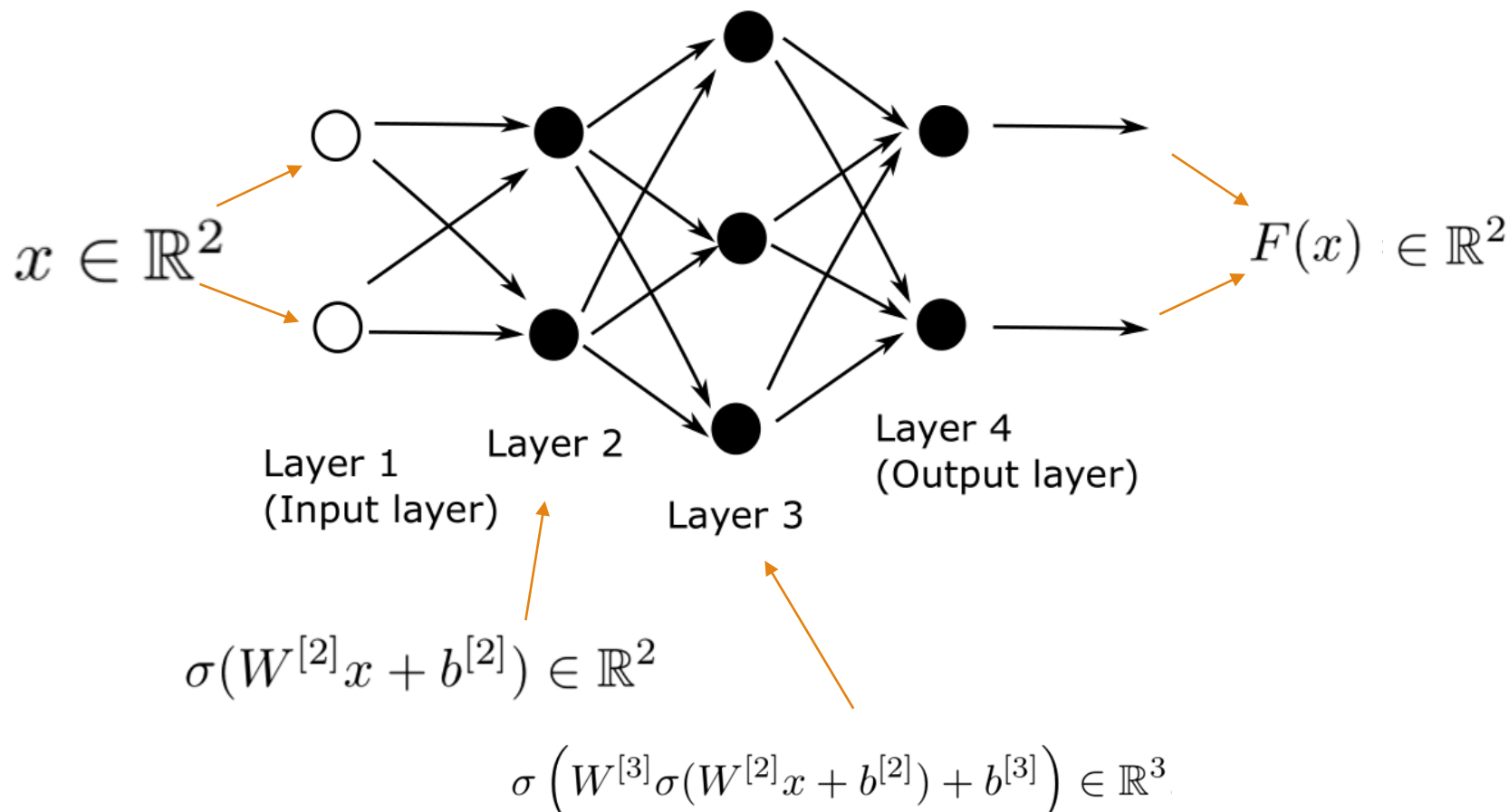
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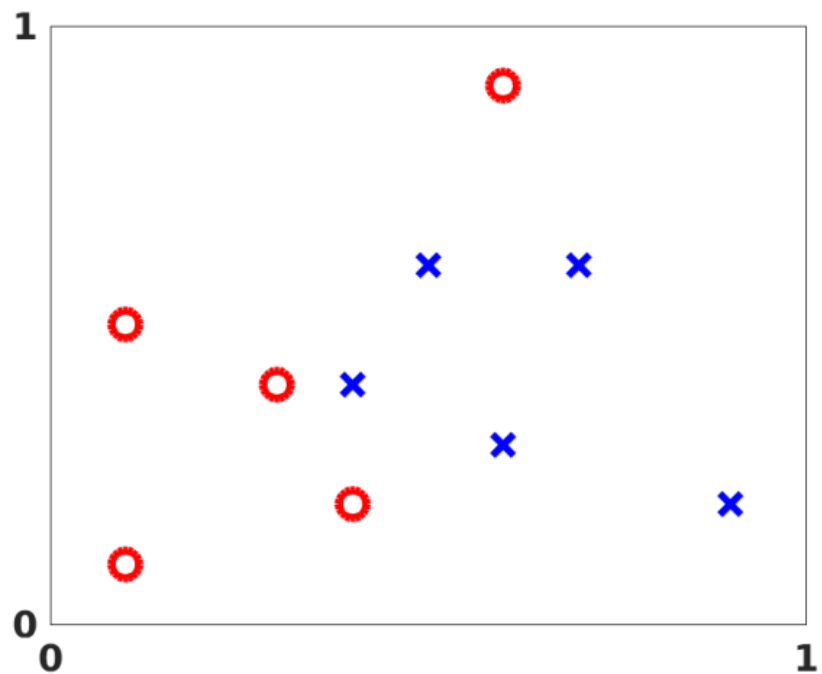
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Final function representing the neural network

