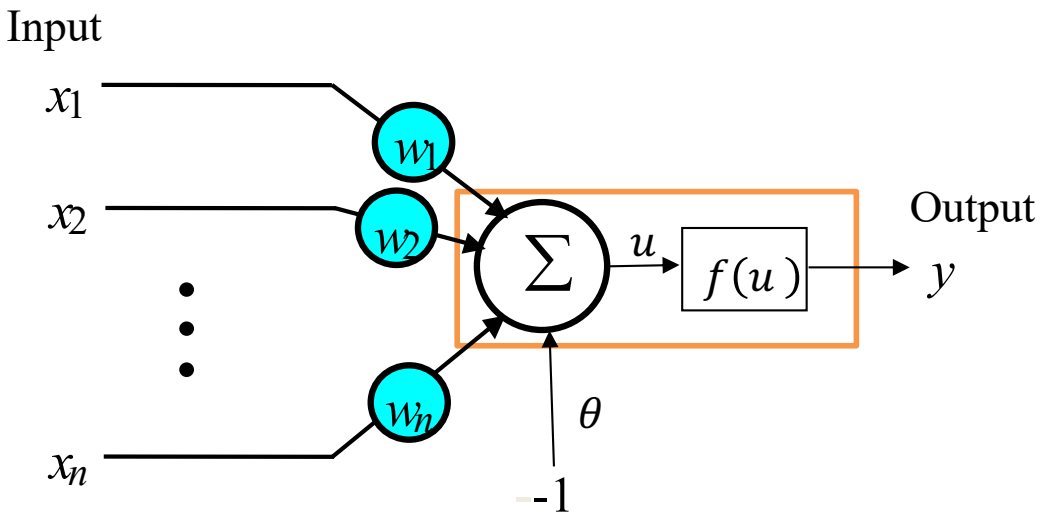
Chapter 1
Fundamentals of Neural Networks

Neural networks and deep learning

Artificial Neuron



Input vector $\boldsymbol{x} = (x_1 \quad x_2 \quad \cdots \quad x_n)^T$
weight vector $\boldsymbol{w} = (w_1 \quad w_2 \quad \cdots \quad w_n)^T$
n is the number of inputs.

Artificial Neuron

An **artificial neuron** is the basic unit of neural networks.

Basic elements of an artificial neuron:

• A set of **input** signals: the input is a vector $\boldsymbol{x} = (x_1 \quad x_2 \quad \cdots \quad x_n)^T$ where n is the number (or the dimension) of input signals. Inputs are also referred to as **features**.

• Inputs are connected to the neuron via synaptic connections whose strengths are represented by their **weights**.

• The weight vector $\boldsymbol{w} = (w_1 \quad w_2 \quad \cdots \quad w_n)^T$ where w_i is the synaptic weight connecting i th input of the neuron.

Notation

Vectors are denoted in bold and
written as horizontally with a transpose (^{T}).

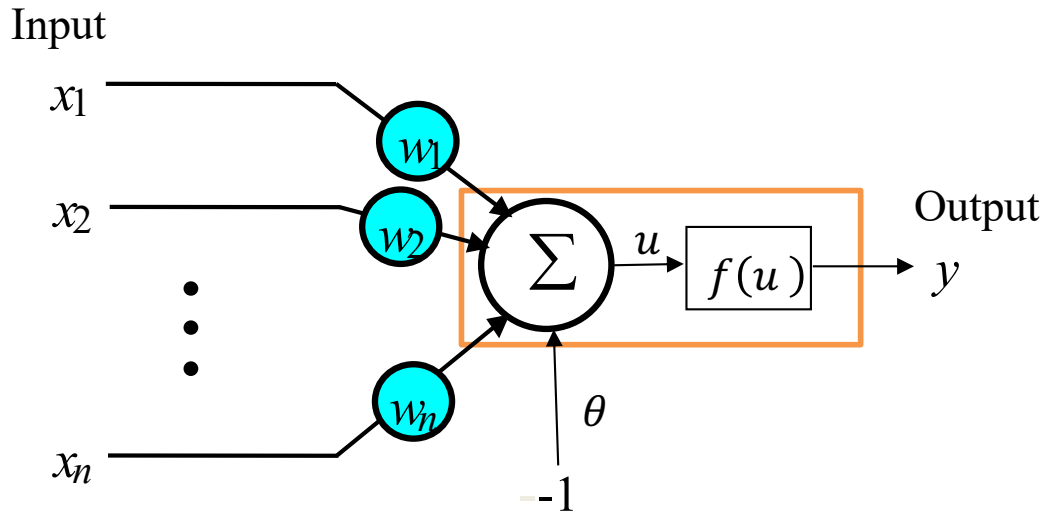
$$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = (w_1 \quad w_2 \quad \cdots \quad w_n)^T$$

Example

$$\boldsymbol{x} = \begin{pmatrix} 1.2 \\ -0.5 \\ 3.5 \\ 2.1 \end{pmatrix} = (1.2 \quad -0.5 \quad 3.5 \quad 2.1)^T$$

$$\boldsymbol{x}^T = (1.2 \quad -0.5 \quad 3.5 \quad 2.1)$$

Artificial Neuron



The total **synaptic input** u to the neuron is given by the sum of the products of the inputs and their corresponding connecting weights minus the **threshold** of the neuron.

The total synaptic input to a neuron, u is given by

$$u = w_1x_1 + w_2x_2 + \cdots w_nx_n - \theta = \sum_{i=1}^{n} w_ix_i - \theta$$

where θ is the threshold of the neuron.

By using vector notations:

$$u = \boldsymbol{w}^T\boldsymbol{x} - \theta$$

Artificial Neuron

The **activation function** f relates synaptic input to the activation of the neuron.

$f(u)$ denotes the **activation** of the neuron.

