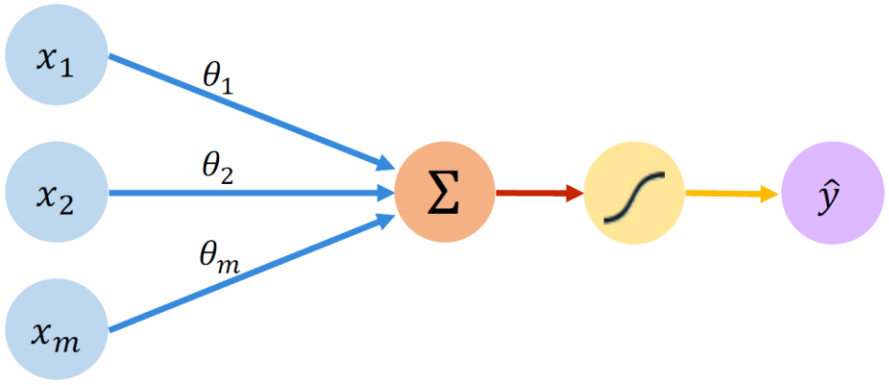
(Artificial) Neural Networks

Industrial AI Lab.

Prof. Seungchul Lee

Perceptron: Forward Propagation



Inputs Weights Sum Non-Linearity Output

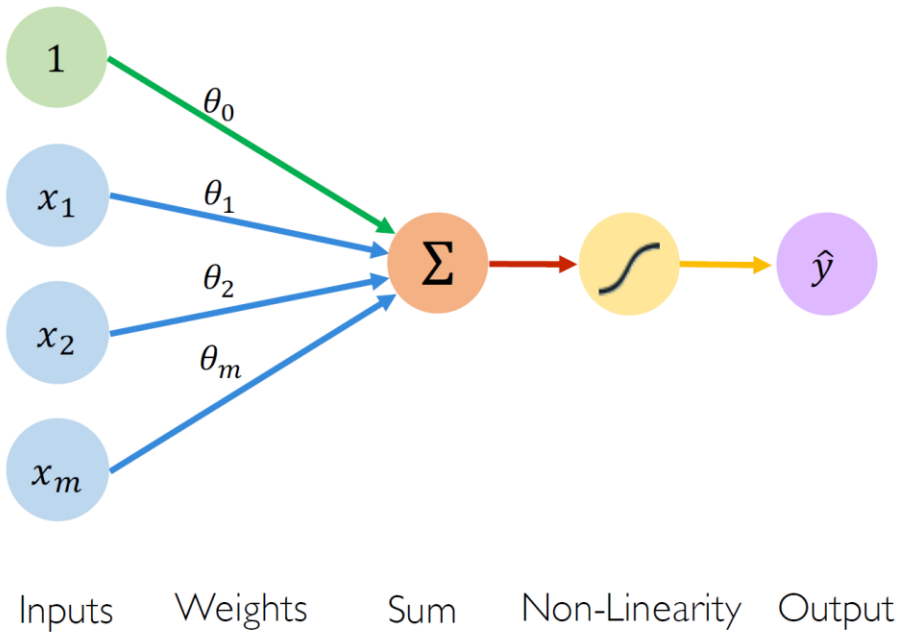
Output

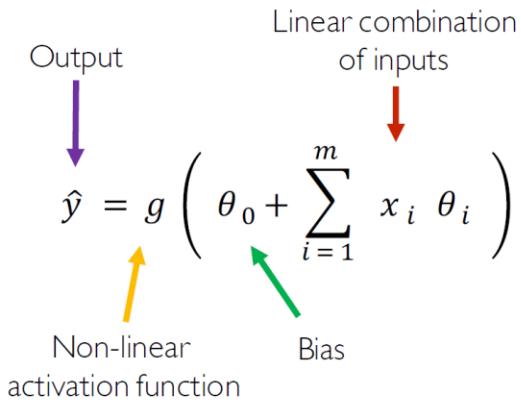
Linear combination of inputs

$$\hat{y} = g\left(\sum_{i=1}^{m} x_i \, \theta_i\right)$$

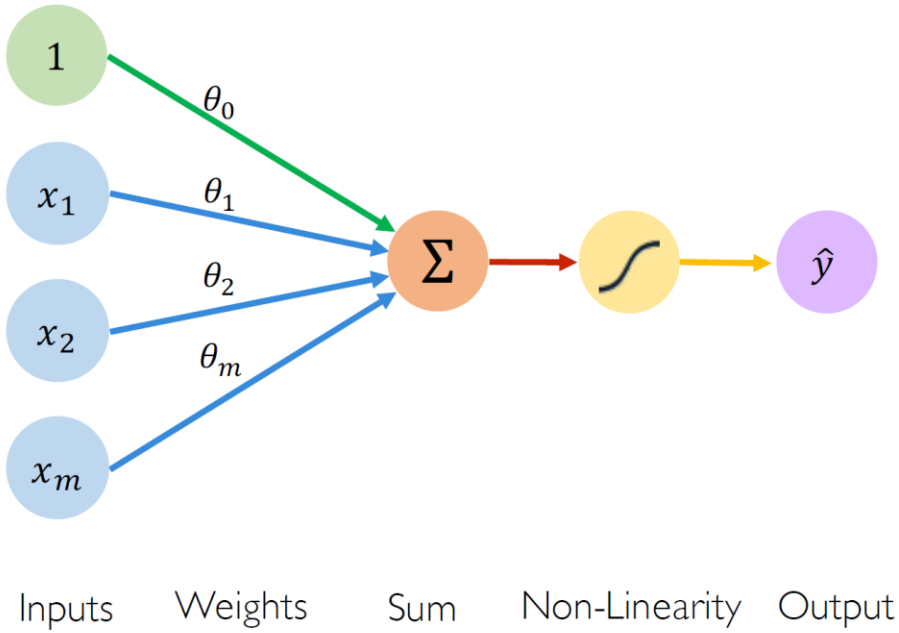
Non-linear activation function

Perceptron: Forward Propagation





Perceptron: Forward Propagation

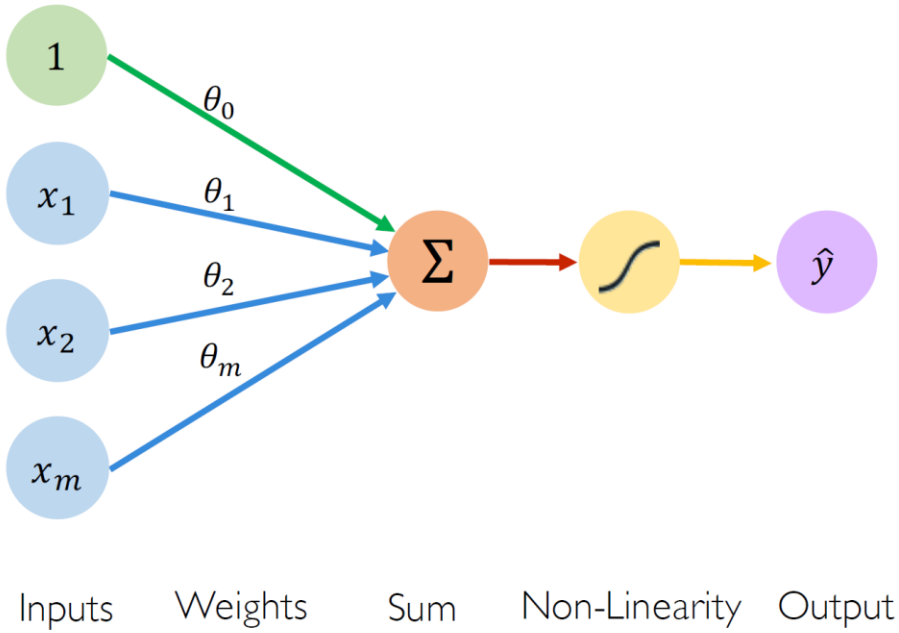


$$\hat{y} = g\left(\theta_0 + \sum_{i=1}^{m} x_i\, \theta_i\right)$$

$$\hat{y} = g\left(\theta_0 + \boldsymbol{X}^T \boldsymbol{\theta}\right)$$

where: $\boldsymbol{X} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$ and $\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_m \end{bmatrix}$

Perceptron: Forward Propagation

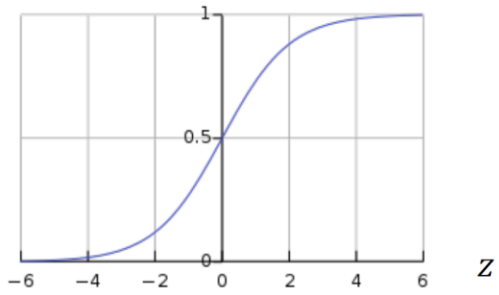


Activation Functions

$$\hat{y} = g(\theta_0 + \boldsymbol{X}^T \boldsymbol{\theta})$$

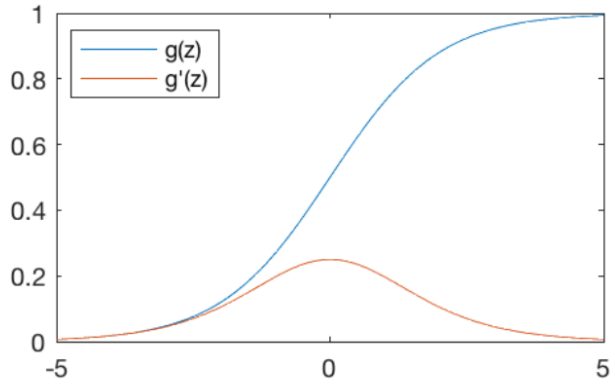
- Example: sigmoid function

$$g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}$$



Common Activation Functions

Sigmoid Function

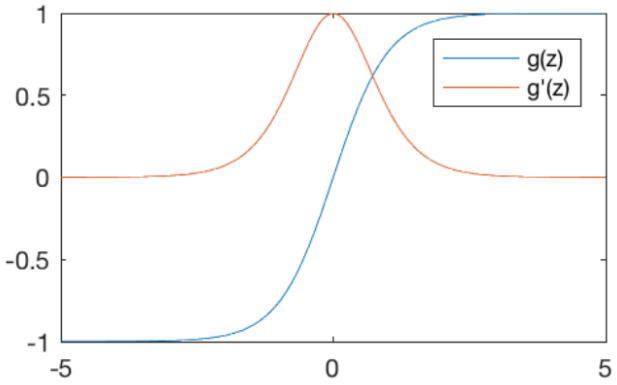


$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

`tf.nn.sigmoid(z)`

Hyperbolic Tangent

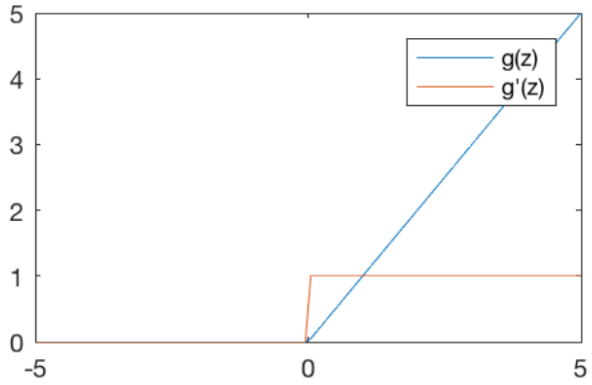


$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

`tf.nn.tanh(z)`

Rectified Linear Unit (ReLU)



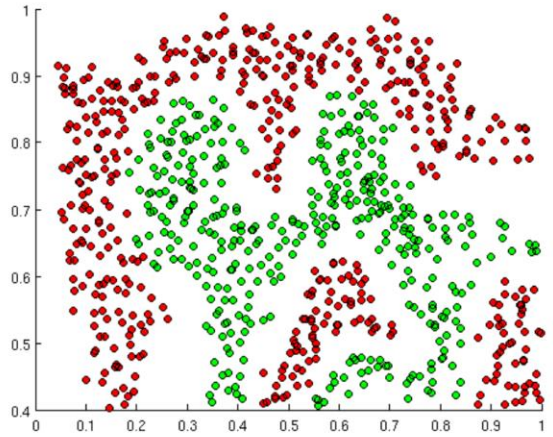
$$g(z) = \max(0, z)$$

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

`tf.nn.relu(z)`

Importance of Activation Functions

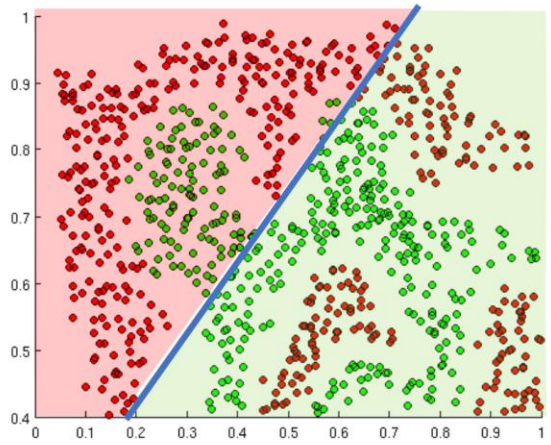
The purpose of activation functions is to ***introduce non-linearities*** *into the network*



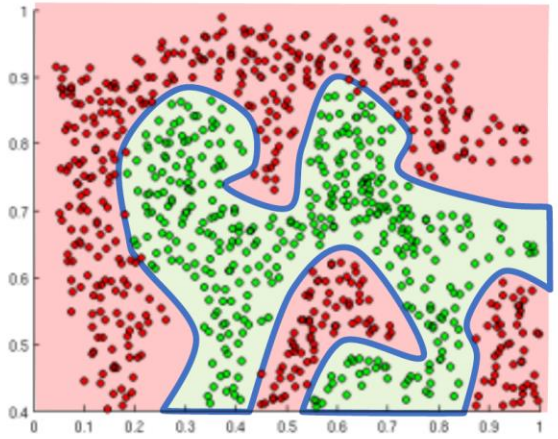
What if we wanted to build a Neural Network to distinguish green vs red points?