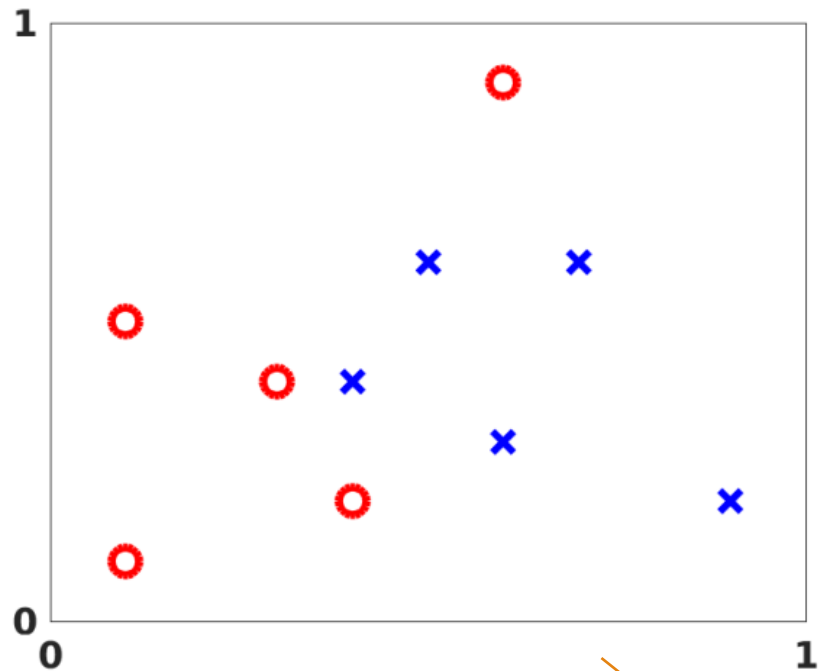
$$F(x) = \sigma \left(W^{[4]} \sigma \left(W^{[3]} \sigma(W^{[2]}x + b^{[2]}) + b^{[3]} \right) + b^{[4]} \right) \in \mathbb{R}^2.$$

Example



Input : labeled data X

Example

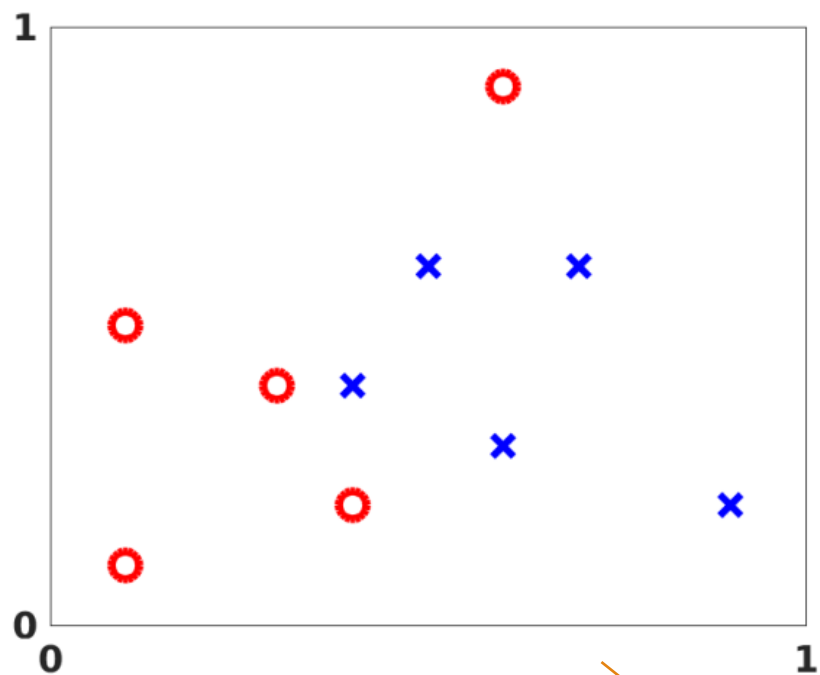


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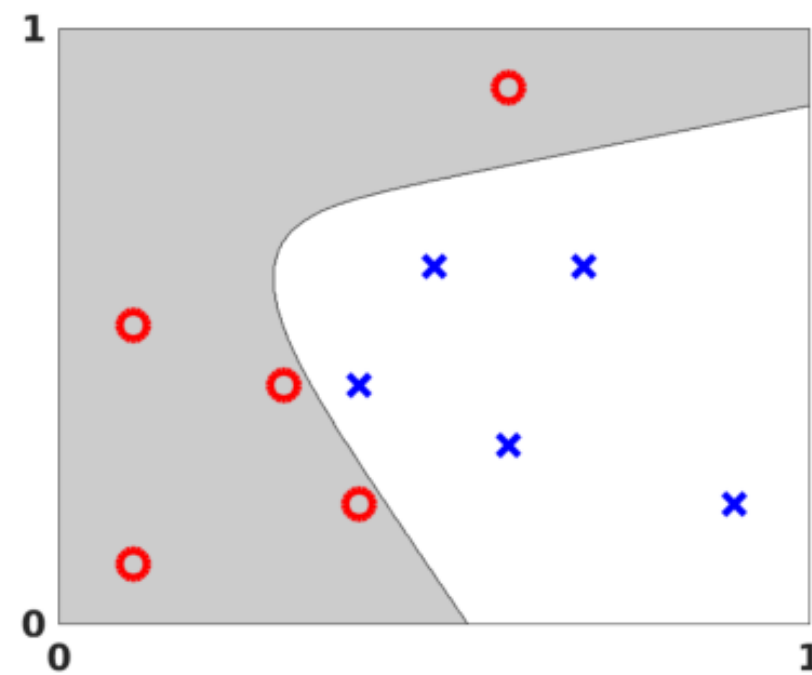
$$\text{Cost} \left(W^{[2]}, W^{[3]}, W^{[4]}, b^{[2]}, b^{[3]}, b^{[4]} \right) = \frac{1}{10} \sum_{i=1}^{10} \frac{1}{2} \|y(x^{\{i\}}) - F(x^{\{i\}})\|_2^2.$$

the difference between the output given by the network and the actual label

Example



Input : labeled data X



Minimize the cost function

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Binary classification

Now suppose that we have data set that consists of images of cats and dogs and we built a neural network that takes as input an image from this data set and gives out a vector in \mathbb{R}^1 (a real number).

How exactly do we use this vector for our classification task ? In general the output $f(x)$ coming from the neural network Does not match the class $\{\pm 1\}$ of the input point x (it could be any real number).



Binary classification

This function takes a tensor of size `input_size` and returns a real number.