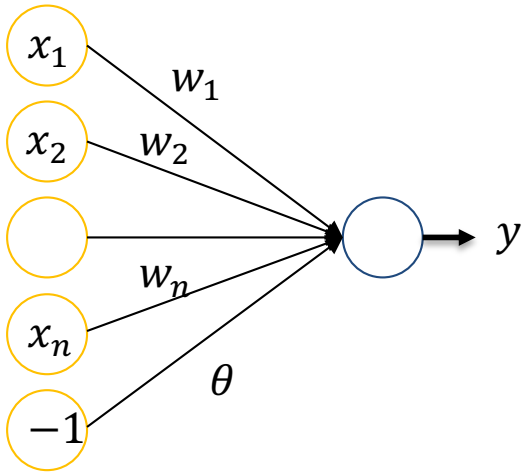
For some neurons, the **output** y is equal to the activation of the neuron.

$$y = f(u)$$

Note that activation is not generally equal to the output of the neuron.

Bias vs Threshold

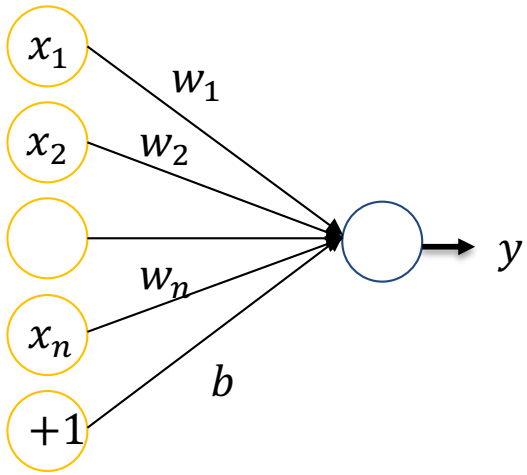
The threshold is often considered as a weight with a fixed input of -1. Often the threshold is represented as a **bias** b that receives constant +1 input.



Threshold

$$u = \boldsymbol{w}^T \boldsymbol{x} - \theta$$

$$y = f(u)$$



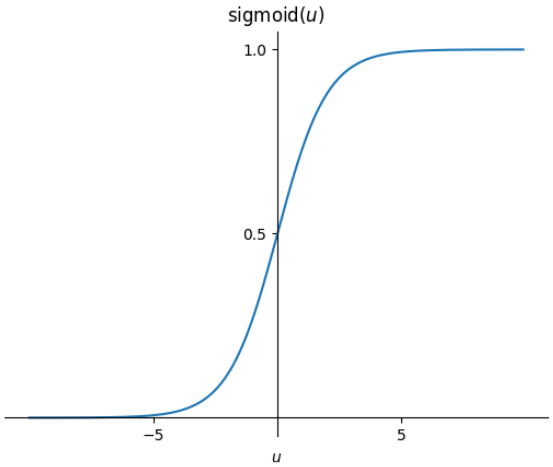
Bias

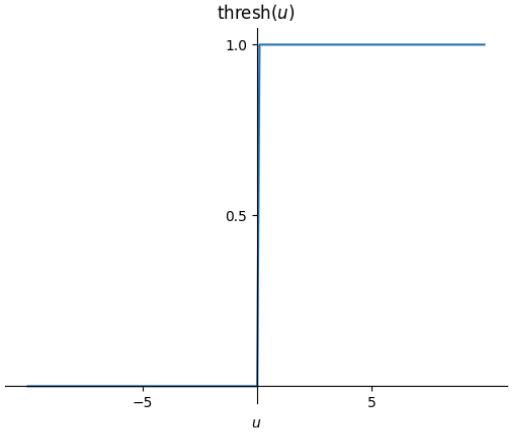
$$u = \boldsymbol{w}^T \boldsymbol{x} + b$$

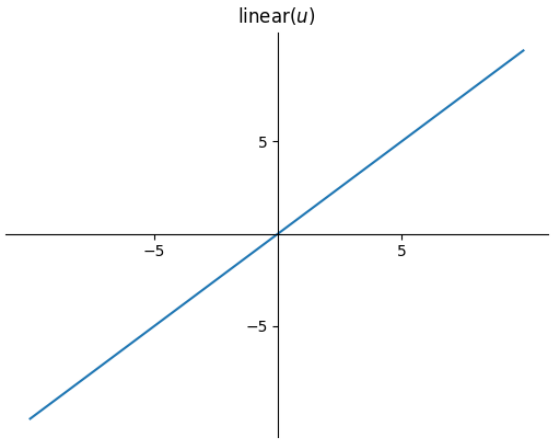
$$y = f(u)$$

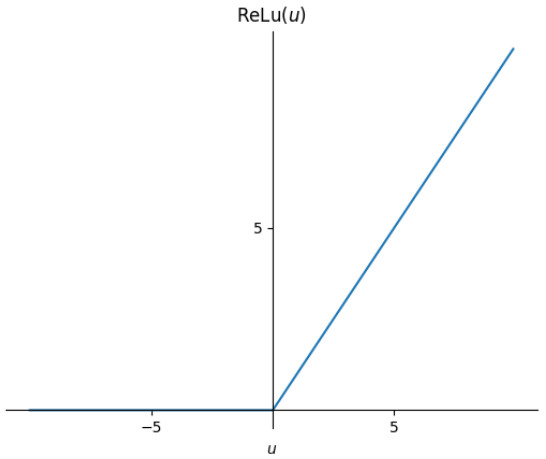
Bias $b = -\theta$

Activation functions









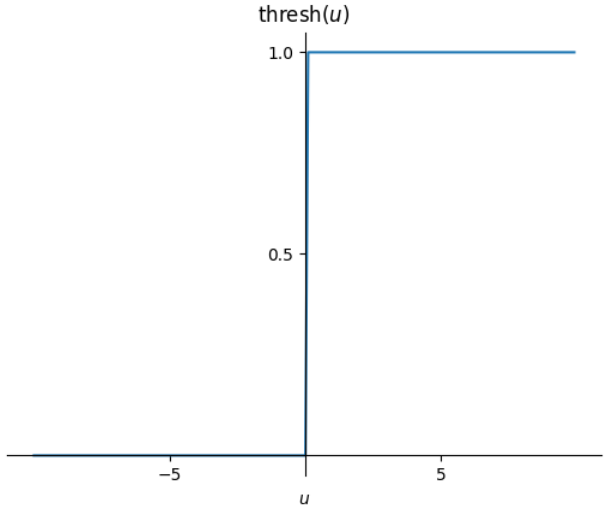
Activation functions

For ***threshold*** **(unit step*)* activation function**, the activation is given by