Importance of Activation Functions

The purpose of activation functions is to ***introduce non-linearities*** *into the network*

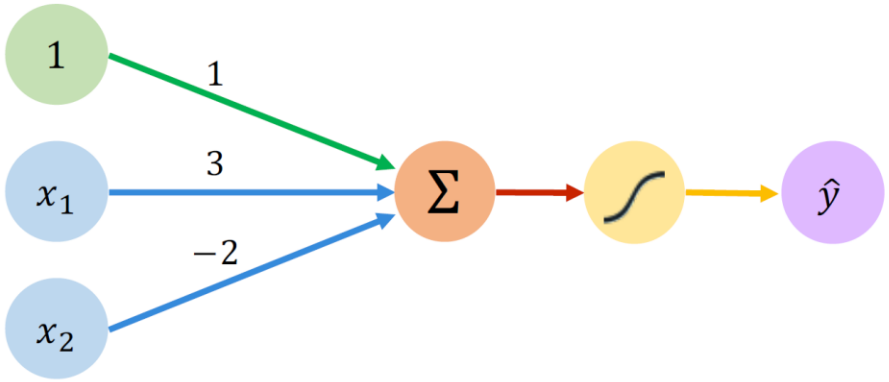


Linear Activation functions produce linear decisions no matter the network size



Non-linearities allow us to approximate arbitrarily complex functions

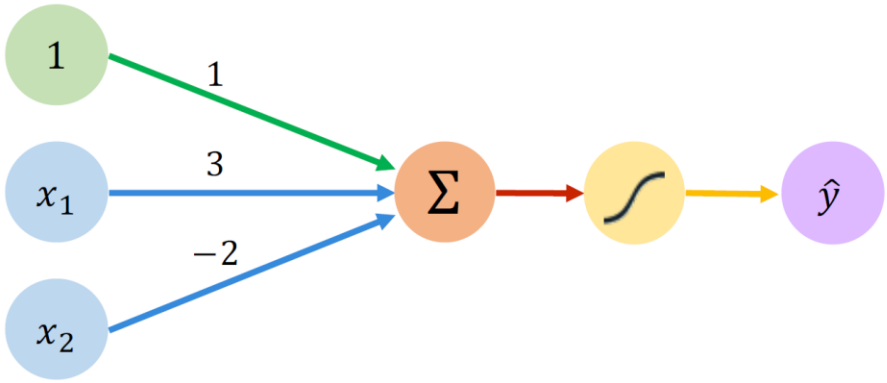
Perceptron: Example



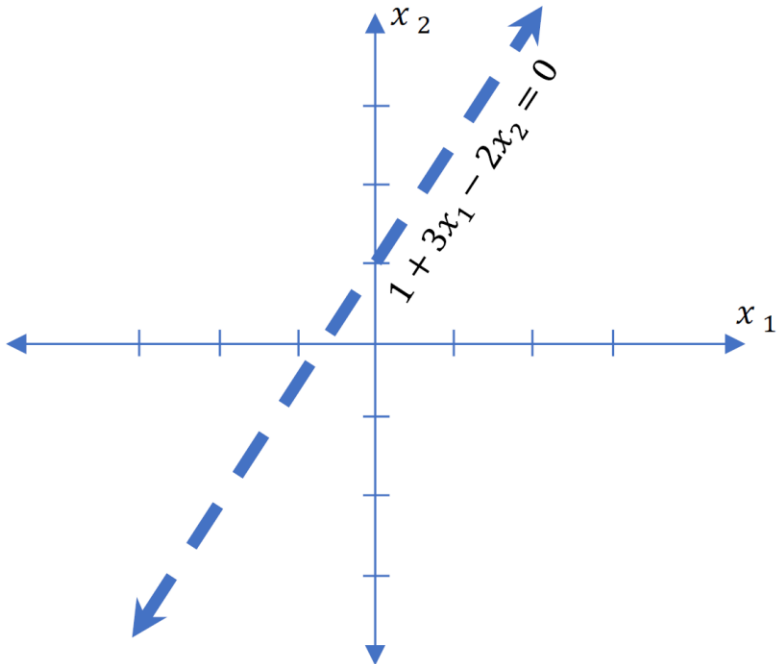
We have: $\theta_0 = 1$ and $\boldsymbol{\theta} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$

$$\hat{y} = g(\theta_0 + \boldsymbol{X}^T \boldsymbol{\theta})$$
$$= g\left(1 + \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 3 \\ -2 \end{bmatrix}\right)$$
$$\hat{y} = g(\underbrace{1 + 3x_1 - 2x_2}_{\text{This is just a line in 2D!}})$$

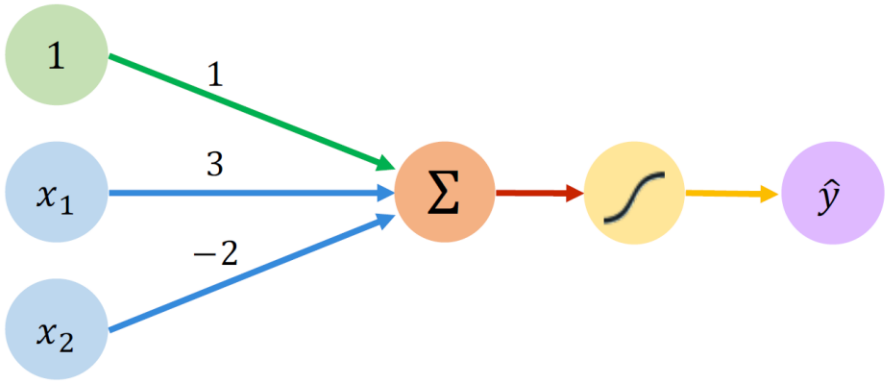
Perceptron: Example



$$\hat{y} = g(1 + 3x_1 - 2x_2)$$



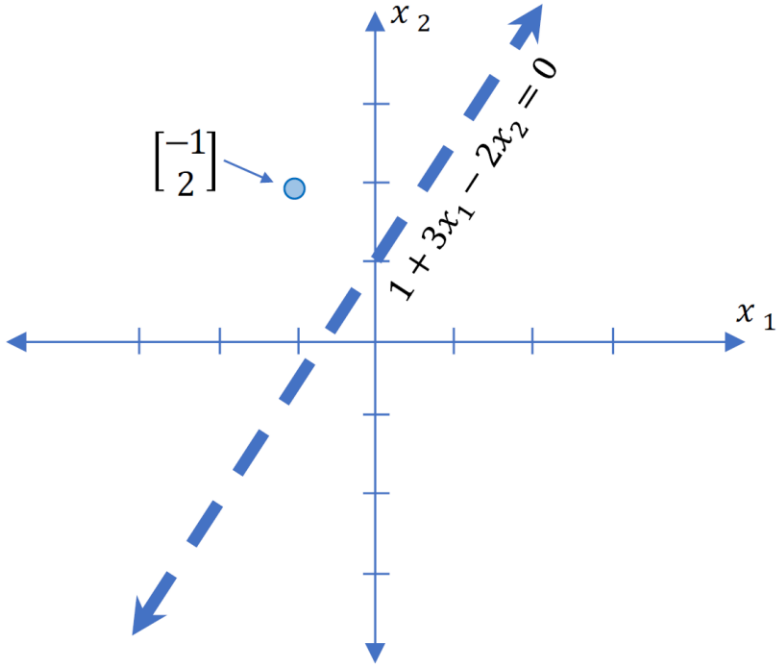
Perceptron: Example



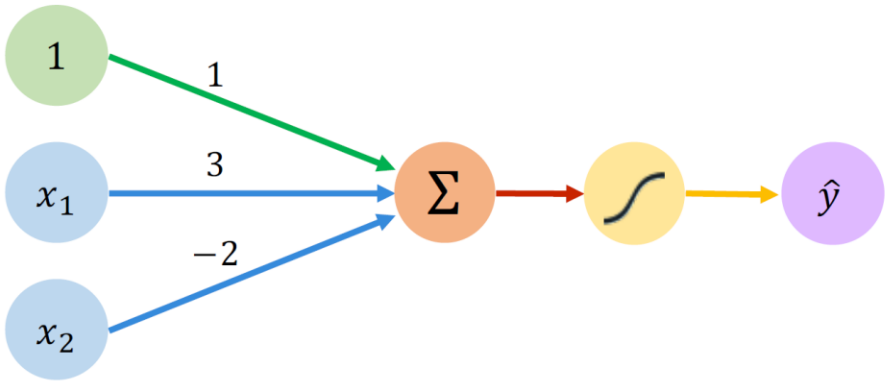
Assume we have input: $\boldsymbol{X} = \begin{bmatrix} -1 \\ 2 \end{bmatrix}$

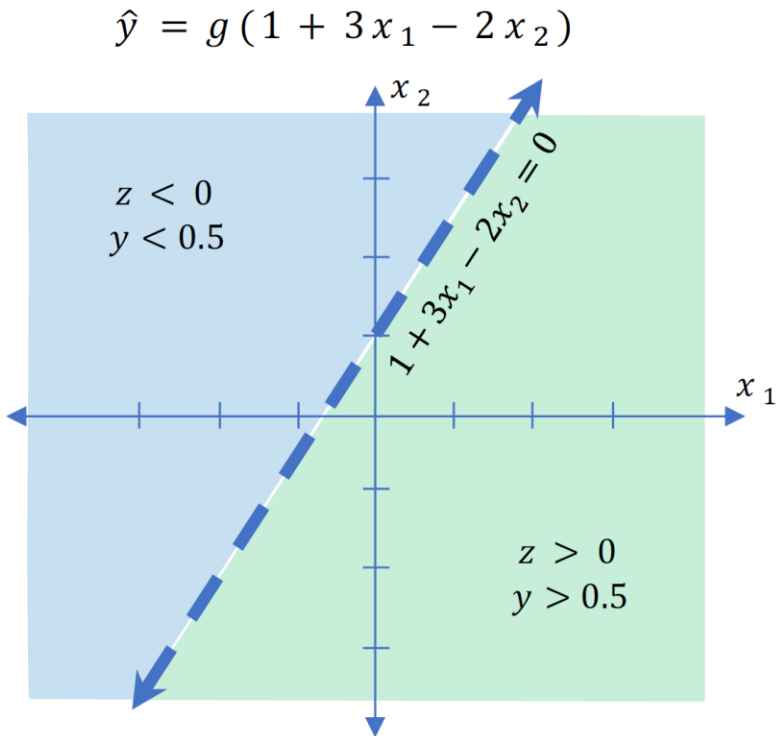
$$\hat{y} = g\left(1 + (3 * -1) - (2 * 2)\right)$$
$$= g(-6) \approx 0.002$$

$$\hat{y} = g(1 + 3x_1 - 2x_2)$$



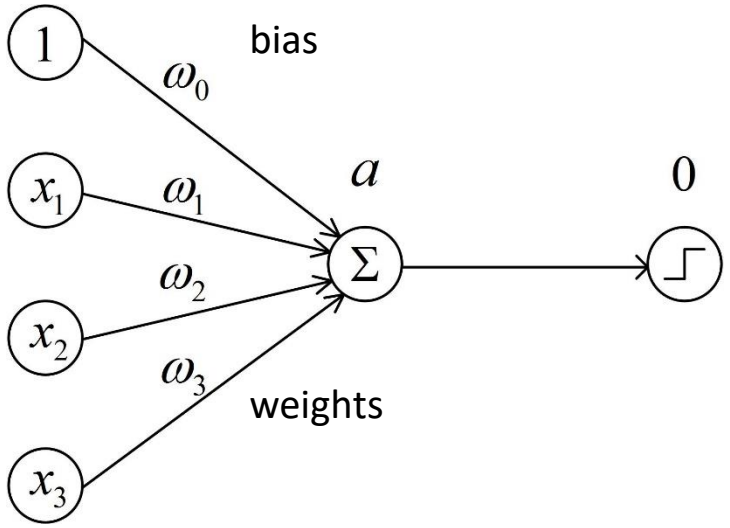
Perceptron: Example



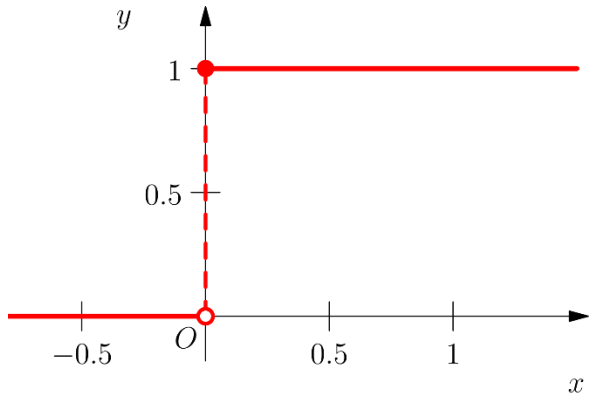


Artificial Neural Networks: Perceptron

- Perceptron for $h(\theta)$ or $h(\omega)$
  - Neurons compute the weighted sum of their inputs
  - A neuron is activated or fired when the sum a is positive



$$a = \omega_0 + \omega_1 x_1 + \cdots$$
$$o = \sigma(\omega_0 + \omega_1 x_1 + \cdots)$$

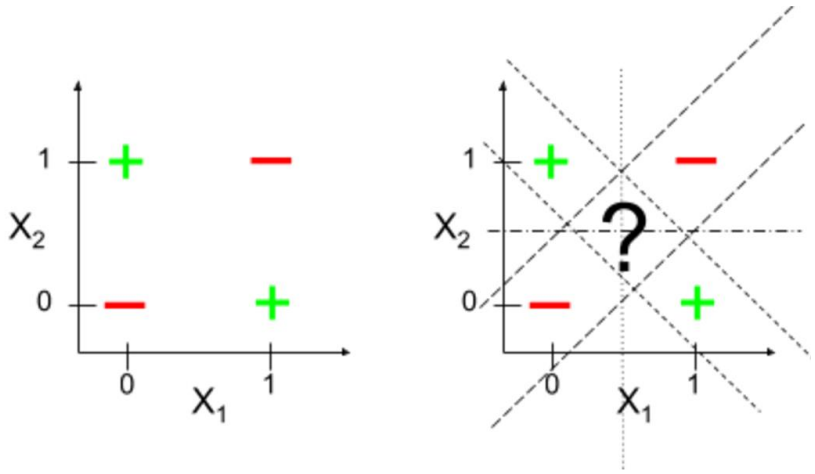


- A step function is not differentiable
- One layer is often not enough

XOR Problem

- Minsky-Papert Controversy on XOR
  - not linearly separable
  - Limitation of perceptron