How can we constrain the output to be between -1 and +1?

```
import torch
import torch.nn as nn

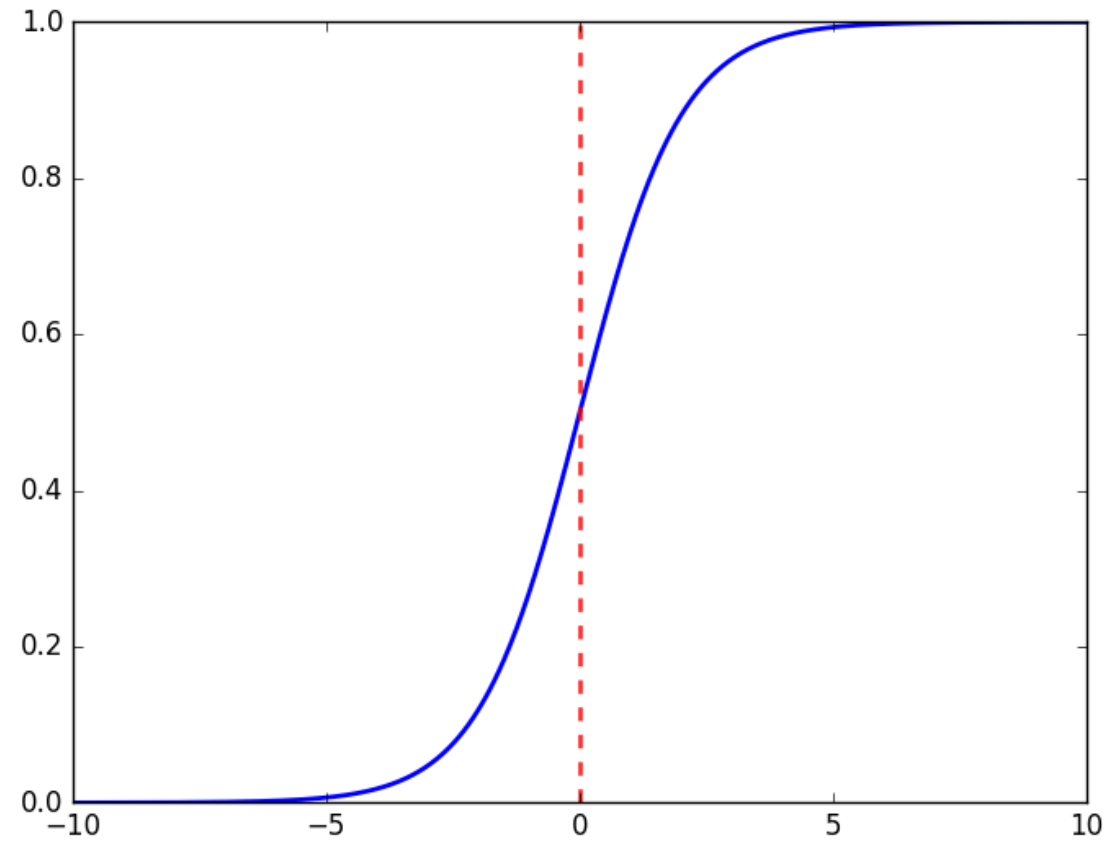
class Net(nn.Module):
    def __init__(self, input_size, hidden_size):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.fc2 = nn.Linear(hidden_size, 1)

    def forward(self, x):
        x = torch.relu(self.fc1(x))
        x = self.fc2(x)
        return x
```

Binary classification

To obtain the required binary classification, we pass the output $f(x)$ through another function :

$$g(z) = 1/(1 + e^{-z})$$



The graph of the sigmoid function

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This function returns an output between 0 and 1. The binary classification is set as follows :

If ($g(z) \geq 0.5$) assign the input the positive class

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Else assign the input to the negative class

But what do we do in the multi-class classification ?

Multi-class classification : the softmax function

In the case of multi-class classification, we use the softmax activation function.
Suppose that we have k classes then the softmax activation function is define by :

$$\text{softmax}(z)_i = \frac{\exp(z_i)}{\sum_{l=1}^k \exp(z_l)}$$

Here z_i represents the i th element of the input to softmax, which corresponds to class i .

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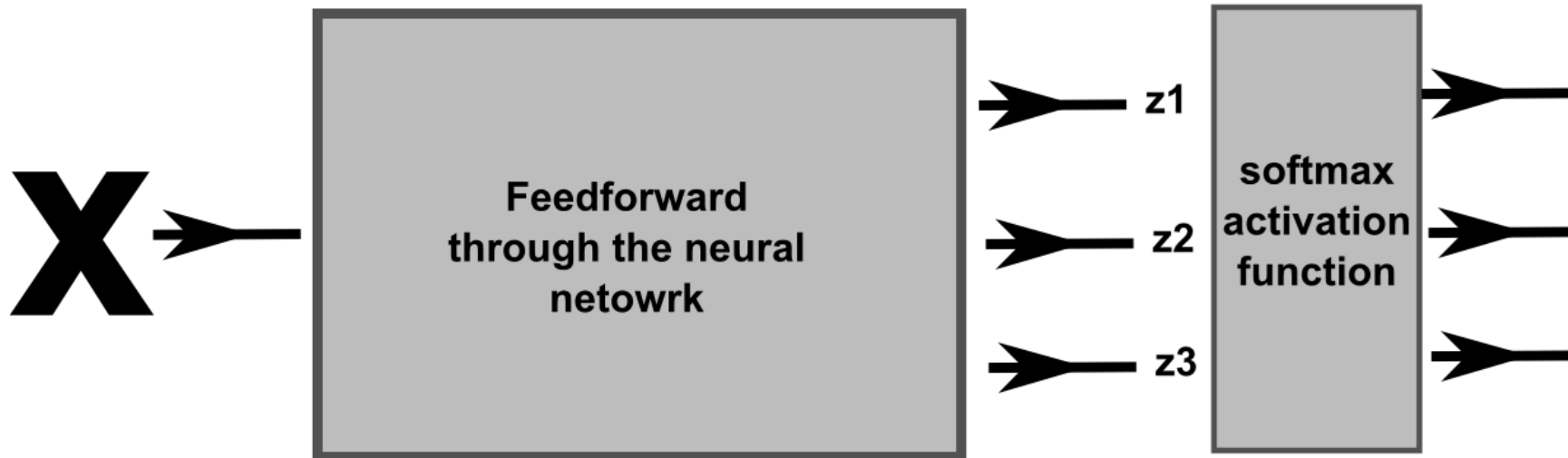
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The softmax function in Python

The softmax function is a mathematical function used to convert a vector of real numbers into a probability distribution.