$$f(u) = theshold(u) = 1(u > 0)$$

where $1(\cdot)$ is the *Indictor function* or *Unit-step function:*

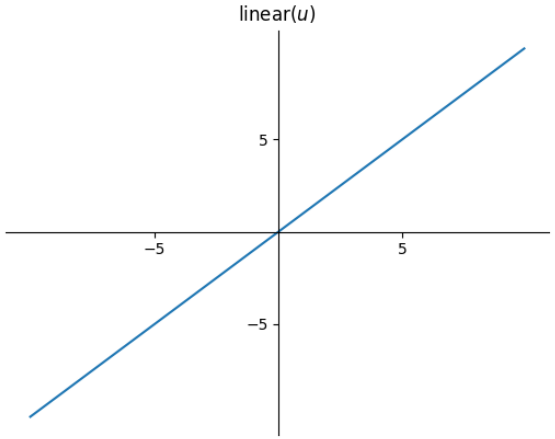
$$1(x) = \begin{cases} 1, & x \text{ is True} \\ 0, & x \text{ is False} \end{cases}$$



Activation functions

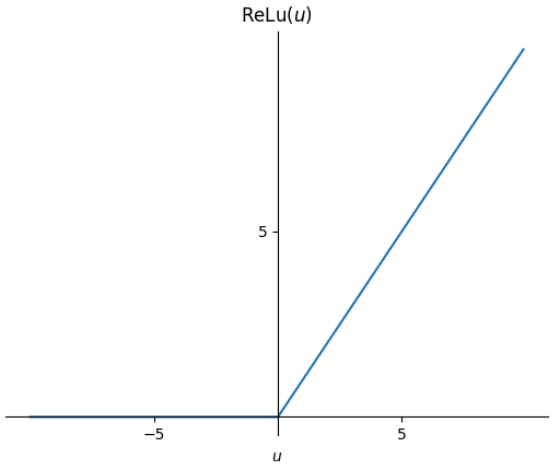
A neuron with ***linear*** activation function can be written as

$$f(u) = linear(u) = u$$



The ***ReLU*** **(rectified-linear unit)** activation function can be written as

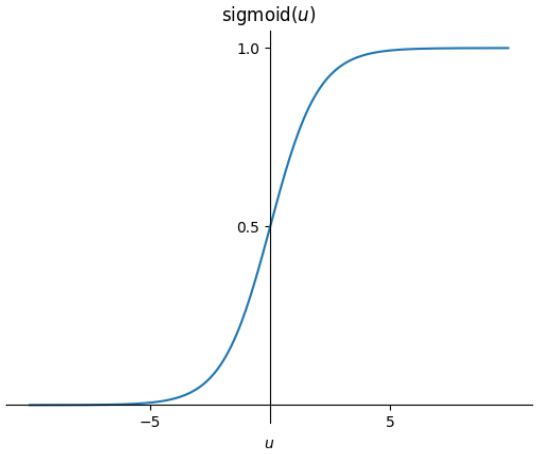
$$f(u) = relu(u) = \max\{0, u\}$$



Sigmoid activation function

The sigmoidal is known as the **logistic function** or simply **sigmoid function**

$$f(u) = sigmoid(u) = \frac{1}{1 + e^{-u}}$$



In general, the ***sigmoid*** activation function can be written as

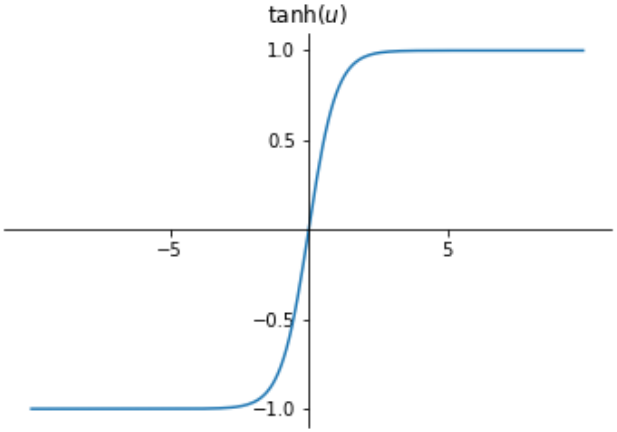
$$f(u) = \frac{a}{1 + e^{-bu}}$$

a is the gain (amplitude) and b is the slope.

But often, $a = 1.0$ and $b = 1.0$.

Tanh activation function

$$f(u) = tanh(u) = \frac{e^{u} - e^{-u}}{e^{u} + e^{-u}}$$

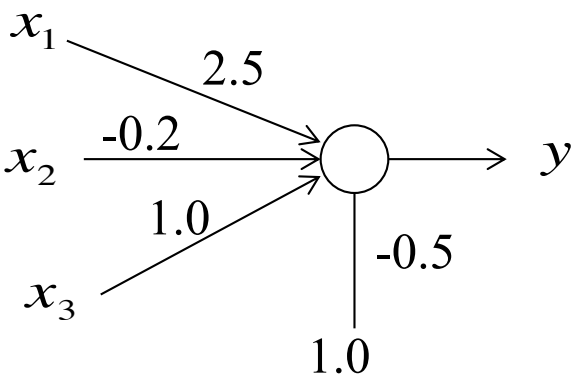


Tanh activation function has the same shape as sigmoidal and spans from -1 and +1. It is also known as **bipolar sigmoidal**.

Sigmoidal is the most pervasive and biologically plausible activation function. Since sigmoid function is *differentiable*, it leads to mathematically attractive neuronal models.

Example 1

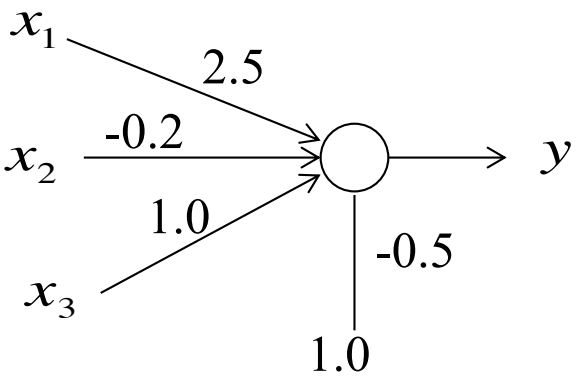
The artificial neuron in the figure receives 3-dimensional inputs $\boldsymbol{x} = (x_1 \quad x_2 \quad x_3)^T$ and has an activation function given by $f(u) = \frac{0.8}{1+e^{-1.2u}}$.