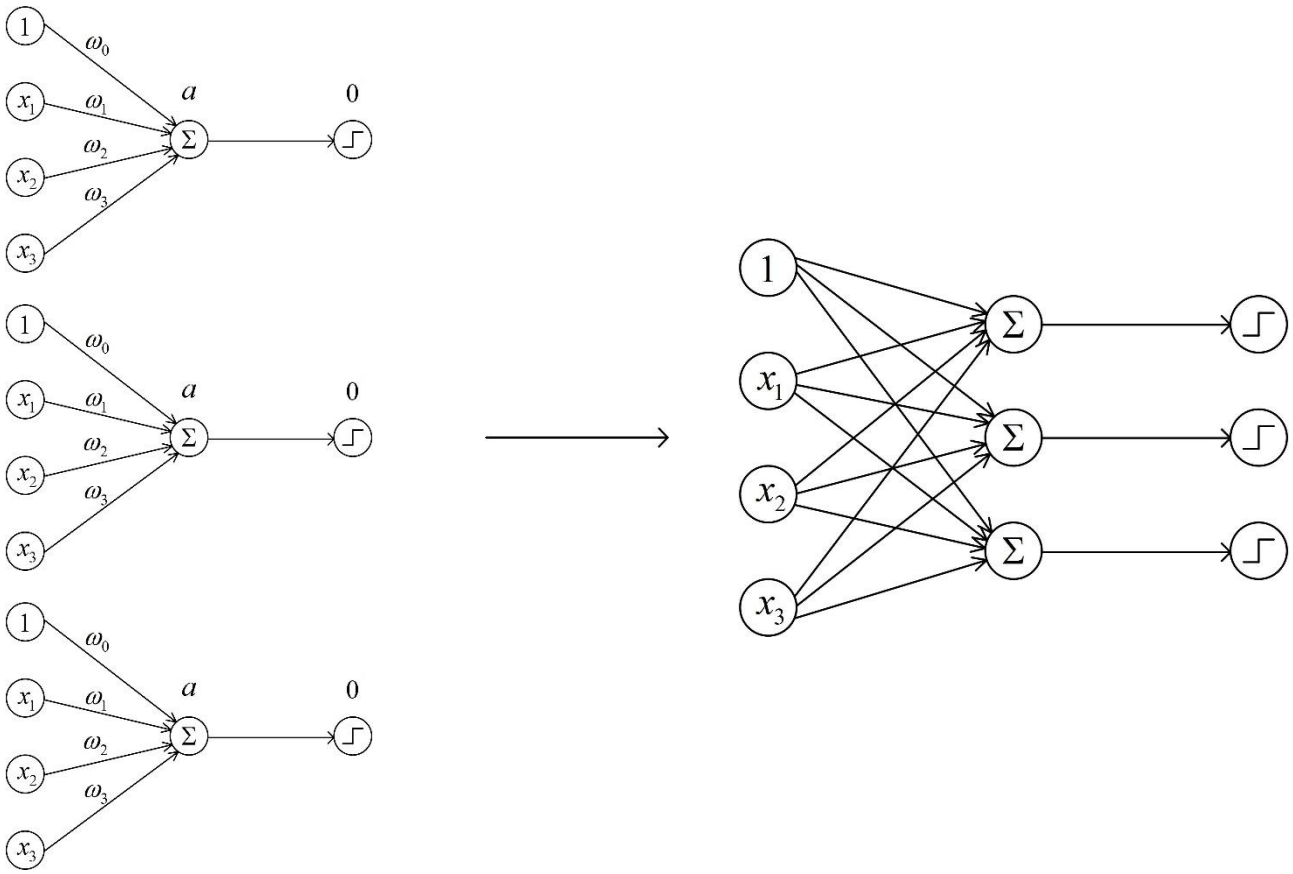
x_1	x_2	x_1 **XOR** x_2
0	0	0
0	1	1
1	0	1
1	1	0



- Single neuron = one linear classification boundary

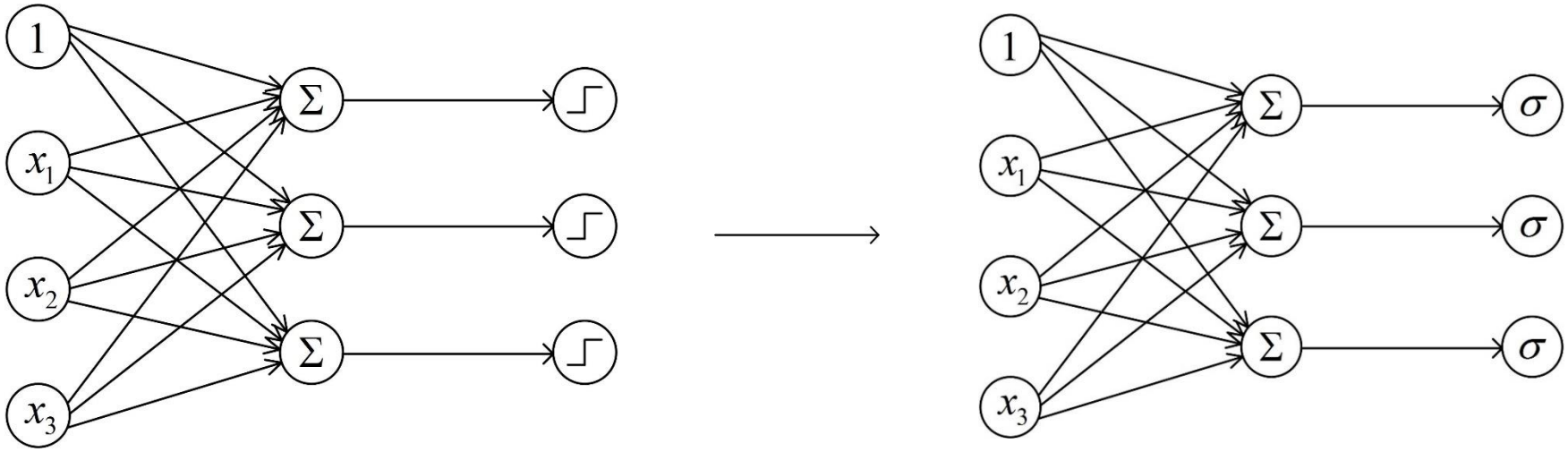
Artificial Neural Networks: MLP

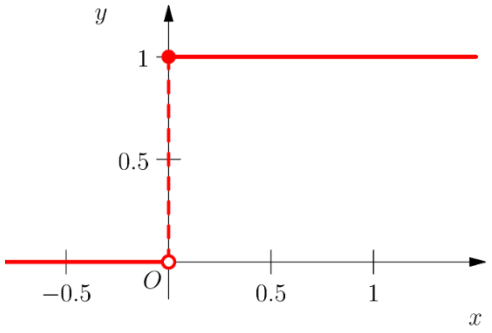
- Multi-layer Perceptron (MLP) = Artificial Neural Networks (ANN)
  - Multi neurons = multiple linear classification boundaries

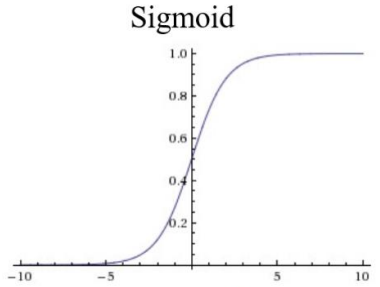


Artificial Neural Networks: Activation Func.

- Differentiable non-linear activation function



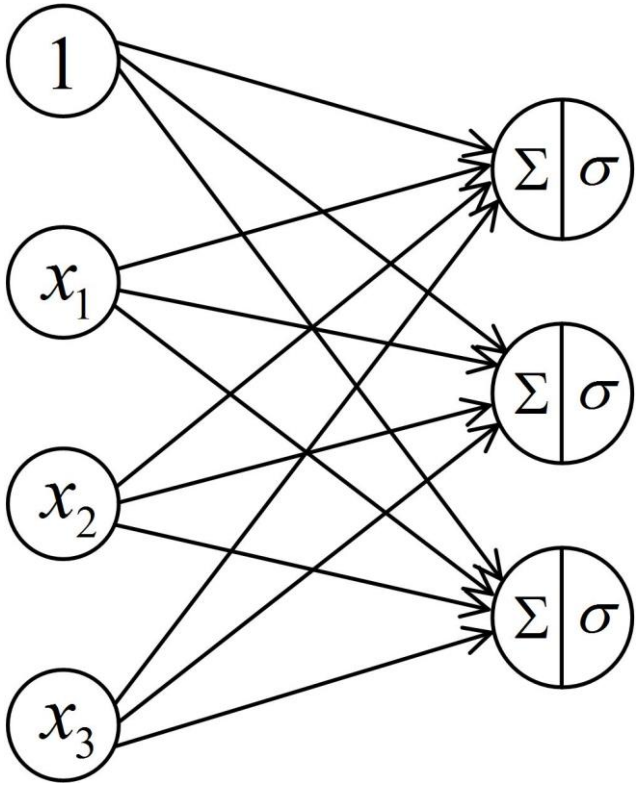




$$g(x) = \frac{1}{1+e^{-x}}$$

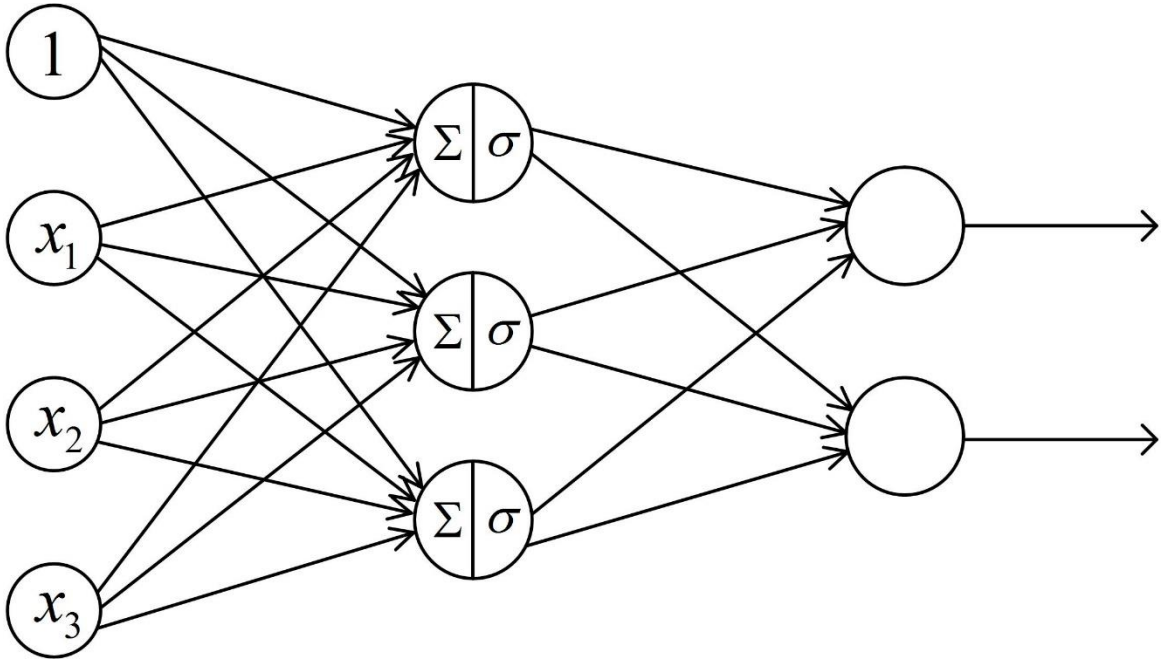
Artificial Neural Networks

- In a compact representation



Artificial Neural Networks

- Multi-layer perceptron
  - Features of features
  - Mapping of mappings



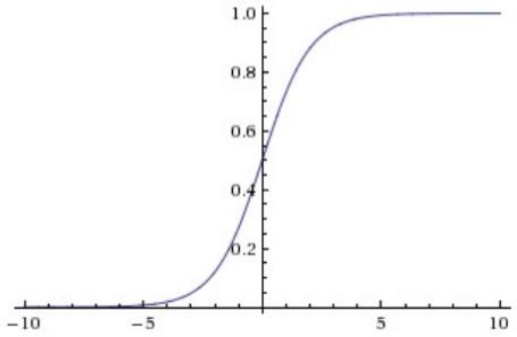
ANN: Transformation

- Affine (or linear) transformation and nonlinear activation layer (notations are mixed: $g = \sigma, \omega = \theta, \omega_0 = b$)

$$o(x) = g\left(\theta^T x + b\right)$$

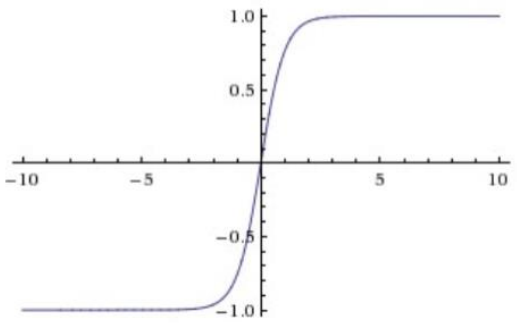
- Nonlinear activation functions ($g = \sigma$)

Sigmoid



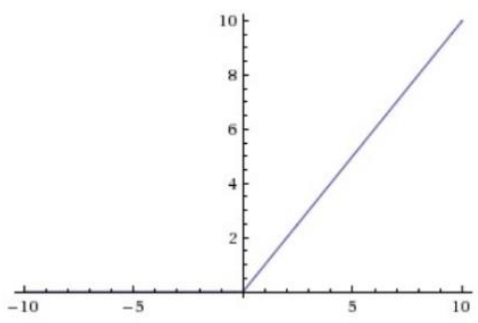
$$g(x) = \frac{1}{1 + e^{-x}}$$

tanh



$$g(x) = \tanh(x)$$

Rectified Linear Unit



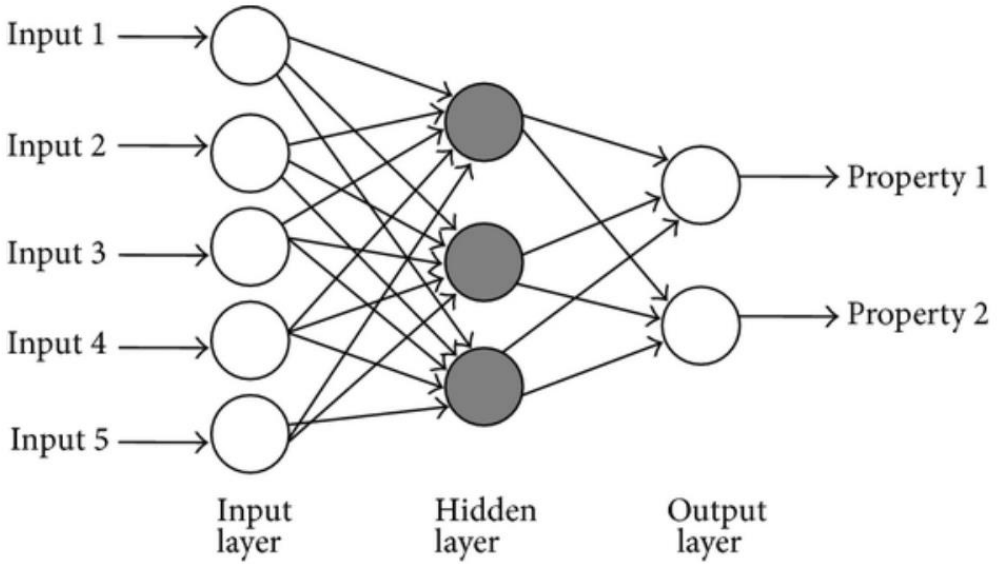
$$g(x) = \max(0, x)$$

ANN: Architecture

- A single layer is not enough to be able to represent complex relationship between input and output

  $\Longrightarrow$ perceptron with many layers and units

$$o_2 = \sigma_2\left(\theta_2^T o_1 + b_2\right) = \sigma_2\left(\theta_2^T \sigma_1\left(\theta_1^T x + b_1\right) + b_2\right)$$