It takes an input vector and returns another vector of the same length, where each element is transformed to a value between 0 and 1, representing the probability of that element being selected. In simple terms, the softmax function normalizes the input vector and makes it easier to interpret as probabilities. Here's a Python example:

```
import numpy as np

def softmax(x):
    exp_values = np.exp(x)
    probabilities = exp_values / np.sum(exp_values)
    return probabilities

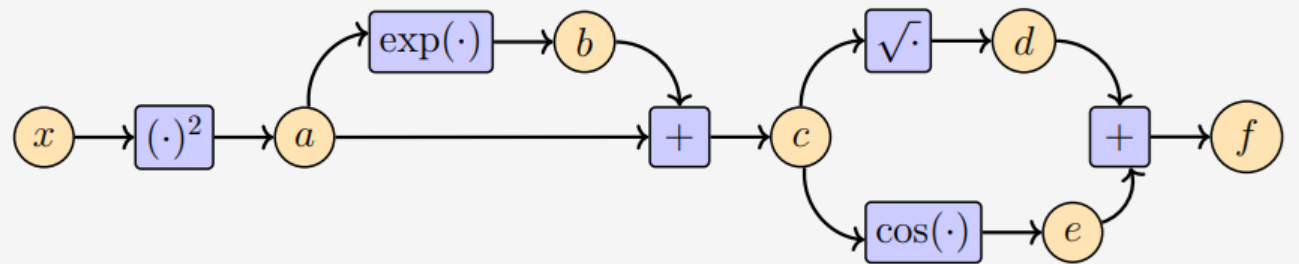
input_vector = np.array([2.0, 1.0, 0.5])
output_vector = softmax(input_vector)
print(output_vector)

[0.62842832 0.2312239 0.14034778]
```

What is a computational graph ?

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2))$$

$$\begin{aligned} a &= x^2, \\ b &= \exp(a), \\ c &= a + b, \\ d &= \sqrt{c}, \\ e &= \cos(c), \\ f &= d + e. \end{aligned}$$



Computation graph of f

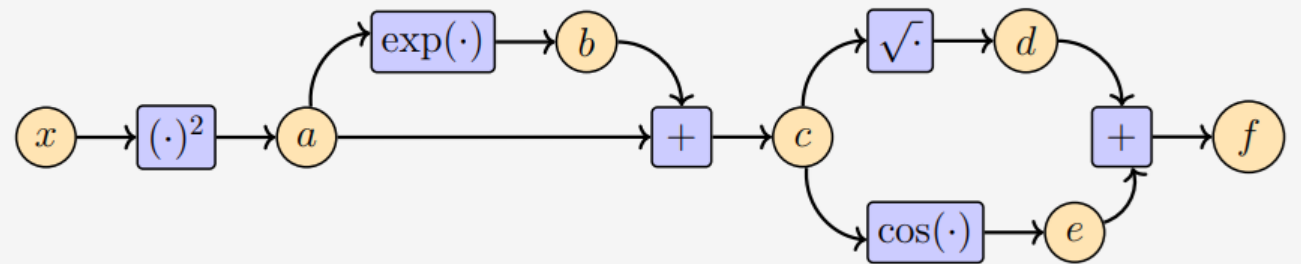
Image source

What is a computational graph ?

- A computational graph, also known as a computational or **directed acyclic graph** (DAG), is a directed graph that represents a computational process or a sequence of computations.
- It is a graph structure where nodes represent operations or computations, and directed edges represent dependencies between these operations.
- Note: yellow nodes in the graph here are placeholders and not really part of the computational graph. They get executed when we insert a certain input to the graph

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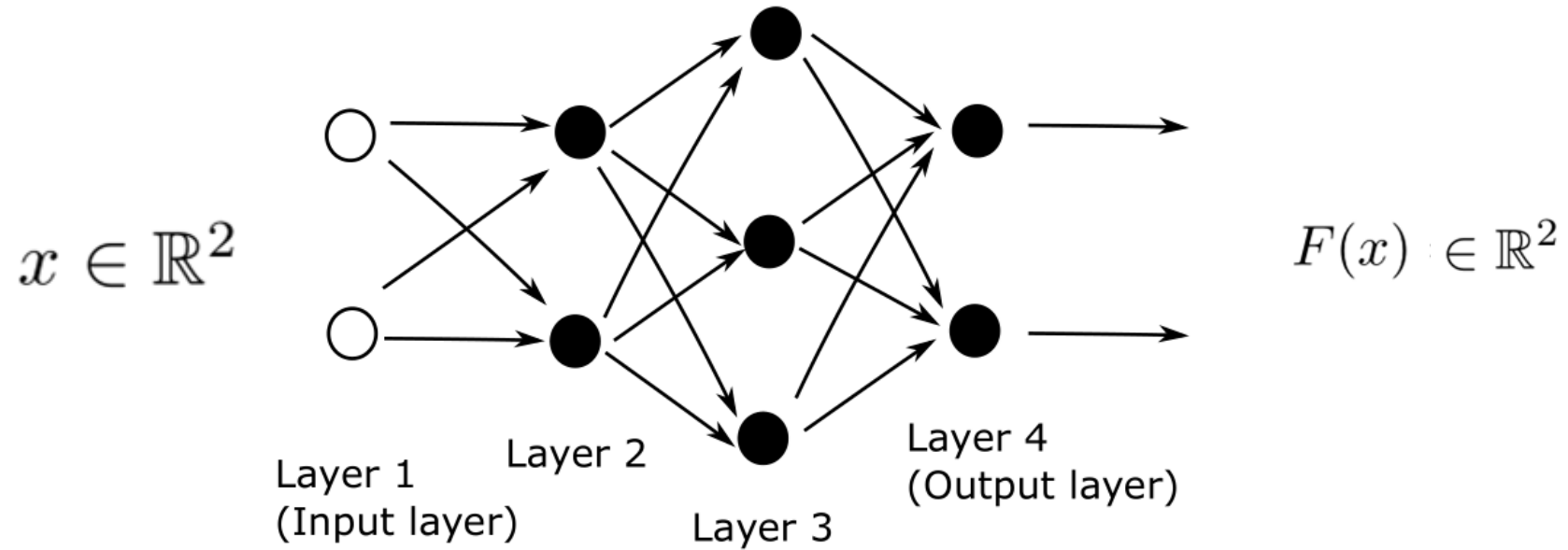
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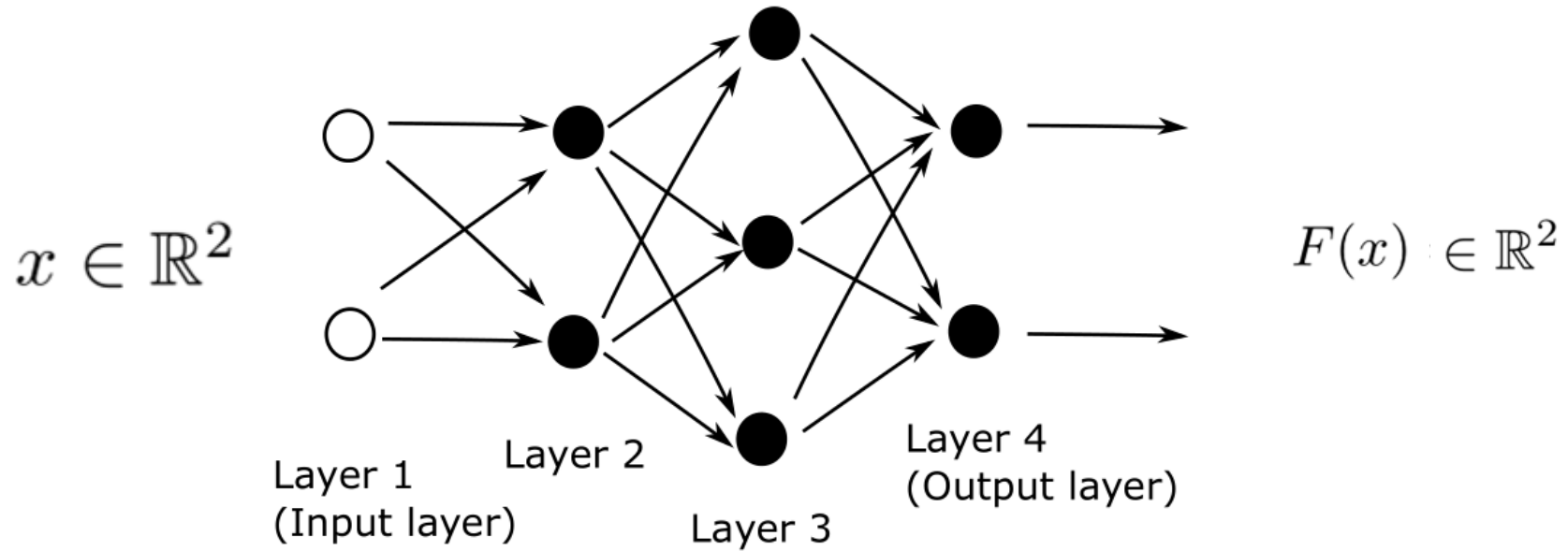
Neural Networks are computational graphs