Find the synaptic input and the output of the neuron for inputs: $\begin{pmatrix} 0.8 \\ 2.0 \\ -0.5 \end{pmatrix}$ and $\begin{pmatrix} -0.4 \\ 1.5 \\ 1.0 \end{pmatrix}$.

Example 1

$$\boldsymbol{w} = \begin{pmatrix} 2.5 \\ -0.2 \\ 1.0 \end{pmatrix}, \qquad b = -0.5$$



Consider $\boldsymbol{x} = \begin{pmatrix} 0.8 \\ 2.0 \\ -0.5 \end{pmatrix}$

Synaptic input $u = \boldsymbol{w}^T \boldsymbol{x} + b = (2.5 \quad -0.2 \quad 1.0) \begin{pmatrix} 0.8 \\ 2.0 \\ -0.5 \end{pmatrix} - 0.5 = 0.6$

Output = $\mathrm{y} = f(u) = \frac{0.8}{1+e^{-1.2u}} = \frac{0.8}{1+e^{-1.2\times 0.6}} = 0.538$

Similarly, for $\boldsymbol{x} = \begin{pmatrix} -0.4 \\ 1.5 \\ 1.0 \end{pmatrix}$, $u = -0.8$ and output $\mathrm{y} = f(u) = 0.222$

PyTorch 2.0

PyTorch/Tensorflow is about processing of **tensors**. Tensor is a multidimensional array.

Rank refers to the number of dimensions and **shape** gives the sizes of each dimension of the tensor.

3. # a rank 0 tensor; a scalar with shape [],

[1., 2., 3.] # a rank 1 tensor; a vector with shape [3]

[[1., 2., 3.], [4., 5., 6.]] # a rank 2 tensor; a matrix with shape [2, 3]

[[[1., 2., 3.]], [[7., 8., 9.]]] # a rank 3 tensor with shape [2, 1, 3]

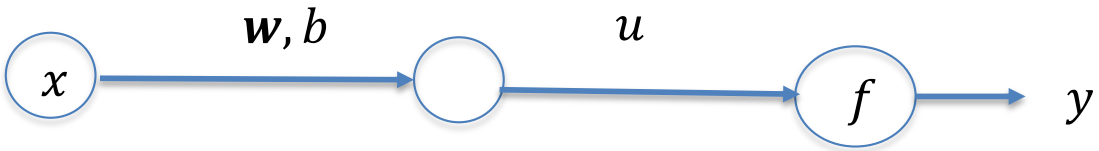
Computational Graph

PyTorch program involves building and evaluation of a **computational graph.**

A computational graph is a series of tensor **operations** arranged into a graph.

- Nodes of the graph represent tensor operations
- Edges represent values (tensors) that follow through the graph

Computational graph of a neuron



multiply
add

$$u = \boldsymbol{w}^T \boldsymbol{x} + b$$
$$\mathrm{y} = f(u)$$

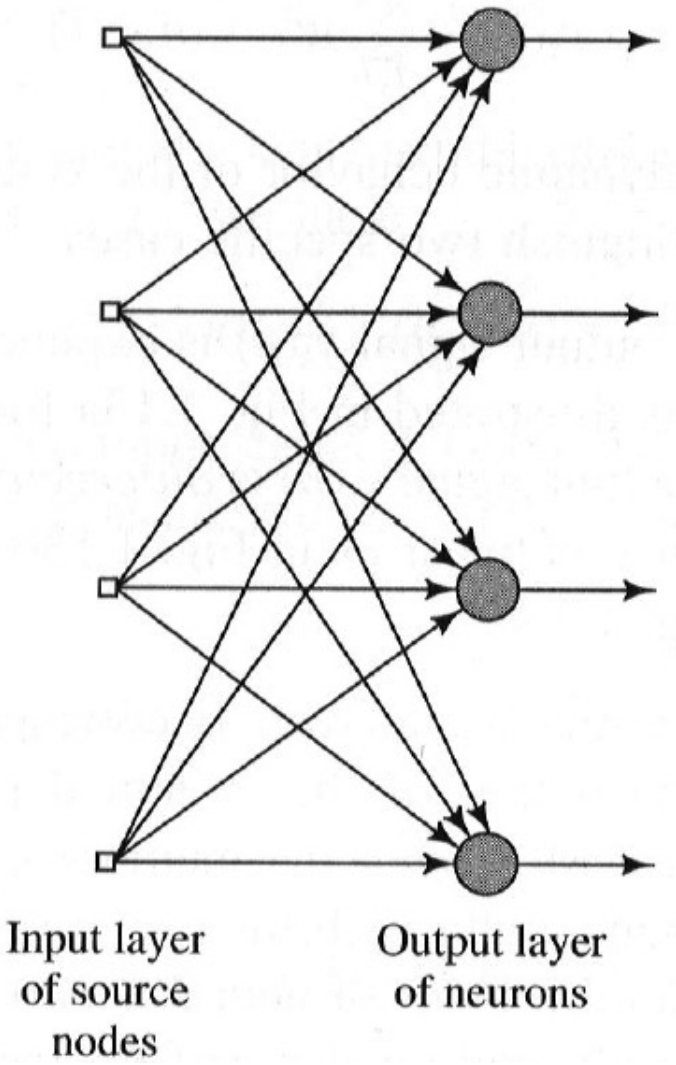
Torch Implementation of Example 1

```
import torch

# a class for neuron
class Neuron():
   # initiate a neuron class with weights and biases (initiate the object)
   def __init__(self):
       self.w = torch.tensor([2.5, -0.2, 1.0])
       self.b = torch.tensor(-0.5)

  # evaluate the neuron (implement a function)
  def __call__(self, x):
      u = torch.inner(self.w, x) + self.b
      y = 0.8/(1+torch.exp(-1.2*u))
   return u, y

# create a neuron
neuron = Neuron()

# evaluate
u, y = neuron(torch.tensor([0.8, 2.0, -0.5]))

# print: u = 0.600, y = 0.538
```