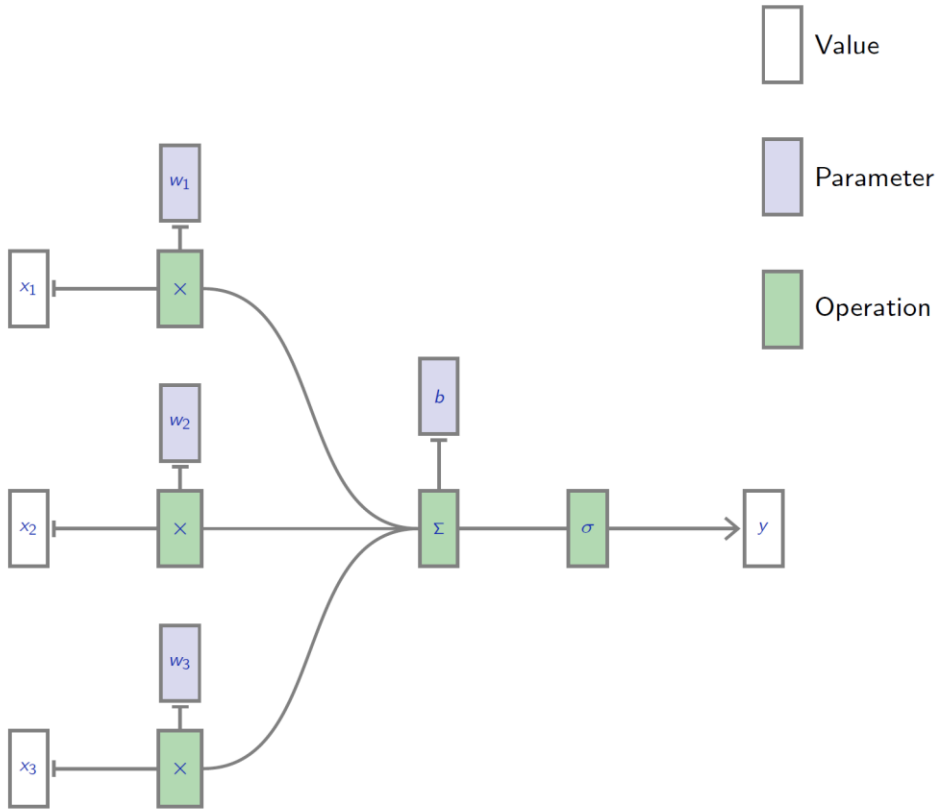
- The perceptron classification rule boils down to

$$f(x) = \sigma(w \cdot x + b).$$

- For neural networks, the function σ that follows a linear operator is called the activation function.

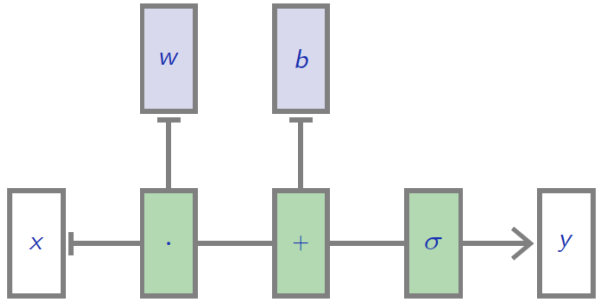
- We can also use tensor operations, as in

$$f(x) = \sigma(w \cdot x + b).$$

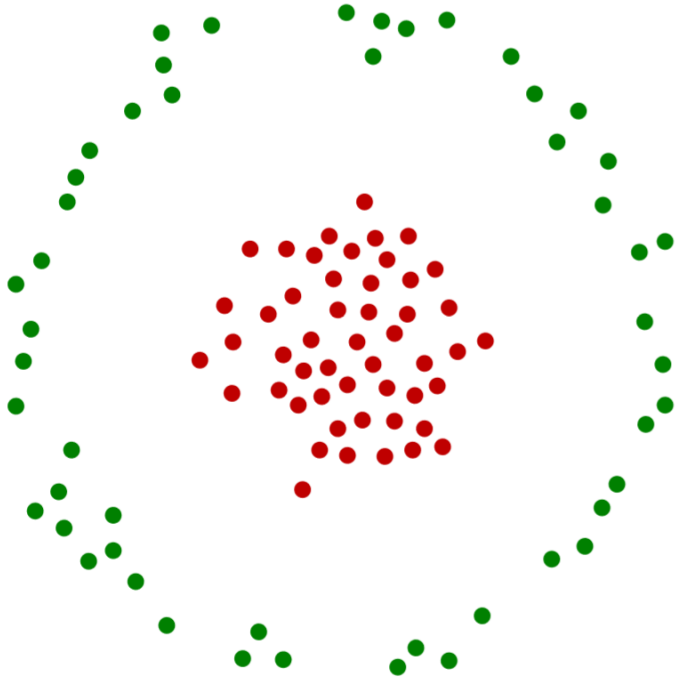


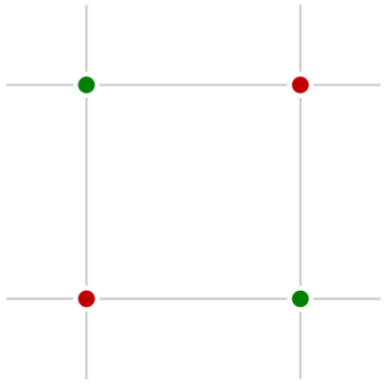
- We can represent this “neuron” as follows:

$$f(x) = \sigma(w \cdot x + b).$$



- The main weakness of linear predictors is their lack of capacity. For classification, the populations have to be linearly separable.

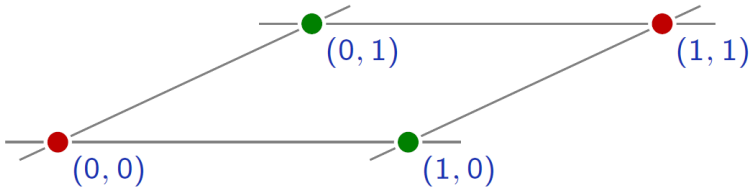




"xor"

- The xor example can be solved by pre-processing the data to make the two populations linearly separable.

$$\Phi : (x_u, x_v) \mapsto (x_u, x_v, x_u x_v).$$



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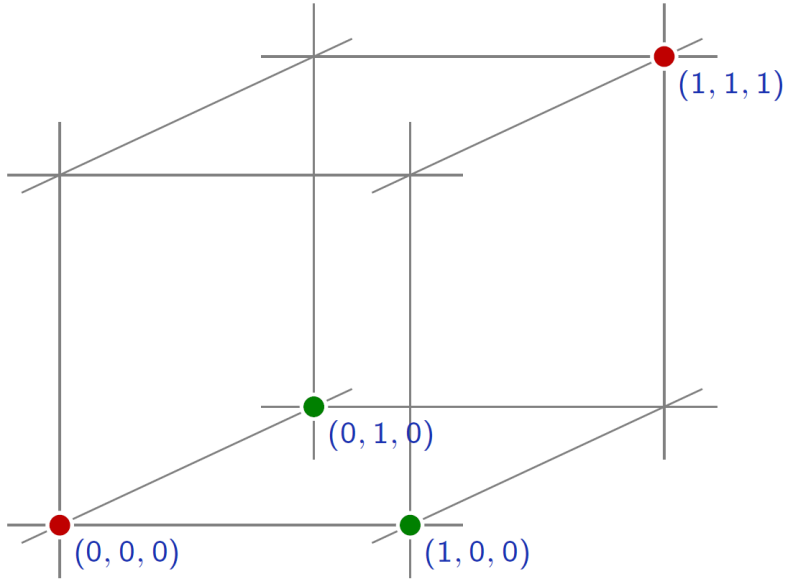

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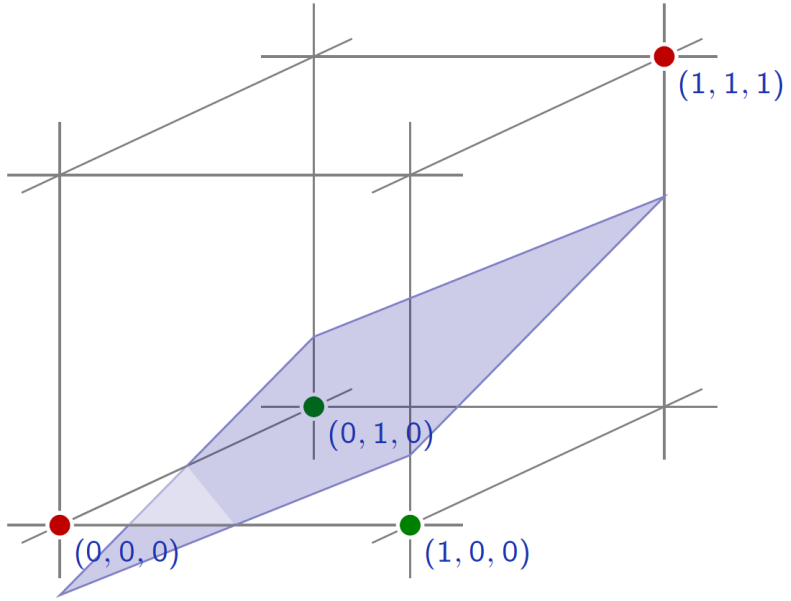
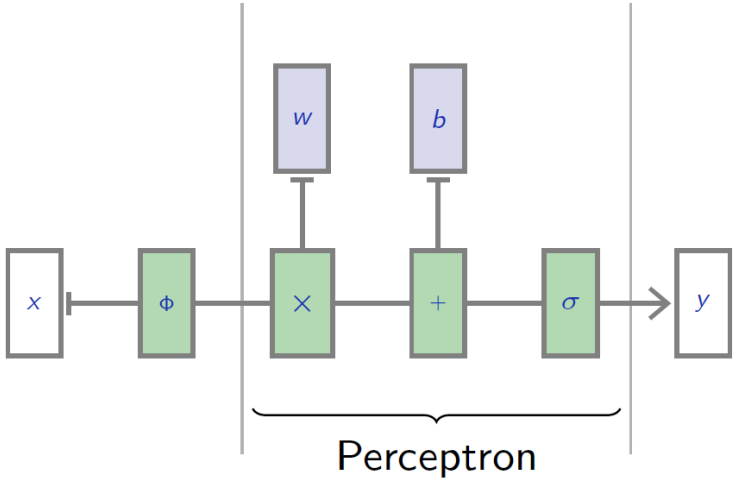
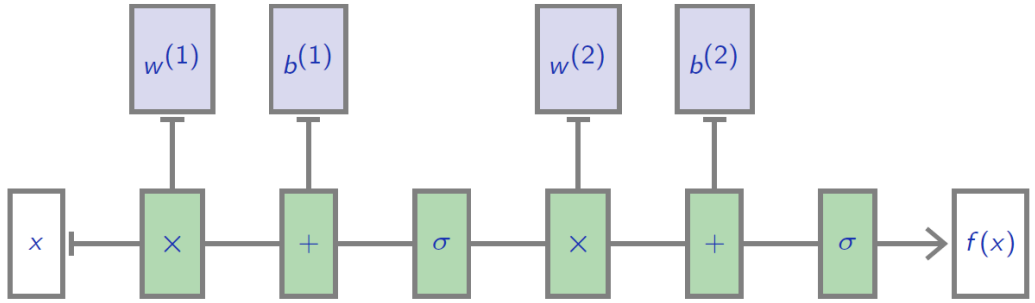


- Nonlinear mapping + neuron

$$\Phi : (x_u, x_v) \mapsto (x_u, x_v, x_u x_v).$$

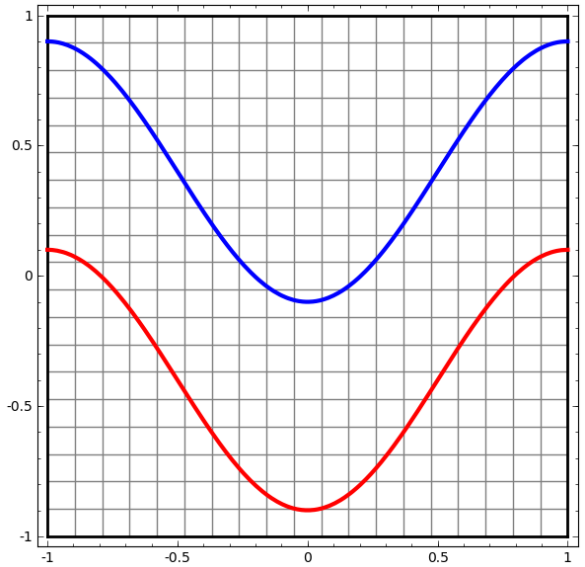


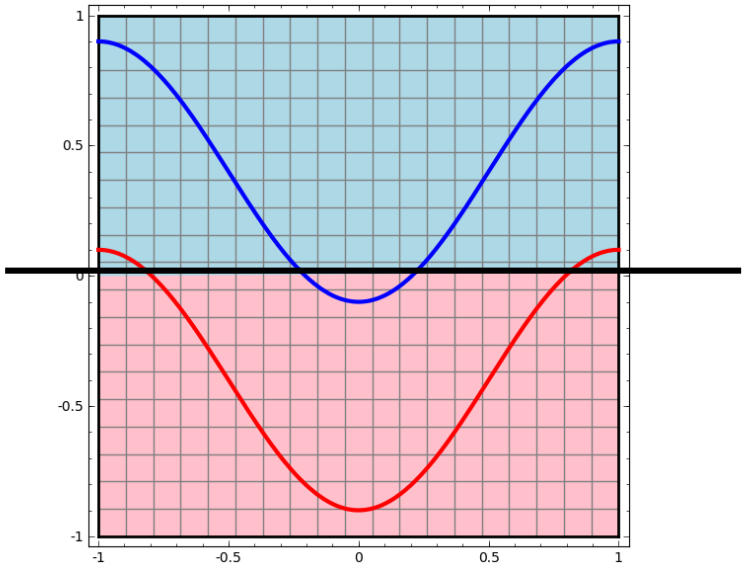
- Nonlinear mapping can be represented by another neurons
- We can generalize an MLP



Linear Classifier

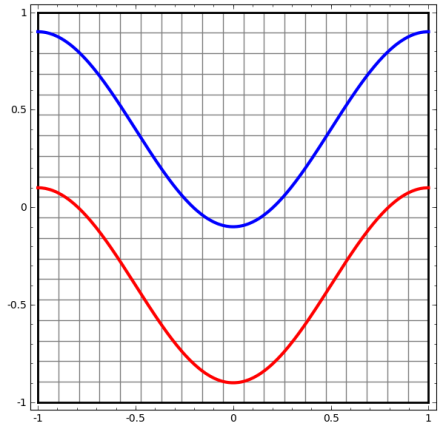
- Perceptron tries to separate the two classes of data by dividing them with a line