Neural networks can be considered as computational graphs.

Why this is a useful fact? Modern DL packages such as tensorflow and pytorch
Use this fact to automatic differentiation

Neural Networks are computational graphs

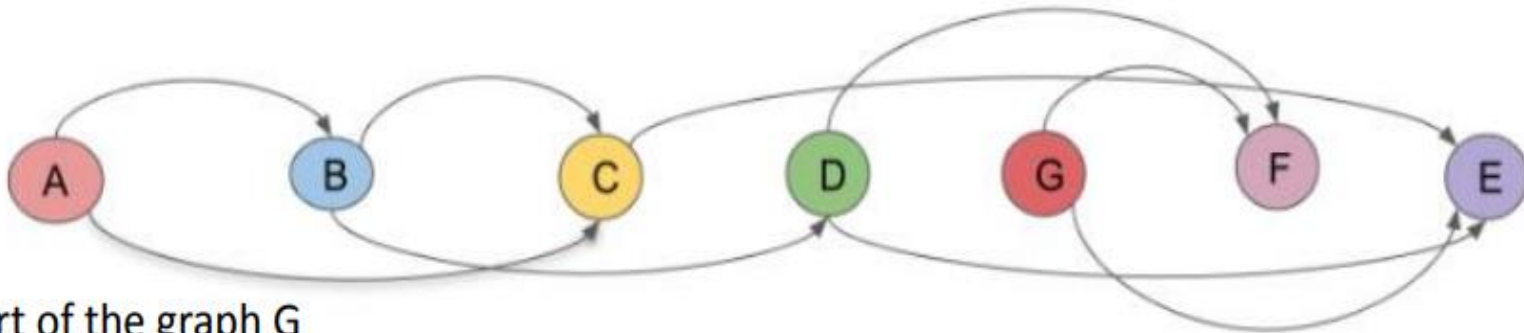
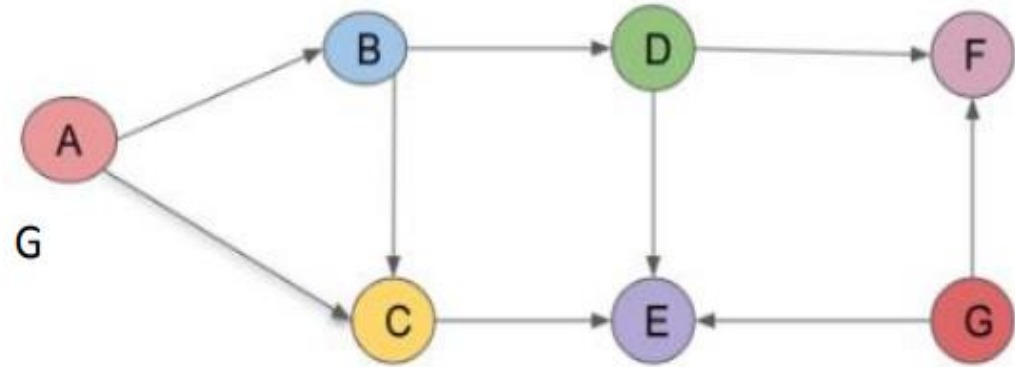


Key fact : feedforward computation of a NN is defined to be the computations that one executes on a computational graph that defines that network given a given input given the topological order of the nodes of the computational graph of a NN