NN Architectures: neuron layers

Single – layer of neurons

• Comprised of an input layer of source units that inject into an output layer of neurons.
• A fully-connected layer

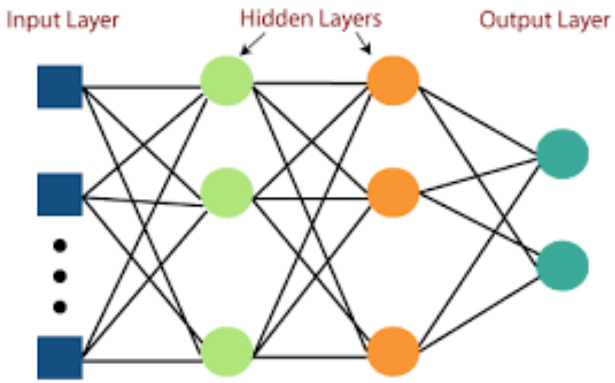


NN architectures: multilayer feedforward networks

• Comprised of more than one layer of neurons. Layers between input source nodes and output layer is referred to as *hidden layers*.

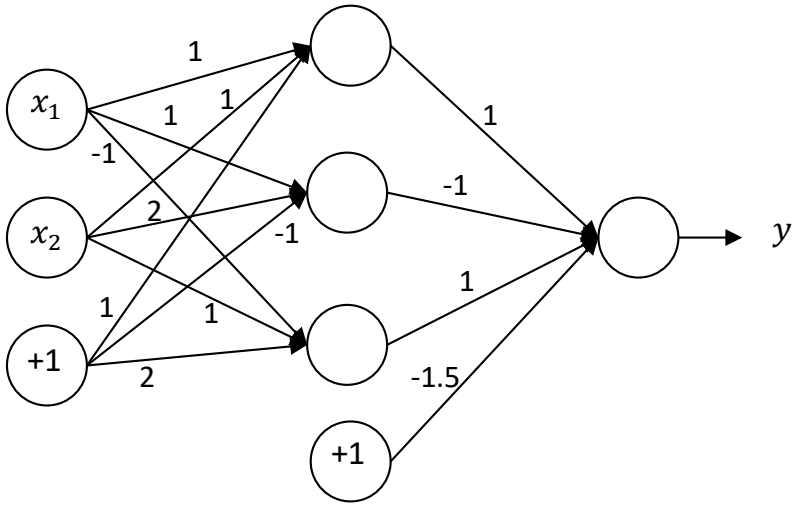
• Multilayer neural networks can handle *more complicated* and *larger scale problems* better than single-layer networks.

• However, training multilayer network may be *more difficult* and *time-consuming*.



Three-layer network

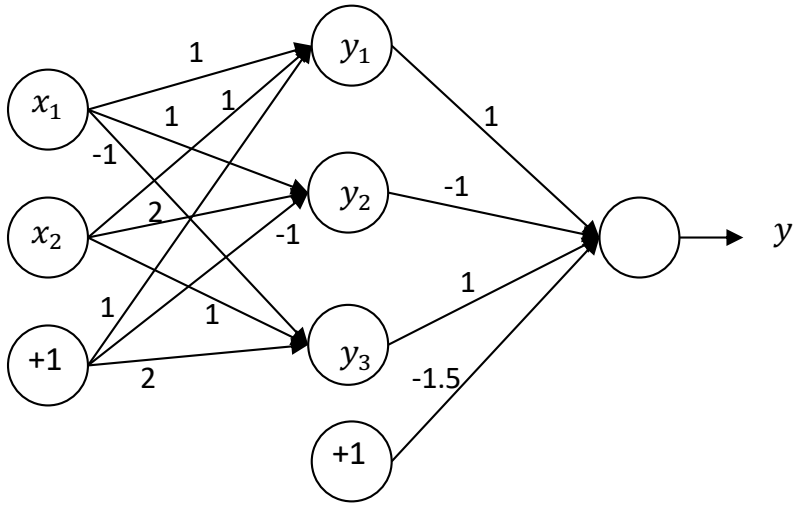
Example 2



Two-layer neural network receives 2-dimensional inputs $(x_1, x_2) \in \boldsymbol{R}^2$ and has one output neuron and three hidden neurons. All the neurons have unit step activation functions. The weights of the connections are given in the figure. Find the space of inputs for which the output $y = 1.0$.

Find the output for inputs $(0.0, 0.0)$, $(2.0, 2.0)$, and $(-1.0, 1.0)$

Example 2



Synaptic inputs:

$$u_1 = x_1 + x_2 + 1$$

Output $y_1 = 1(u_1 > 0)$

$$u_2 = x_1 + 2x_2 - 1$$

$$y_2 = 1(u_2 > 0)$$

$$u_3 = -x_1 + x_2 + 2$$

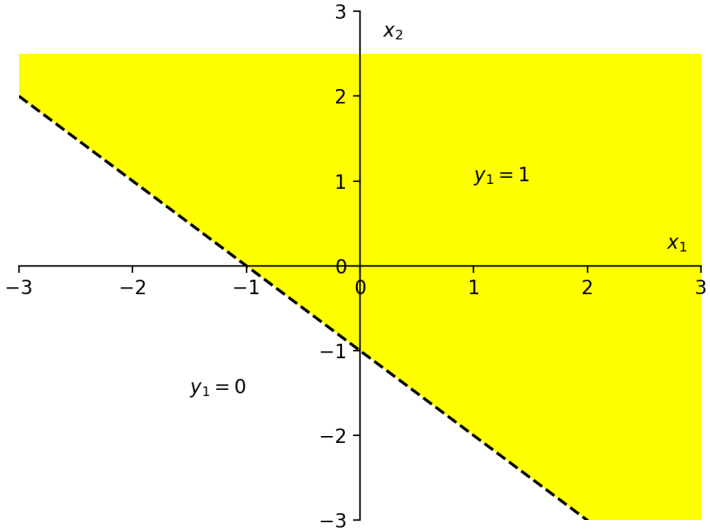
$$y_3 = 1(u_3 > 0)$$

$$u = y_1 - y_2 + y_3 - 1.5$$

$$y = 1(u > 0)$$

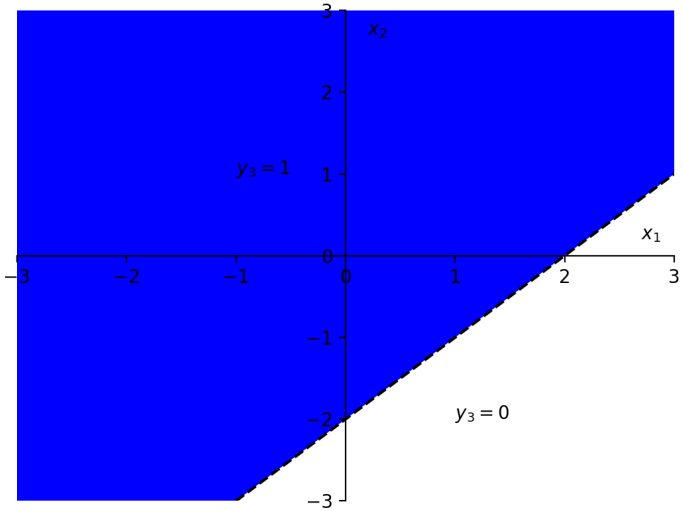
$$y_1 = f(u_1) = 1(u_1 > 0)$$

Boundary: $u_1 = x_1 + x_2 + 1 = 0 \rightarrow x_2 = -x_1 - 1$

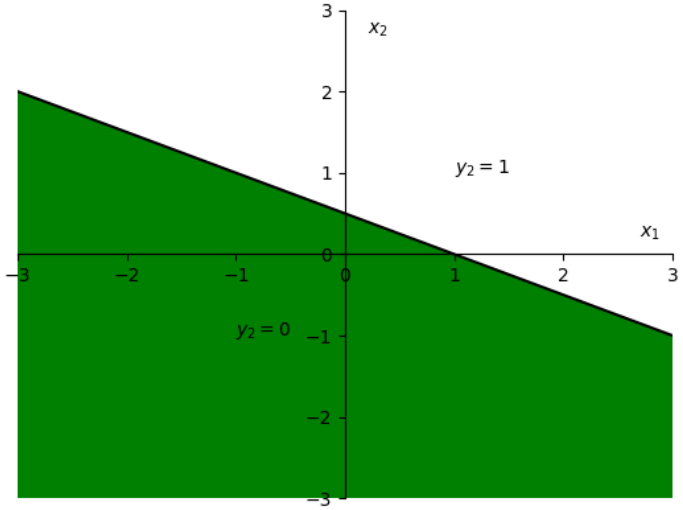


The boundary line is obtained by setting $u_1 = 0$; and for one side of the boundary, $y = 1$ and on other side $y_1 = 0$.

$$u_3 = x_2 - x_1 + 2 = 0 \rightarrow x_2 = x_1 - 2$$



$$u_2 = 2x_2 + x_1 - 1 = 0 \rightarrow x_2 = -0.5x_1 + 0.5$$



Output layer neuron:

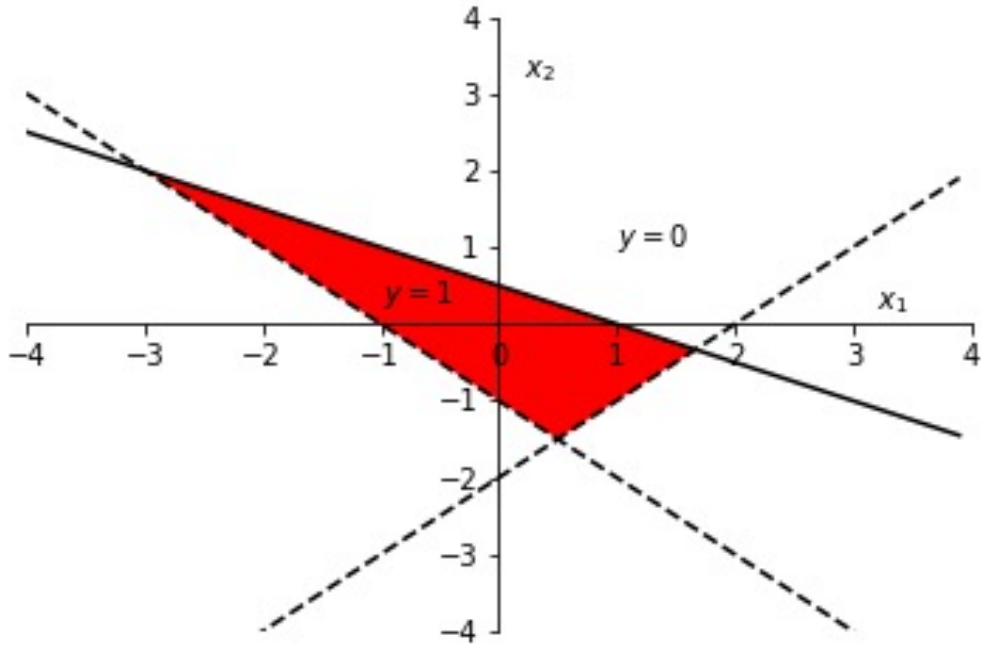
$$u = y_1 - y_2 + y_3 - 1.5$$
$$y = 1(u > 0)$$

Note that $y_1, y_2, y_3 \in \{0, 1\}$

y_1	y_2	y_3	u	y
0	0	0	-1.5	0
0	0	1	-0.5	0
0	1	0	-2.5	0
0	1	1	-1.5	0
1	0	0	-0.5	0
1	0	1	0.5	1
1	1	0	-1.5	0
1	1	1	-0.5	0

$$Y = Y_1 \overline{Y_2} Y_3$$

$y = 1$ region is given by the intersection of regions: y_1=1, y_2=0, and y_3=1.