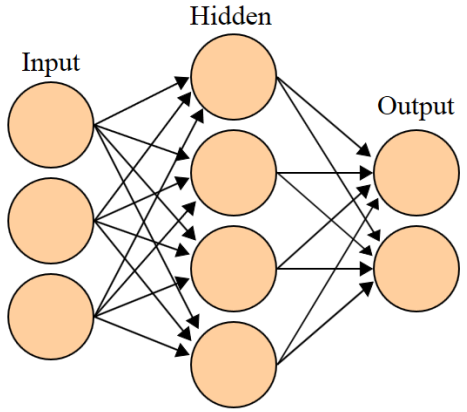


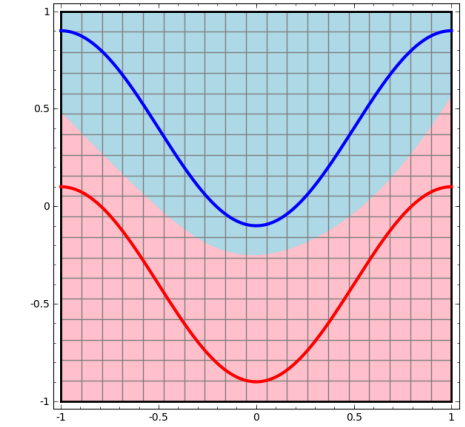


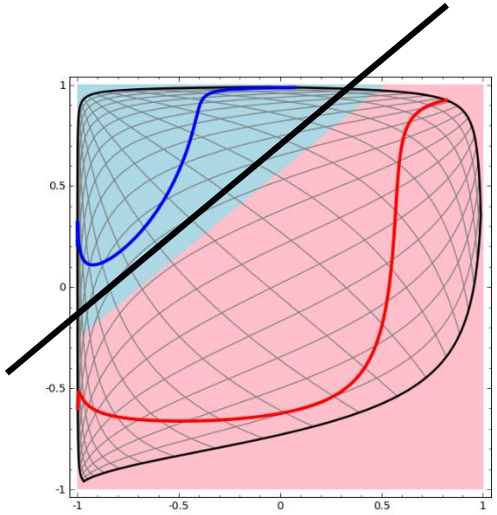
Neural Networks

- The hidden layer learns a representation so that the data is linearly separable





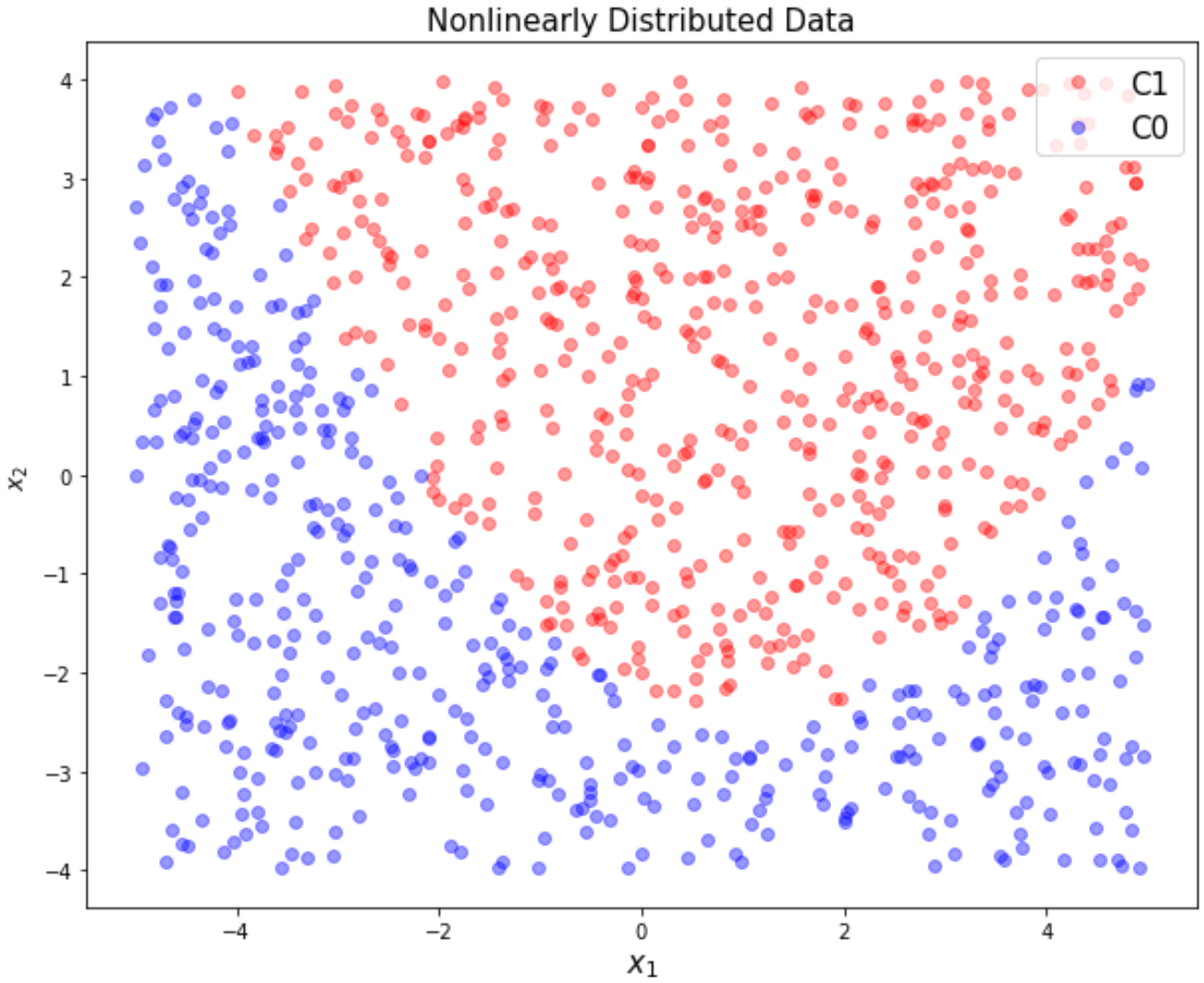




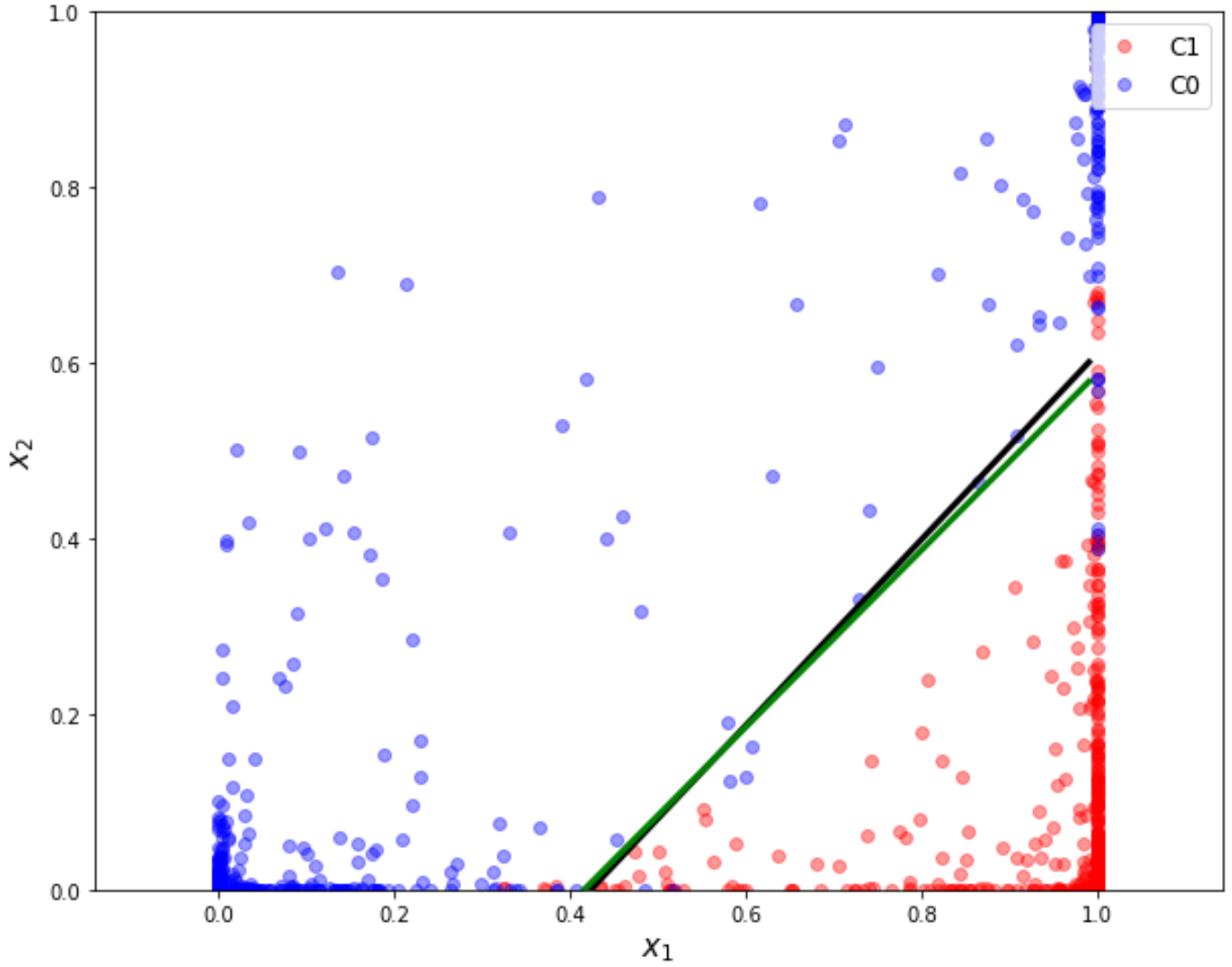
Understanding a Network's Behavior

- Understanding what is happening in a deep architectures after training is complex and the tools we have at our disposal are limited.
- We can look at
  - the network's parameters, filters as images,
  - internal activations as images,
  - distributions of activations on a population of samples,
  - derivatives of the response(s) wrt the input,
  - maximum-response synthetic samples,
  - adversarial samples.