Recall topological sort

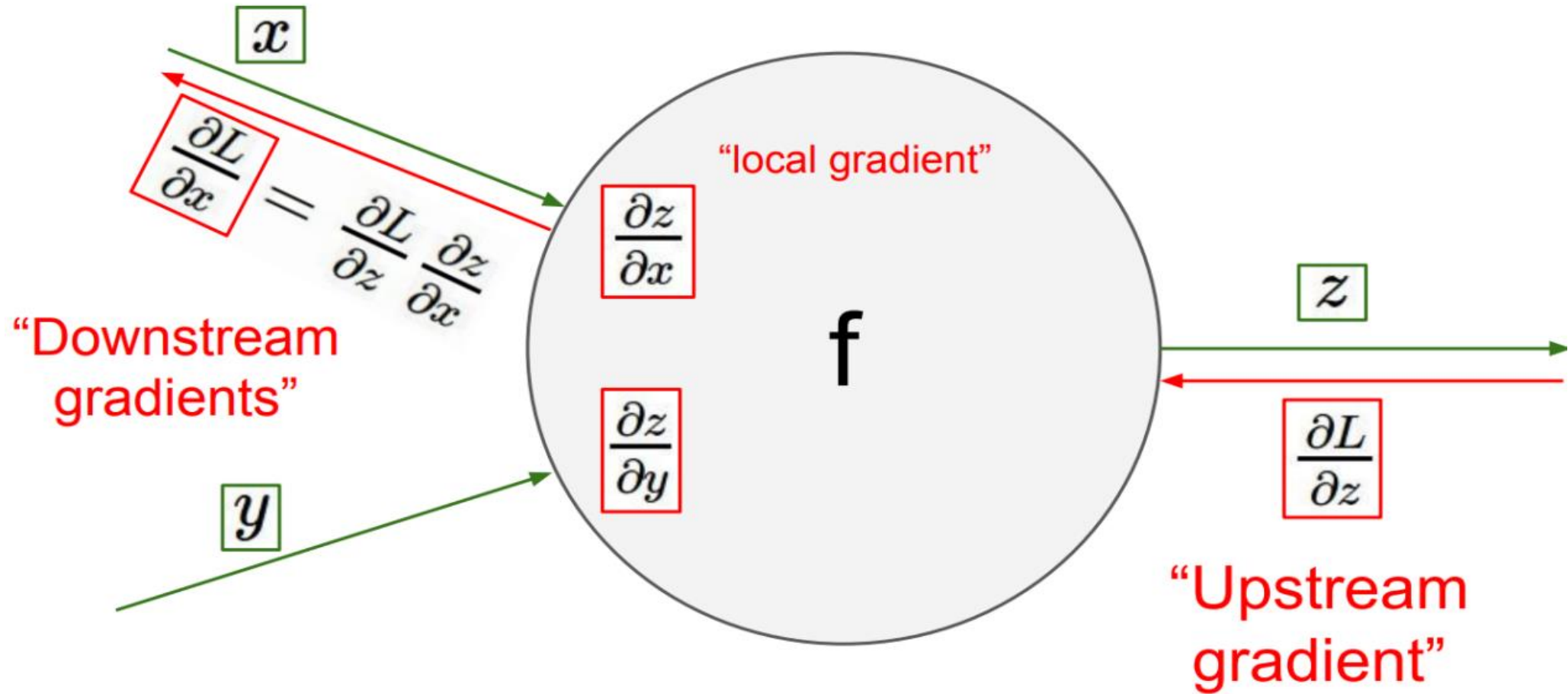
Recall that a topological sort of a DAG is a linear ordering of its vertices such that for every directed edge uv from vertex u to vertex v , u comes before v in the ordering.

Example



A topological sort of the graph G

Backprop in nutshell



Backprop in nutshell

More general :

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

1. Write an **algorithm** for evaluating the function $y = f(\mathbf{x})$. The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the “**computation graph**”)
2. Visit each node in **topological order**.
For variable u_i with inputs v_1, \dots, v_N
 - a. Compute $u_i = g_i(v_1, \dots, v_N)$
 - b. Store the result at the node

Backward Computation

1. **Initialize** all partial derivatives dy/du_i to 0 and $dy/dy = 1$.
2. Visit each node in **reverse topological order**.
For variable $u_i = g_i(v_1, \dots, v_N)$
 - a. We already know dy/du_i
 - b. Increment dy/dv_j by $(dy/du_i)(du_i/dv_j)$
(Choice of algorithm ensures computing (du_i/dv_j) is easy)

Return partial derivatives dy/du_i for all variables

The approximation power of neural networks

Approximation Theorems using shallow NN

Let $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ be a nonconstant, **bounded**, and **continuous** function

(You may think about this function as Relu if you like). Consider summation of the form :

$$\sum_{i=1}^N v_i \varphi (w_i x + b_i)$$

Real numbers (the weights)