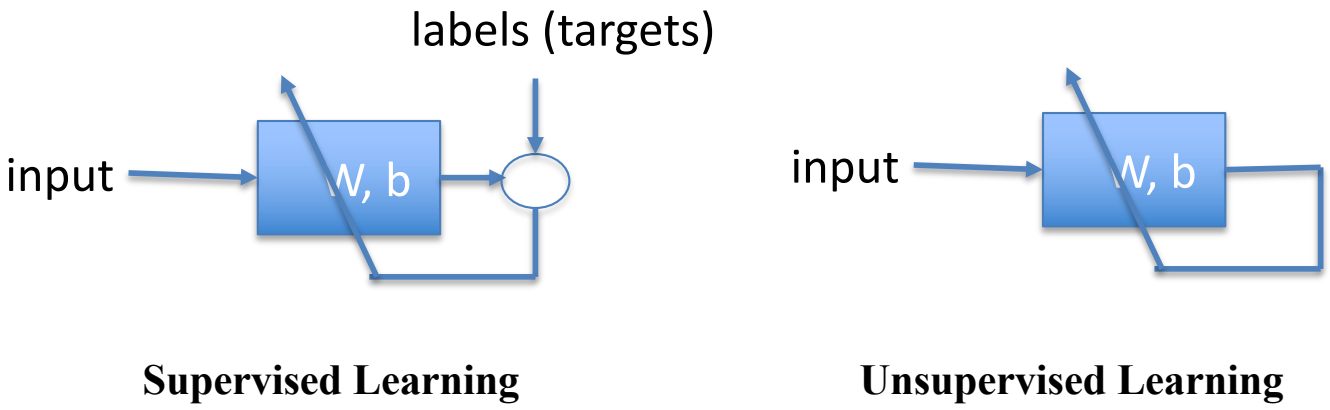
$$x = (0.0, 0.0) \rightarrow y = 1$$
$$x = (2.0, 2.0) \rightarrow y = 0$$
$$x = (-1.0, 1.0) \rightarrow y = 1$$

Note that networks of *discrete perceptrons* (neurons with threshold activation functions) can implement Boolean functions.

Training (or learning) of neural networks

Neural networks attain their operating characteristics through **learning** (or **training**) with training examples. During training, the weights or the strengths of connections are gradually adjusted iteratively to achieve their desirable labels (or **targets**).

Training may be either **supervised** or **unsupervised**.



Supervised Learning **Unsupervised Learning**

Supervised and unsupervised learning

Supervised Learning:
For each training input pattern, the network is presented with the correct **target label** (the desired output).

Unsupervised Learning:
For each training input pattern, the network adjusts weights *without knowing* the correct target.

In unsupervised training, the network **self-organizes** to classify similar input patterns into clusters.

Supervised learning

Learning of a neuron or neural network is usually performed in order to minimize a **cost function** (**loss function** or **error function**).

The cost function $J(\boldsymbol{W}, \boldsymbol{b})$ is of an artificial neuron is typically a multi-dimensional function that depends on weights $\boldsymbol{W}$ and the biases $\boldsymbol{b}$. The neuron learning attempts to find the optimal weights $\boldsymbol{W}^*$ and biases $\boldsymbol{b}^*$ that minimize the error function:

$$\boldsymbol{W}^*, \boldsymbol{b}^* = arg \min_{\boldsymbol{W}, \boldsymbol{b}} J(\boldsymbol{W}, \boldsymbol{b})$$

Given a set of training patterns, the parameters (weights and biases) minimizing cost function are learned in an iterative procedure. In each iteration, small changes of weights $\Delta\boldsymbol{W}$ and biases $\Delta\boldsymbol{b}$ are made:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} + \Delta\boldsymbol{W}$$
$$\boldsymbol{b} \leftarrow \boldsymbol{b} + \Delta\boldsymbol{b}$$

Gradient descent learning

The grading descent procedure states that the weights $\boldsymbol{W}$ (and biases $\boldsymbol{b}$) are updated during learning by searching in the direction of and proportional the **negative gradient** of the cost function.

That is, the change of the weight vector:

$$\Delta \boldsymbol{W} \propto -\frac{\partial J(\boldsymbol{W},\boldsymbol{b})}{\partial \boldsymbol{w}}$$

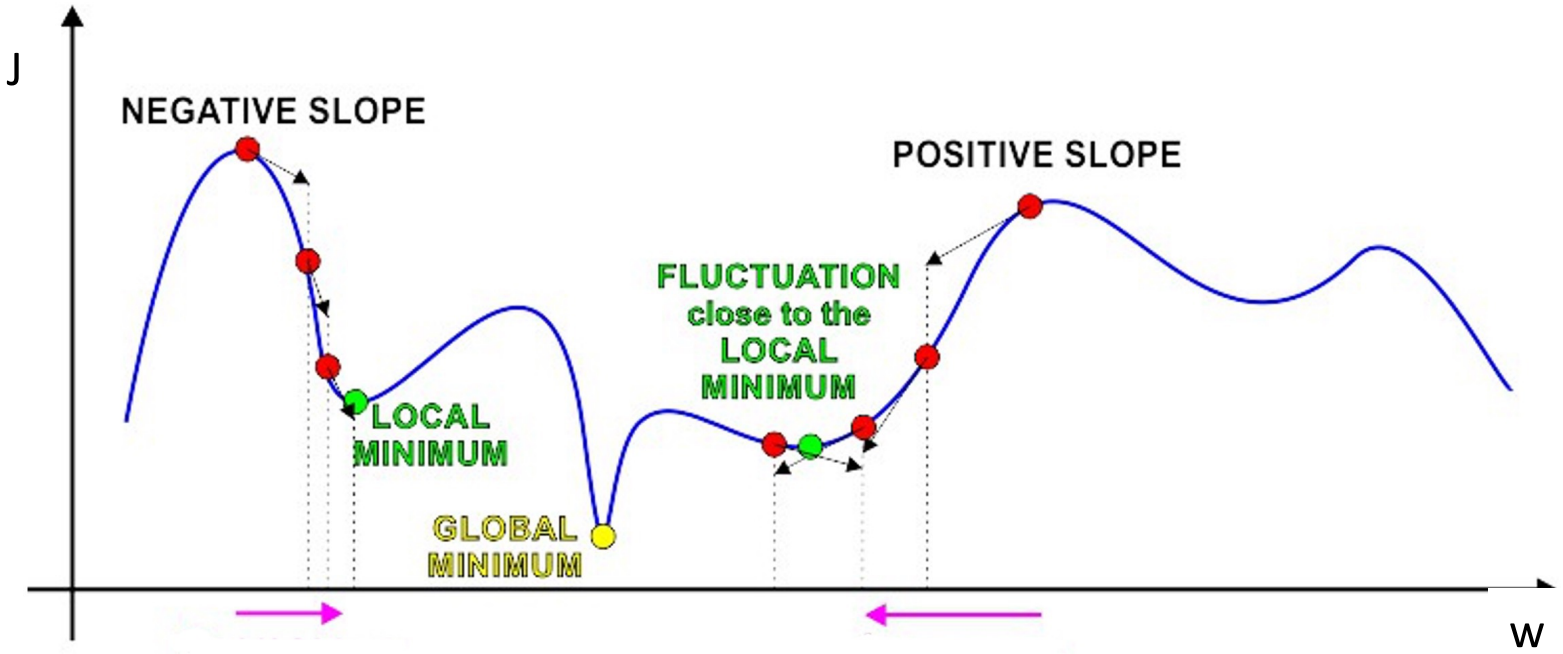
$$\Delta \boldsymbol{W} = -\alpha \frac{\partial J(\boldsymbol{W},\boldsymbol{b})}{\partial \boldsymbol{W}}$$