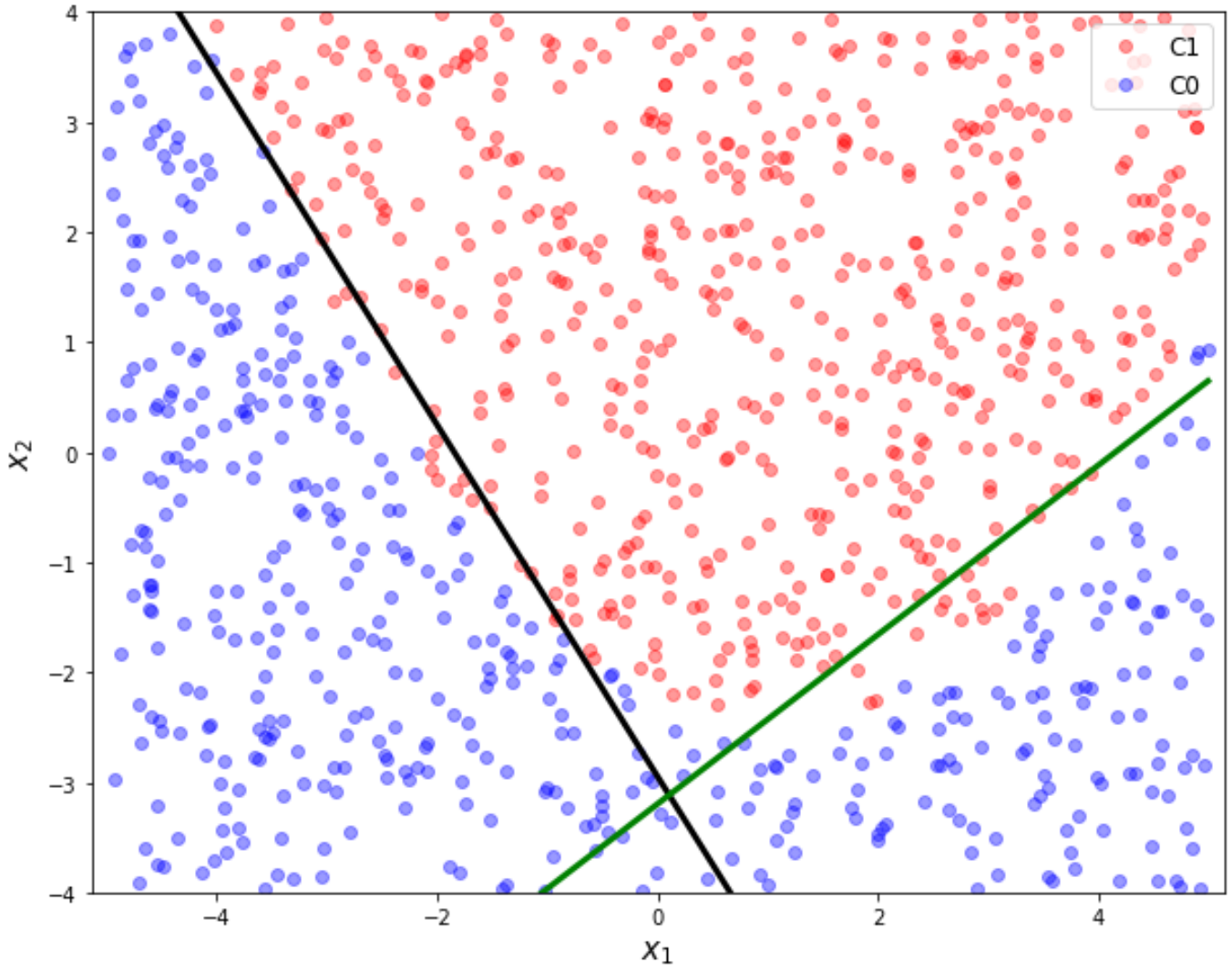
Nonlinearly Distributed Data



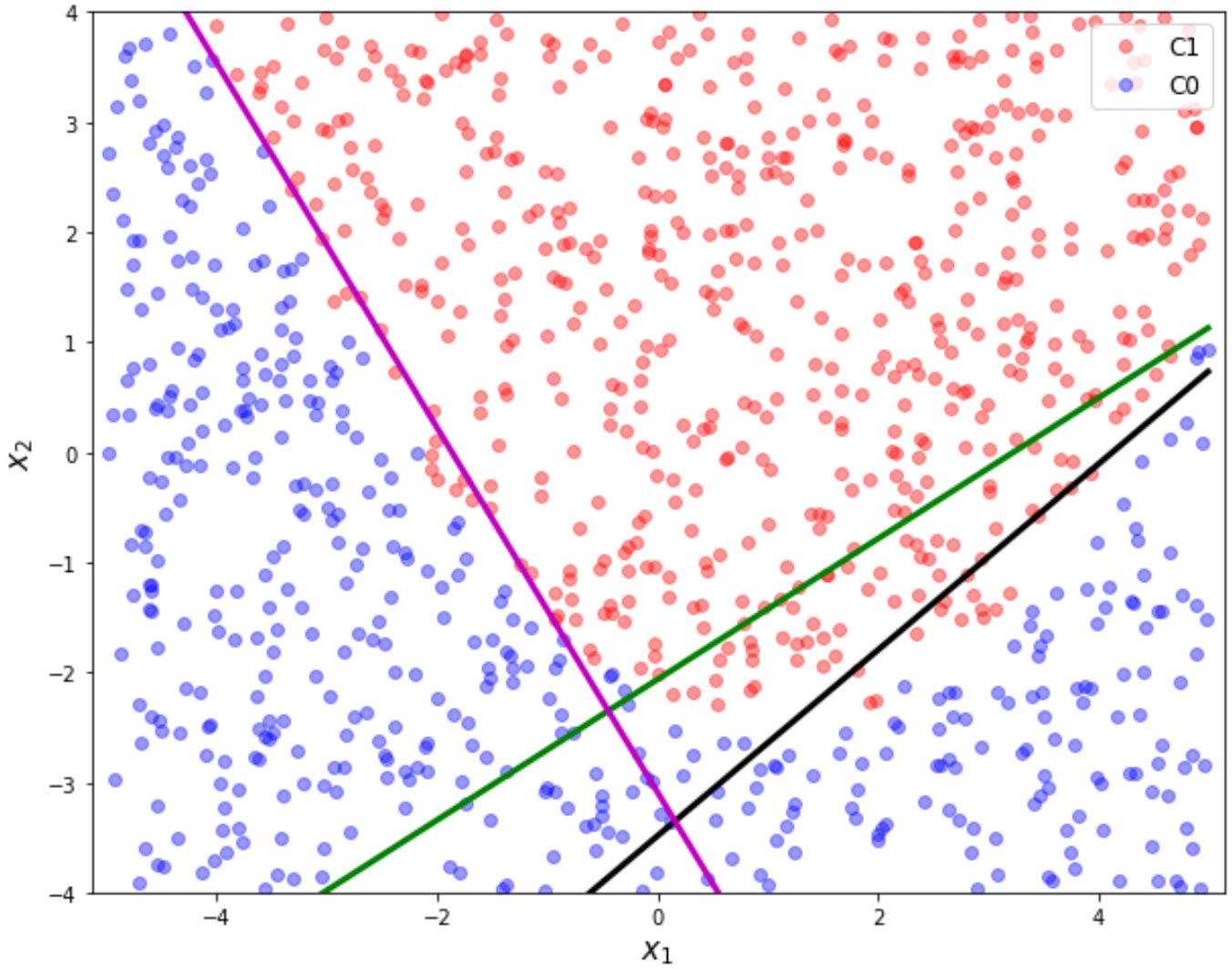
Multi Layers

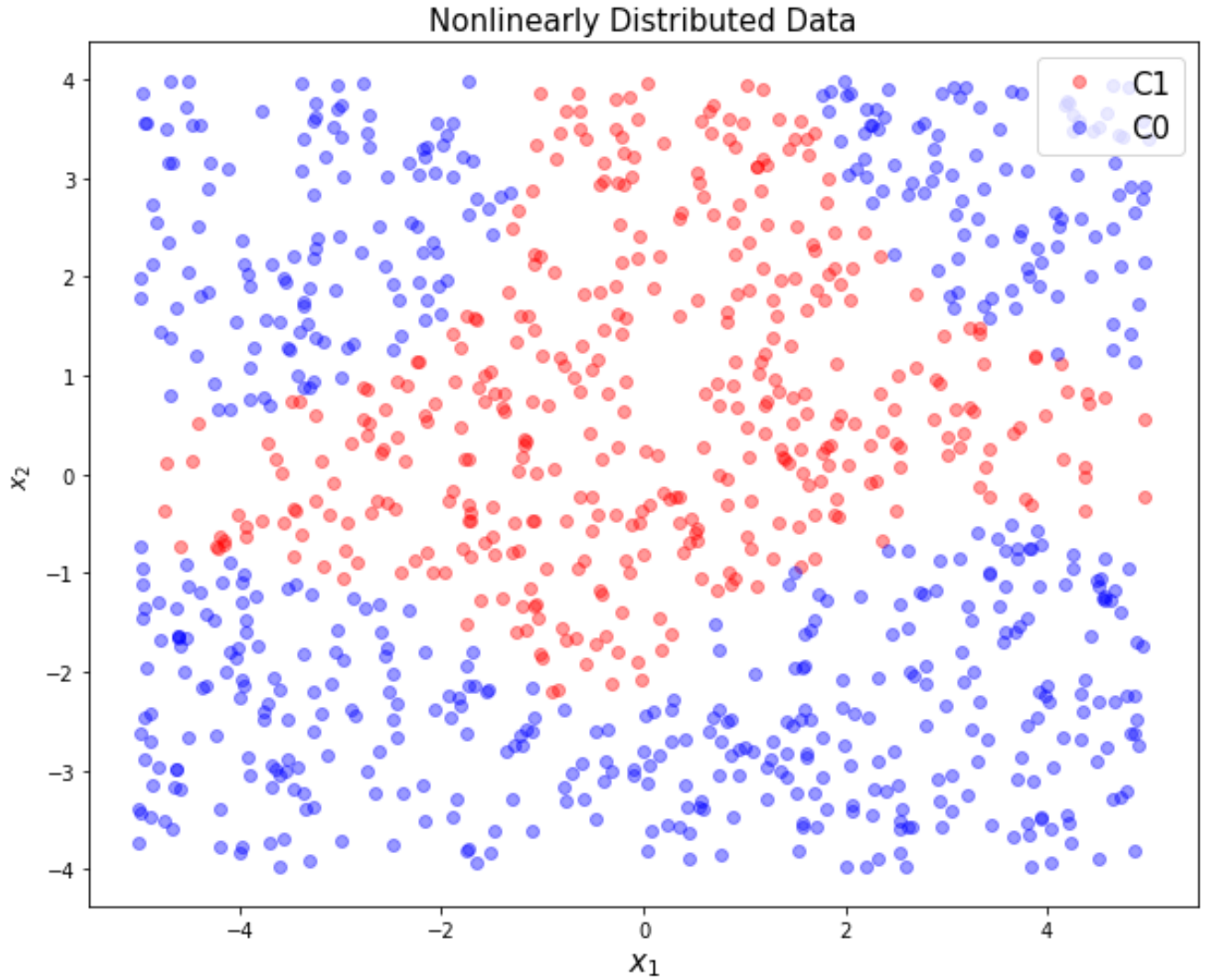


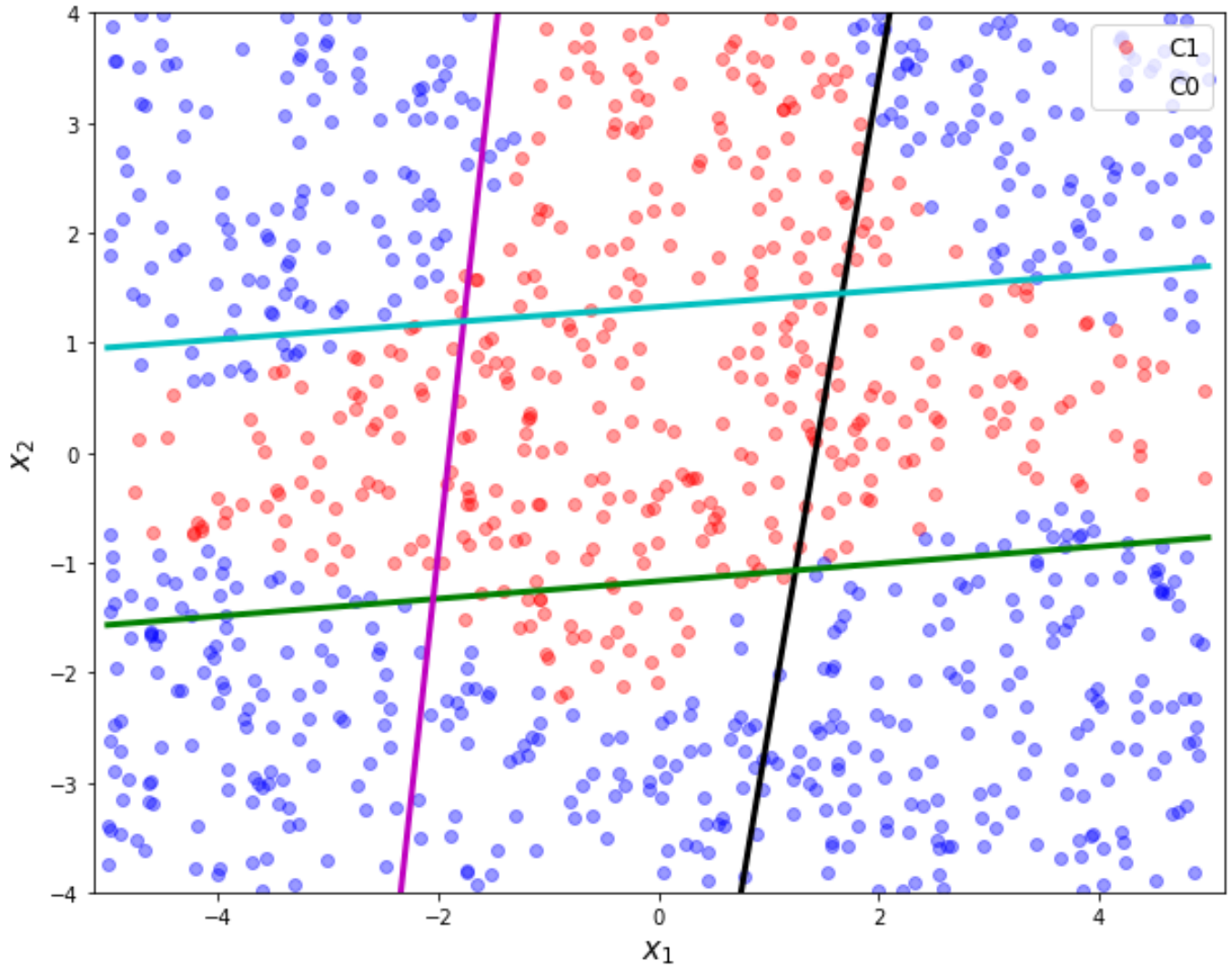
Multi Layers



Multi Neurons




Nonlinearly Distributed Data
C1
C0
x_1
x_2
4
3
2
1
0
−1
−2
−3
−4
−4
−2
0
2
4


C1
C0
x_1
x_2
4
3
2
1
0
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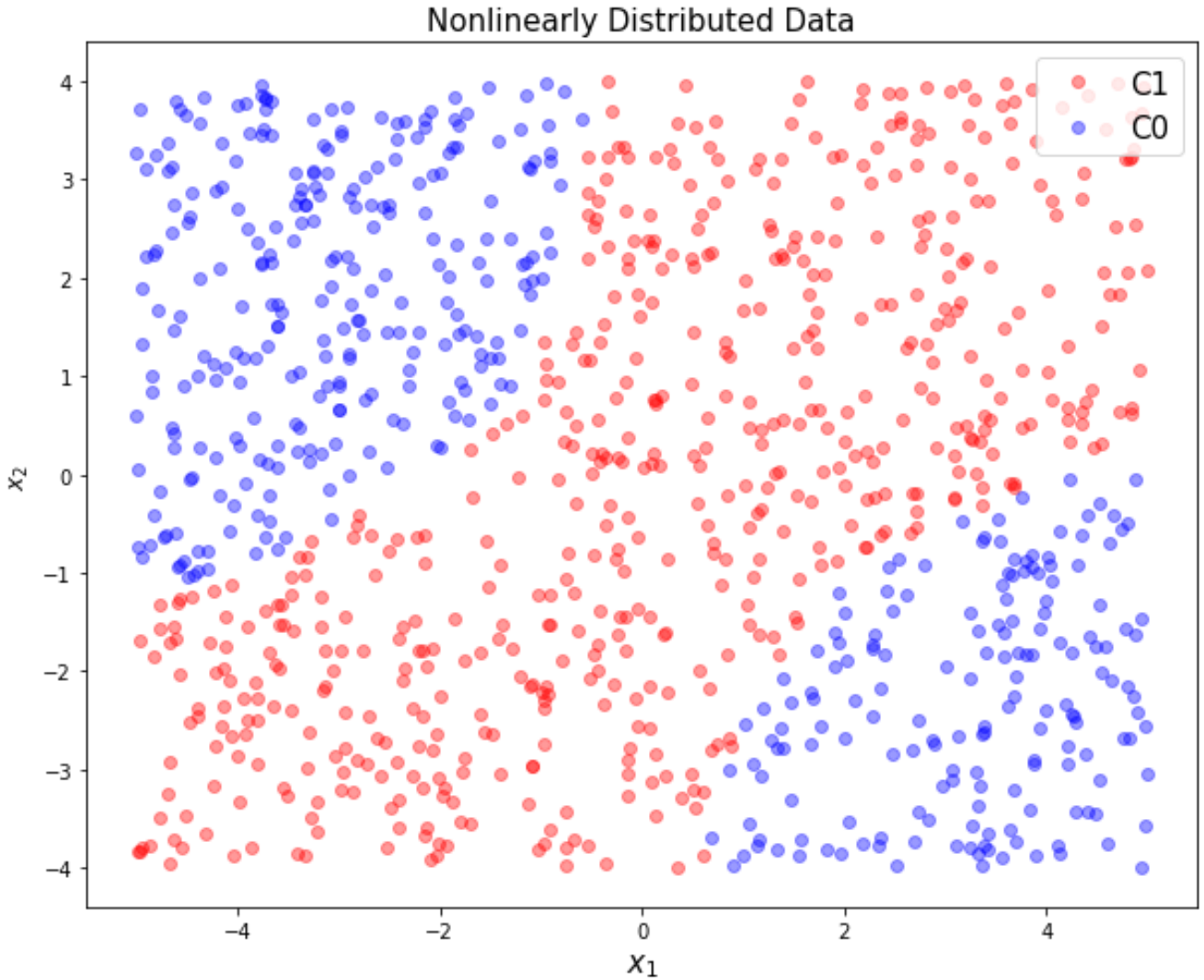
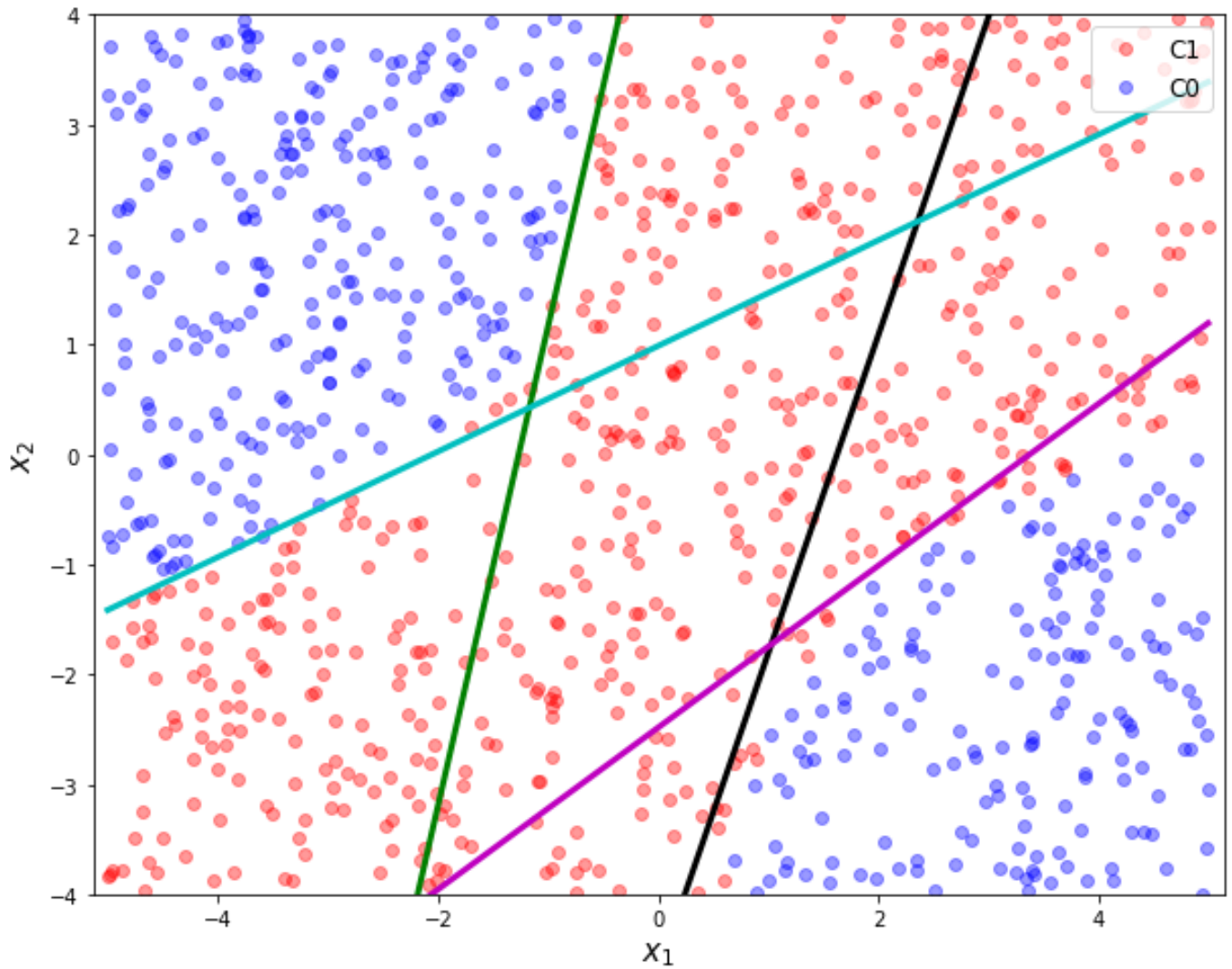
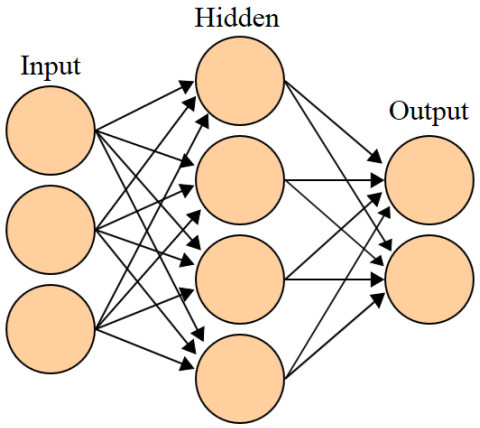
−2
−3
−4
−4
−2
0
2
4