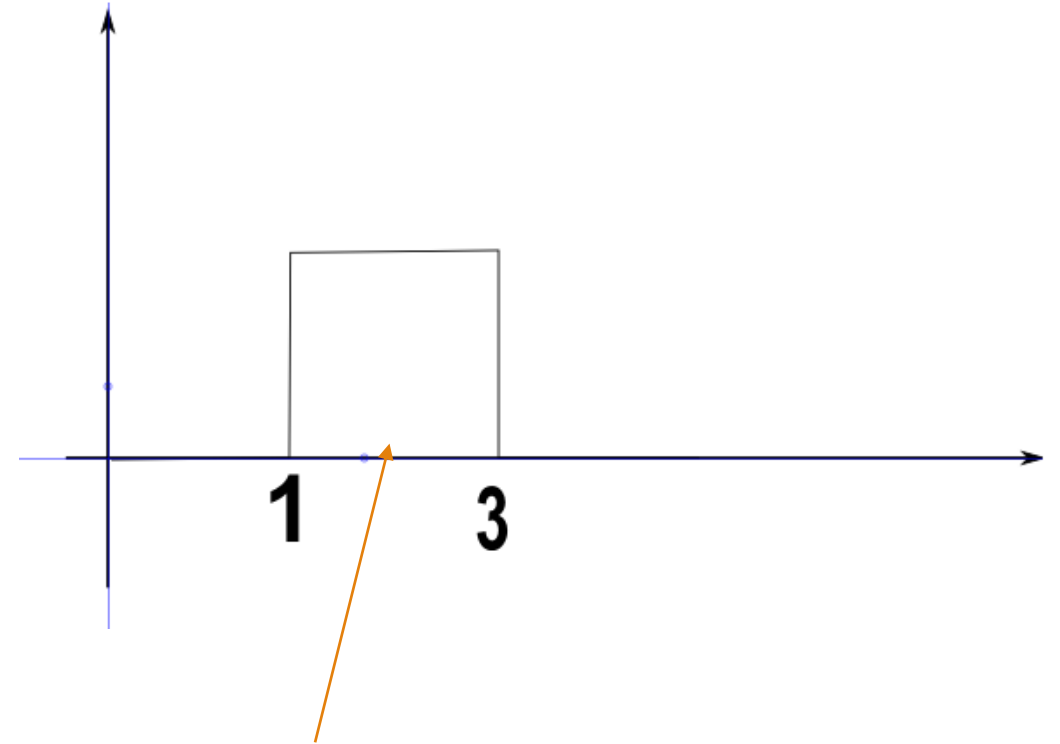
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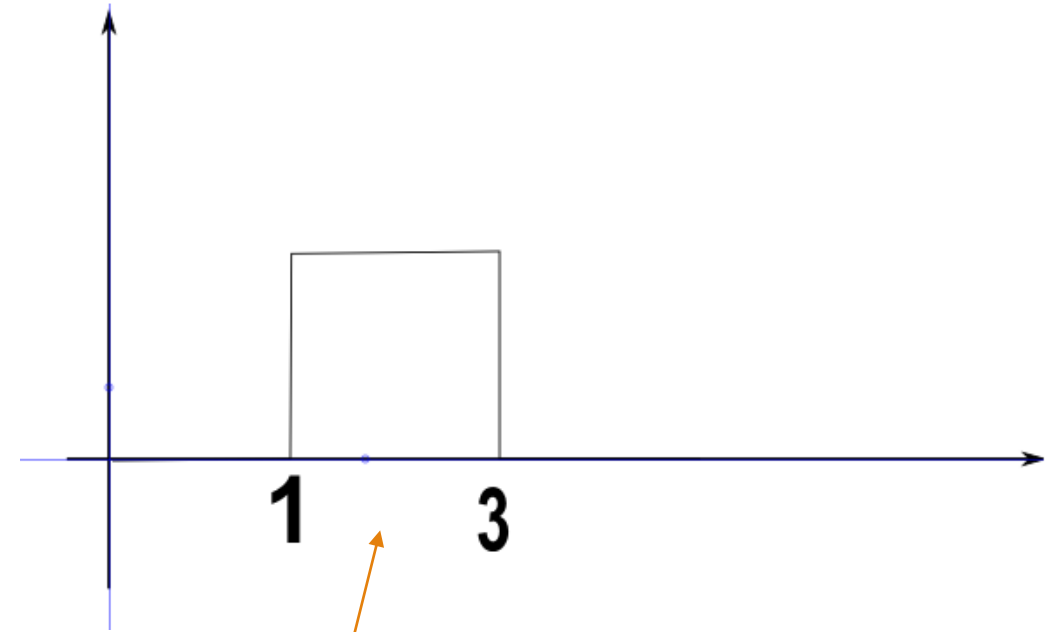
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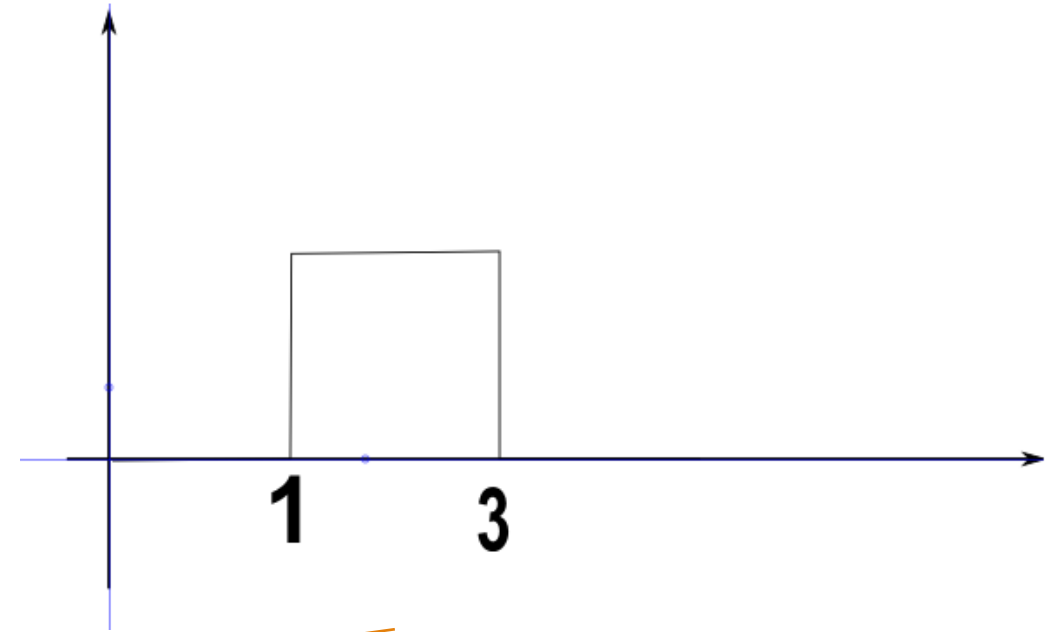
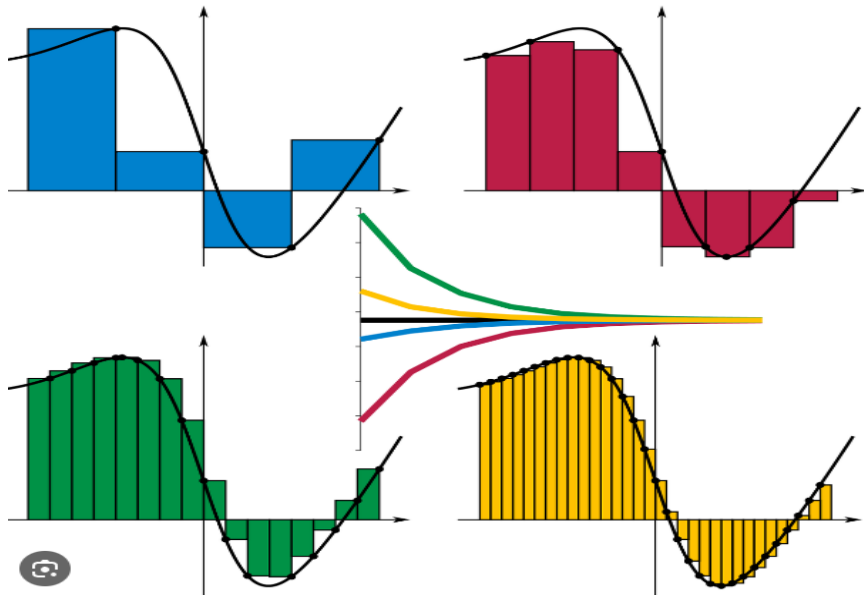
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Can you imagine building more complex functions if we have more
Summations and maybe vary the weights ? –what are the functions you can build?