where $\frac{\partial J(\boldsymbol{W},\boldsymbol{b})}{\partial \boldsymbol{W}}$ is the gradient (partial derivative) of cost with respect to weight $\boldsymbol{W}$ and α is *learning factor* or *learning rate*. $\alpha \in (0.0, 1.0]$.

The **gradient descent equations** for learning the weights is given by substituting above in

$$\boldsymbol{W} \leftarrow \boldsymbol{W} + \Delta \boldsymbol{W}$$

Gradient Descent Leaning



Gradient descent learning

The **gradient descent equations** for the weights is given by

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \frac{\partial J(\boldsymbol{W}, \boldsymbol{b})}{\partial \boldsymbol{W}}$$

Similarly, for the bias

$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \frac{\partial J(\boldsymbol{W}, \boldsymbol{b})}{\partial \boldsymbol{b}}$$

Notation: $\nabla_{\boldsymbol{W}} J = \frac{\partial J(\boldsymbol{W}, \boldsymbol{b})}{\partial \boldsymbol{W}}$ and $\nabla_{\boldsymbol{b}} J = \frac{\partial J(\boldsymbol{W}, \boldsymbol{b})}{\partial \boldsymbol{b}}$.

Gradient descent learning is given by

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} J$$
$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \nabla_{\boldsymbol{b}} J$$

Note: Will drop the arguments in J.

Gradient descent learning

Given a set of training examples
Initialize weight $\boldsymbol{W}$ and bias $\boldsymbol{b}$
Set the learning parameter α
Iterate until convergence:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} J$$
$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \nabla_{\boldsymbol{b}} J$$

Convergence is achieved by observing one of the following:

1. No changes in weights and biases
2. No difference between the outputs and targets
3. No decrease in the cost function J

Training dataset

Training data are also referred to as **training examples** or **training patterns.** For supervised learning, a training pattern consists of a pair consisting of input pattern and the corresponding target.

A training dataset is a set of training examples: $\{(\boldsymbol{x}_p, d_p)\}_{p=1}^{P}$
or $\{(\boldsymbol{x}_1, d_1), (\boldsymbol{x}_2, d_2), \cdots (\boldsymbol{x}_P, d_P)\}$

$\boldsymbol{x}_p$ is the input (features) and d_p is the target (desired label) of p th training pattern. P is the number of examples in the dataset.

The input is usually n-dimensional and written as:

$$\boldsymbol{x}_p = (x_{p1}, x_{p2}, \cdots x_{pn})^T$$

Stochastic Gradient Descent (SGD) learning

Given training examples $\{(\boldsymbol{x}_p, d_p)\}_{p=1}^{P}$

Set learning factor α

Initialize $(\boldsymbol{W}, \boldsymbol{b})$

Iterate until convergence:

for each pattern $(\boldsymbol{x}_p, d_p)$:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} J_p$$

$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \nabla_{\boldsymbol{b}} J_p$$

- In each **epoch** or cycle of iteration, the learning takes place individually over every pattern
- The cost J_p is individually computed from the output and the target of the p th training pattern.

Batches of Data

Inputs are often presented as a batch in a **data matrix** $\boldsymbol{X}$ and a **target vector** $\boldsymbol{d}$. The input datapoints (or patterns) are written as rows in the data matrix and the targets are written into a single vector in the target vector.

Given a training dataset $\{(\boldsymbol{x}_p, d_p)\}_{p=1}^{P}$.

Data matrix:

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1{}^T \\ \boldsymbol{x}_2{}^T \\ \vdots \\ \boldsymbol{x}_P{}^T \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ x_{P1} & x_{P2} & \cdots & x_{Pn} \end{pmatrix}$$

Target vector:

$$\boldsymbol{d} = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_P \end{pmatrix}$$

(Batch) Gradient descent learning

Given a set of training patterns: $(\boldsymbol{X}, \boldsymbol{d})$
Set learning factor α
Initialize $(\boldsymbol{W}, \boldsymbol{b})$
Iterate until convergence:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} J$$
$$b \leftarrow b - \alpha \nabla_b J$$

The cost J is computed using <u>all</u> the training patterns.
That is, using $(\boldsymbol{X}, \boldsymbol{d})$
In each epoch, the weights are updated once considering all the input patterns.

Summary

- Analogy between biological and artificial neurons
- Transfer function of artificial neuron:

$$u = \boldsymbol{w}^T \boldsymbol{x} + b$$
$$y = f(u)$$

- Types of activation functions: sigmoid, threshold, linear, ReLU, and tanh.
- Given inputs, to find the outputs for simple feedforward networks
- Supervised and unsupervised learning
- Gradient descent learning:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} J$$
$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \nabla_{\boldsymbol{b}} J$$

- Stochastic gradient descent (SGD) and batch gradient descent (GD)