Nonlinearly Distributed Data
C1
C0
x_1
x_2
4
3
2
1
0
−1
−2
−3
−4
−4
−2
0
2
4


C1
C0
x_1
x_2
4
3
2
1
0
−1
−2
−3
−4
−4
−2
0
2
4

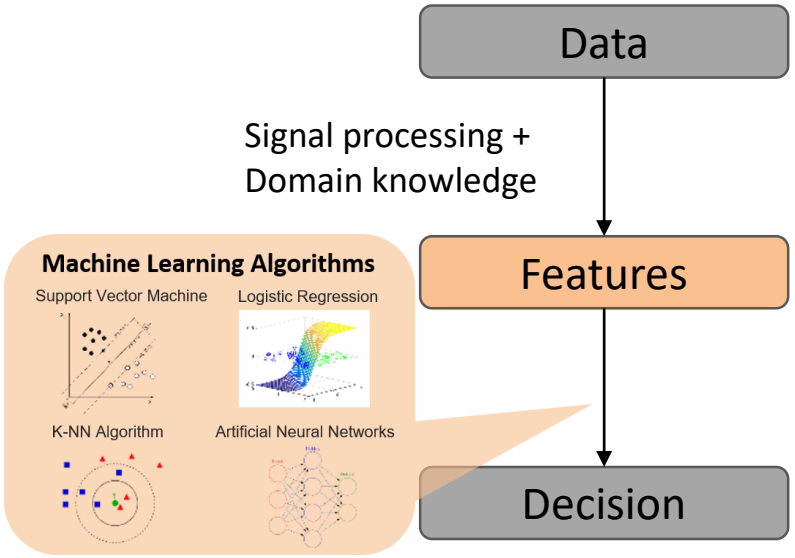
Summary

- Learning weights and biases from data using gradient descent

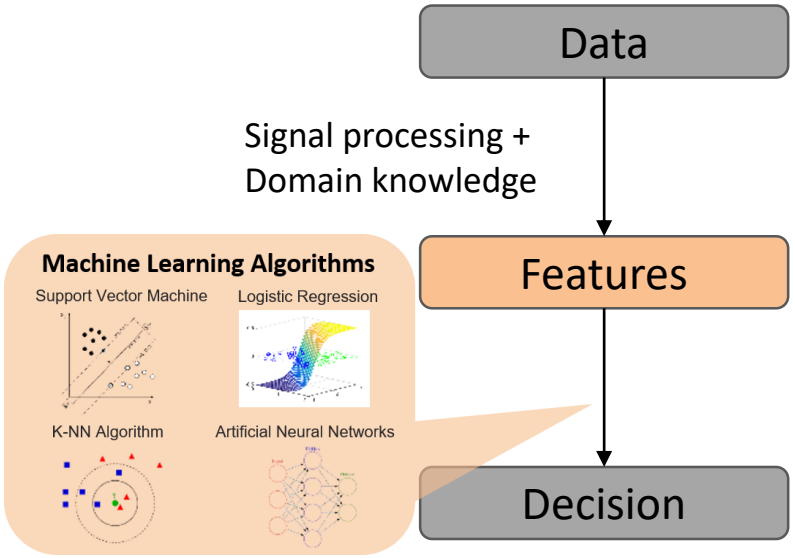


$$x \rightarrow \boxed{\hat{y} = f_{\omega_1,\cdots,\omega_k}(x)} \rightarrow y$$