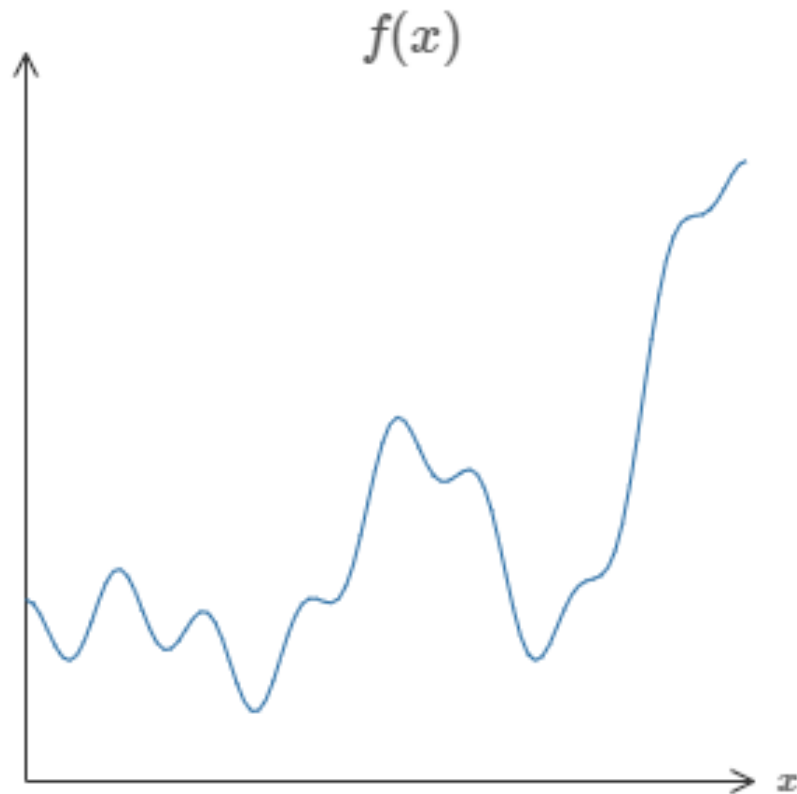
Approximation Theorems using shallow NN



Familiar ? Riemann sum from Calc?

Approximation Theorems using shallow NN

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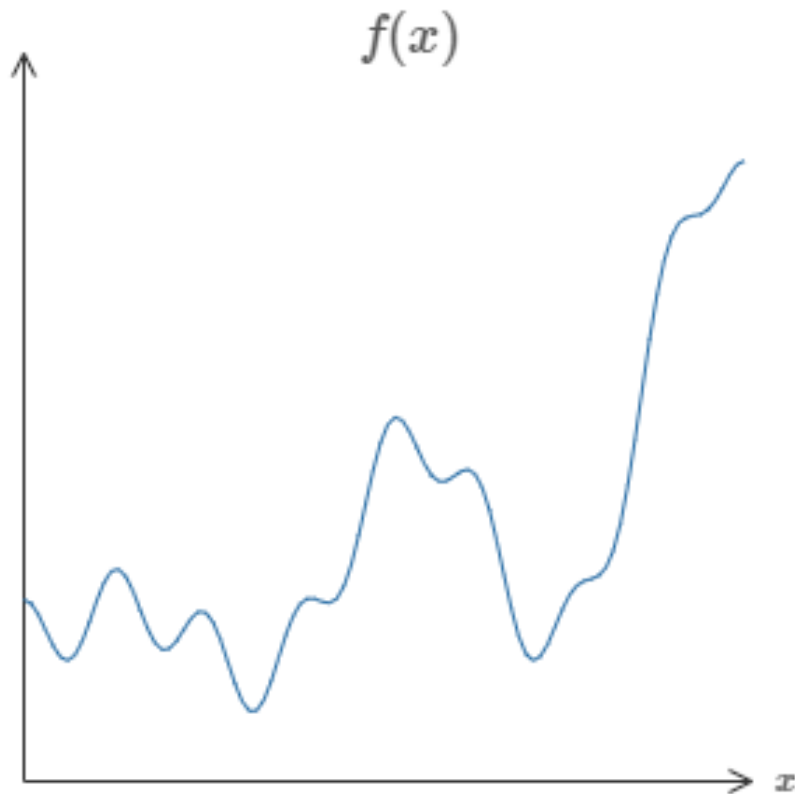


$$\sum_{i=1}^N v_i \varphi(w_i x + b_i)$$

Given a function f as above, can we find v_i 's, w_i 's, and b_i 's such that the summation above is as close we like to f ?

Approximation Theorems using shallow NN

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Given a function f as above, can we find v_i 's, w_i 's, and b_i 's such that the summation above is as close we like to f ?

It turns out that the answer is yes as long as we are willing to increase N (increase number of kernels).
Let's [see](#) a few examples.

Approximation Theorems using shallow NN

It turns out that this theorem generalizes to higher dimension the same way :

The following summations:

$$\sum_{i=1}^N v_i \varphi (w_i^T x + b_i) \quad \begin{array}{l} w_i \in \mathbb{R}^m \\ v_i, b_i \in \mathbb{R} \end{array}$$

can approximate any continuous real valued function on $[0,1]^m$.

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Universal approximation theorem. Let $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ be a nonconstant, **bounded**, and **continuous** function (called the *activation function*). Let I_m denote the m -dimensional **unit hypercube** $[0, 1]^m$. The space of real-valued continuous functions on I_m is denoted by $C(I_m)$. Then, given any $\varepsilon > 0$ and any function $f \in C(I_m)$, there exist an integer N , real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ for $i = 1, \dots, N$, such that we may define:

$$F(x) = \sum_{i=1}^N v_i \varphi (w_i^T x + b_i)$$

as an approximate realization of the function f ; that is,

$$|F(x) - f(x)| < \varepsilon$$