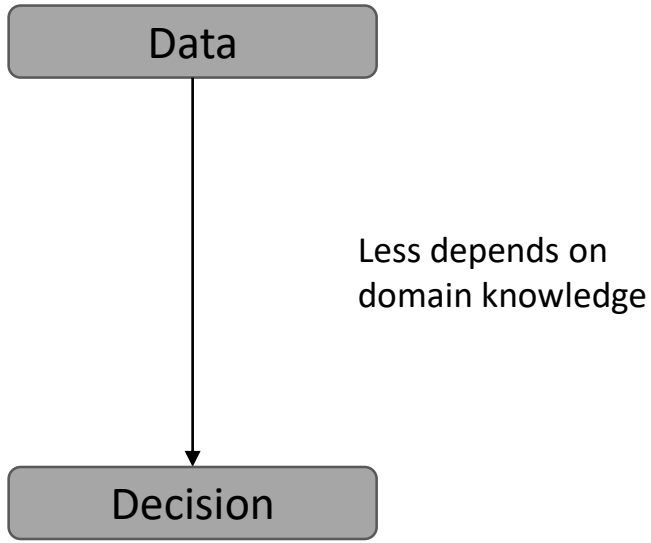
Machine Learning



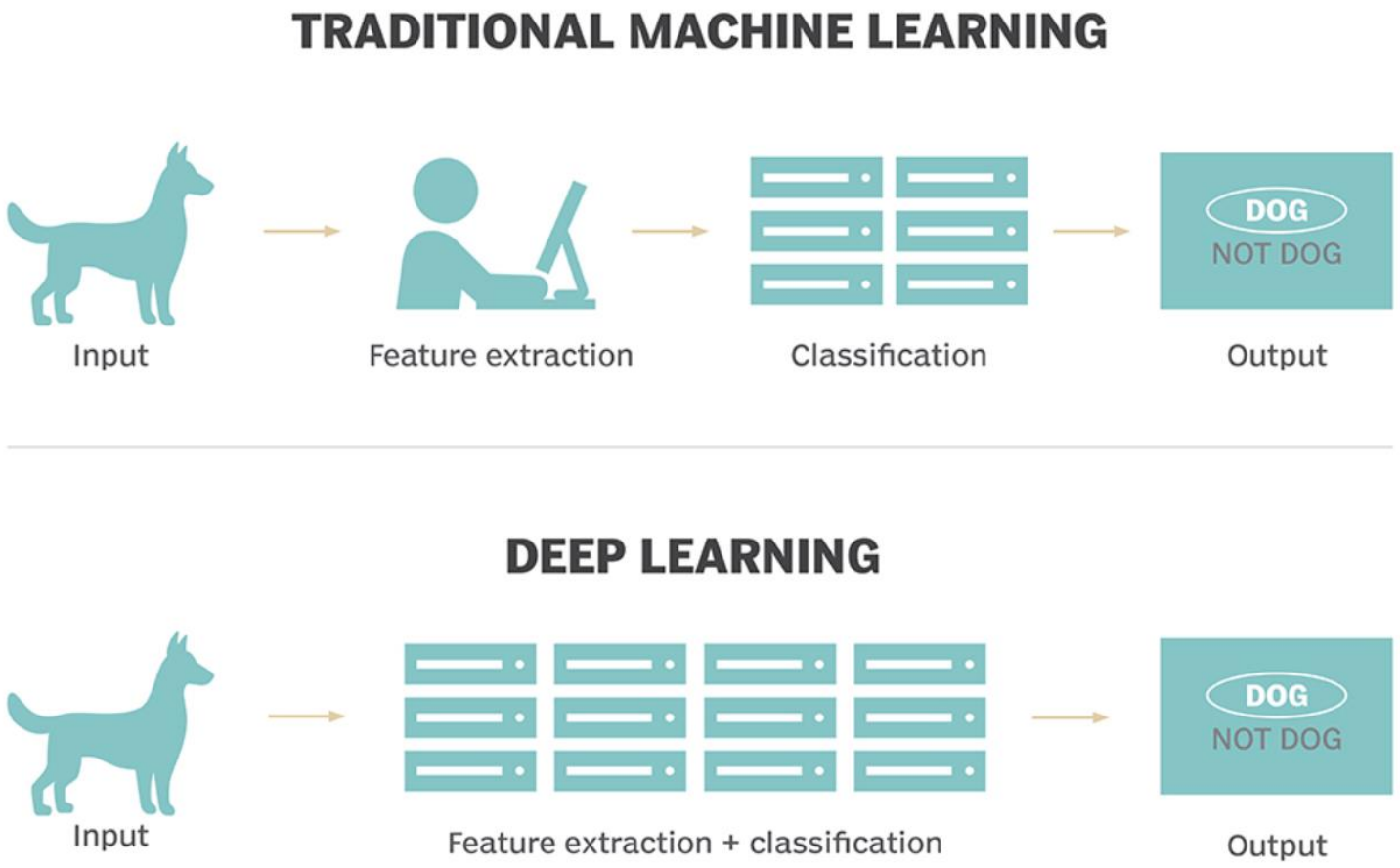
Machine Learning



Deep Learning

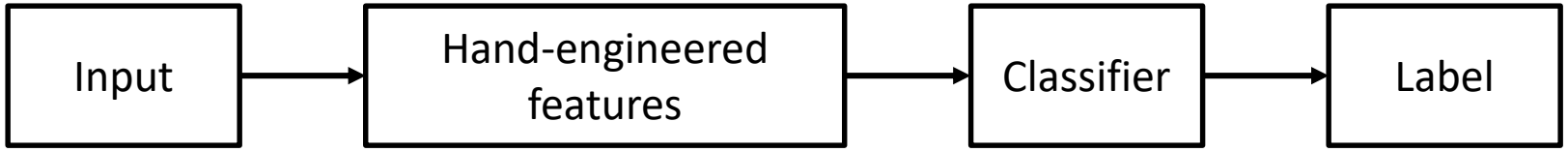


Recall Supervised Learning Setup

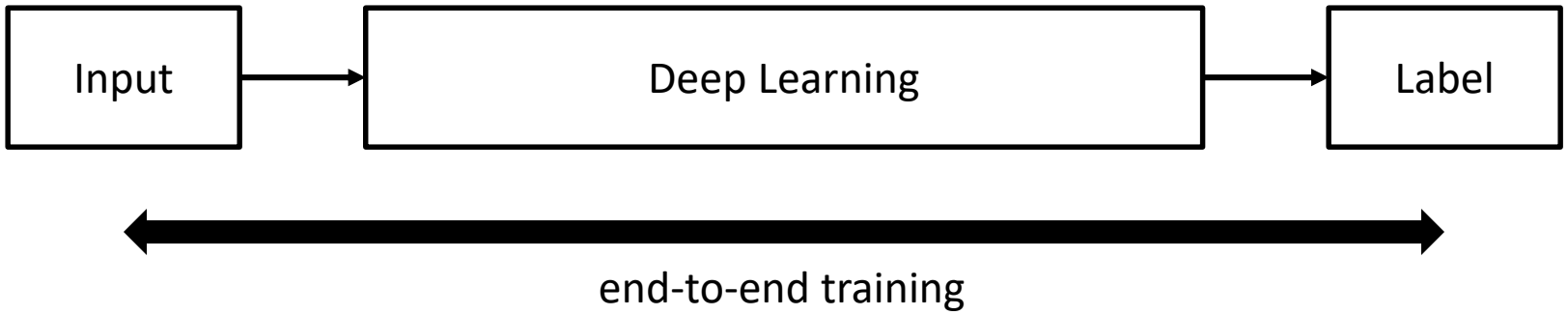


Machine Learning and Deep Learning

- Machine Learning



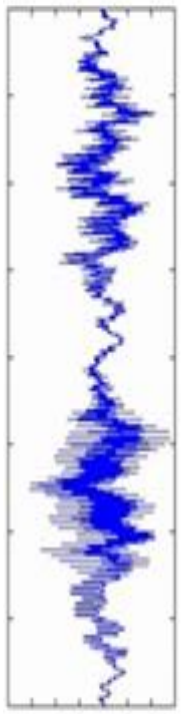
- Deep supervised learning

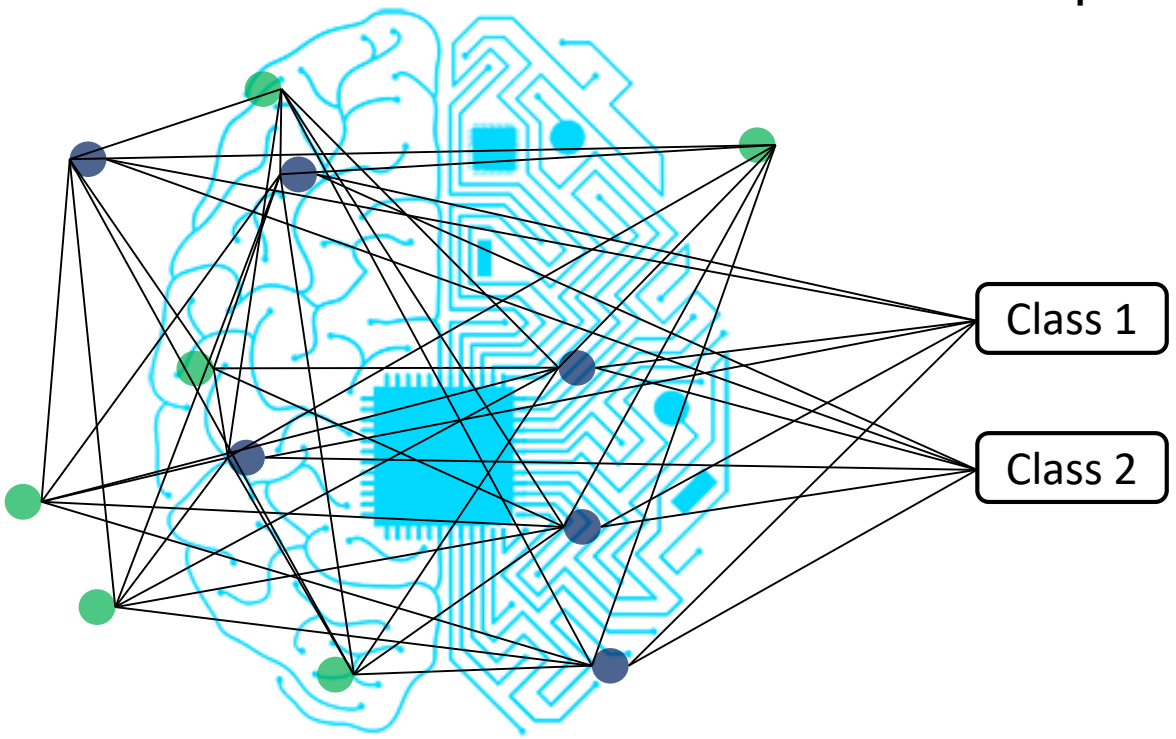


Artificial Neural Networks

- Complex/Nonlinear universal function approximator
  - Linearly connected networks
  - Simple nonlinear neurons

Input

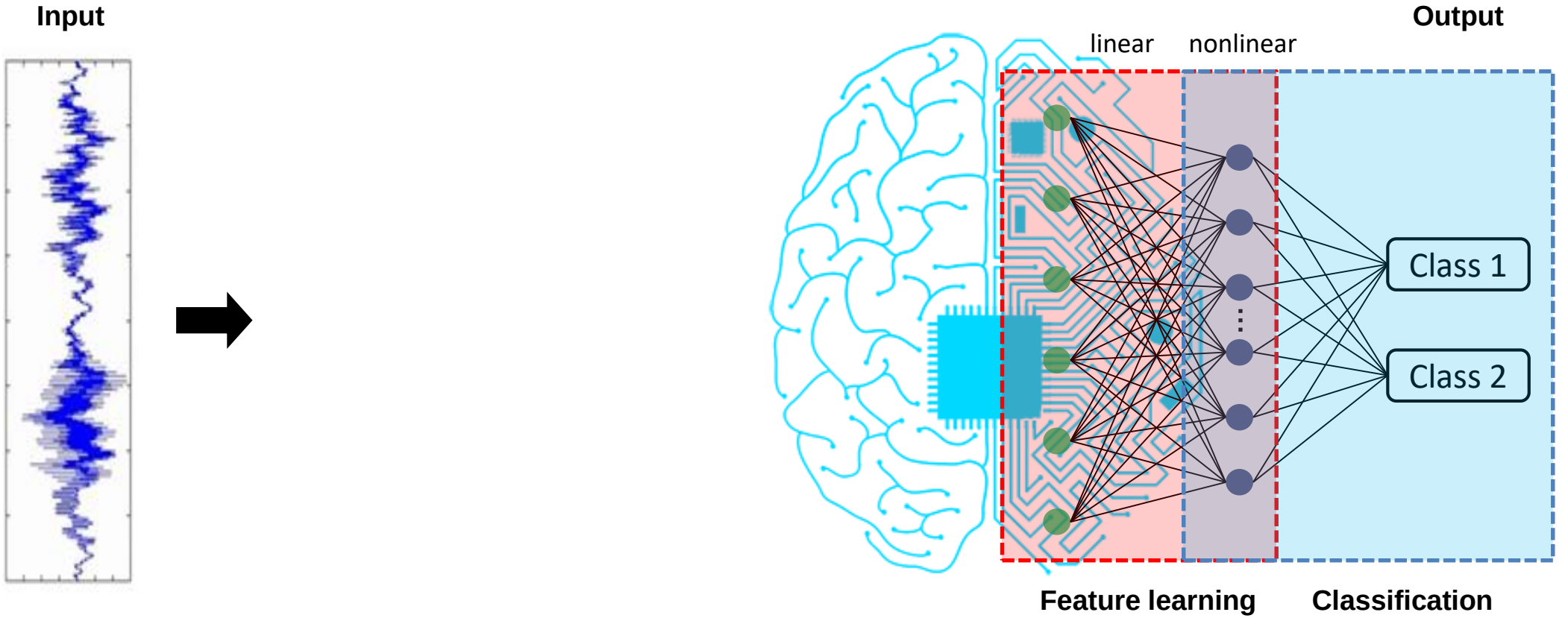




Output

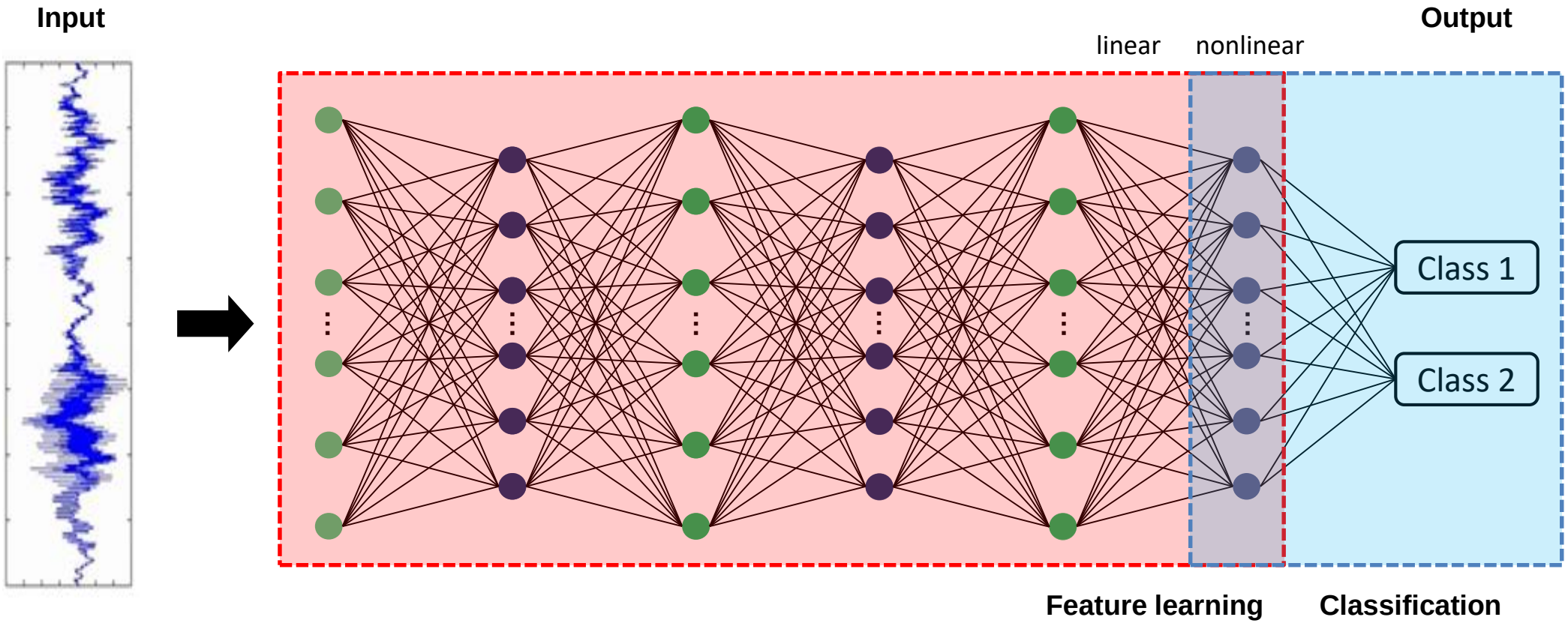
Artificial Neural Networks

- Complex/Nonlinear universal function approximator
  - Linearly connected networks
  - Simple nonlinear neurons



Deep Artificial Neural Networks

- Complex/Nonlinear universal function approximator
  - Linearly connected networks
  - Simple nonlinear neurons



Training: Backpropagation

Training Neural Networks: Optimization

- Learning or estimating weights and biases of multi-layer perceptron from training data

- 3 key components
  - objective function $f(\cdot)$
  - decision variable or unknown θ
  - constraints $g(\cdot)$

- In mathematical expression

$$\begin{aligned} \min_{\theta} \quad & f(\theta) \\ \text{subject to} \quad & g_i(\theta) \leq 0, \qquad i = 1, \cdots, m \end{aligned}$$

Training Neural Networks: Loss Function

- Measures error between target values and predictions

$$\min_{\theta} \sum_{i=1}^{m} \ell\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$$

- Example
  - Squared loss (for regression):

$$\frac{1}{N} \sum_{i=1}^{N} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

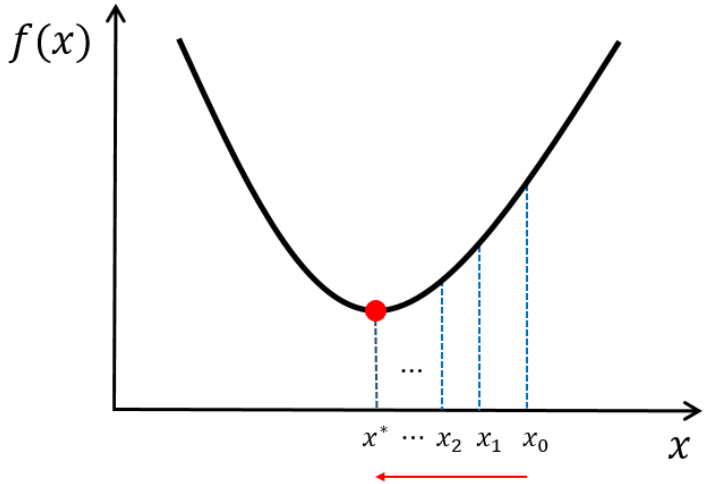
  - Cross entropy (for classification):

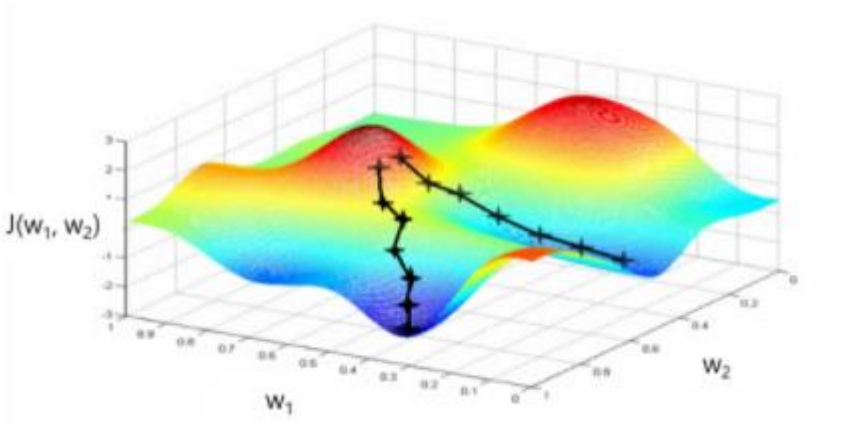
$$-\frac{1}{N} \sum_{i=1}^{N} y^{(i)} \log\left(h_\theta\left(x^{(i)}\right)\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_\theta\left(x^{(i)}\right)\right)$$

Training Neural Networks: Gradient Descent

- Negative gradients points directly downhill of the cost function
- We can decrease the cost by moving in the direction of the negative gradient (α is a learning rate)

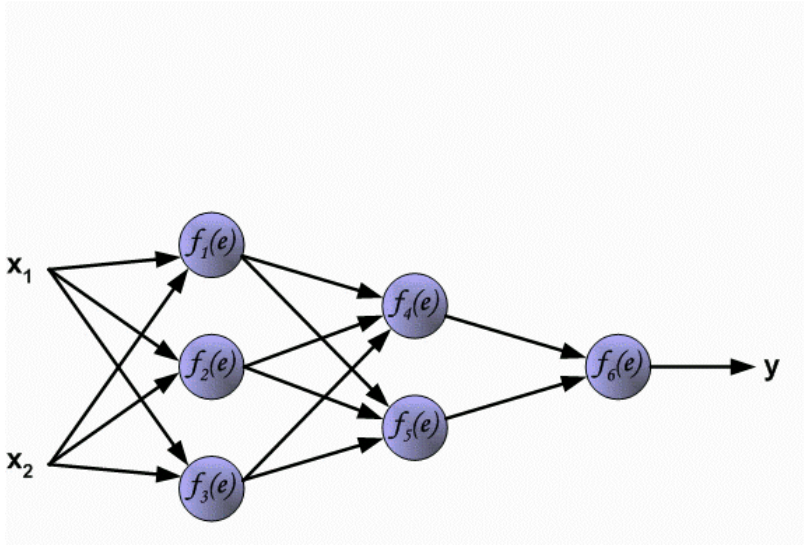
$$\theta := \theta - \alpha \nabla_\theta \left(h_\theta \left(x^{(i)} \right), y^{(i)} \right)$$





Training Neural Networks: Backpropagation Learning

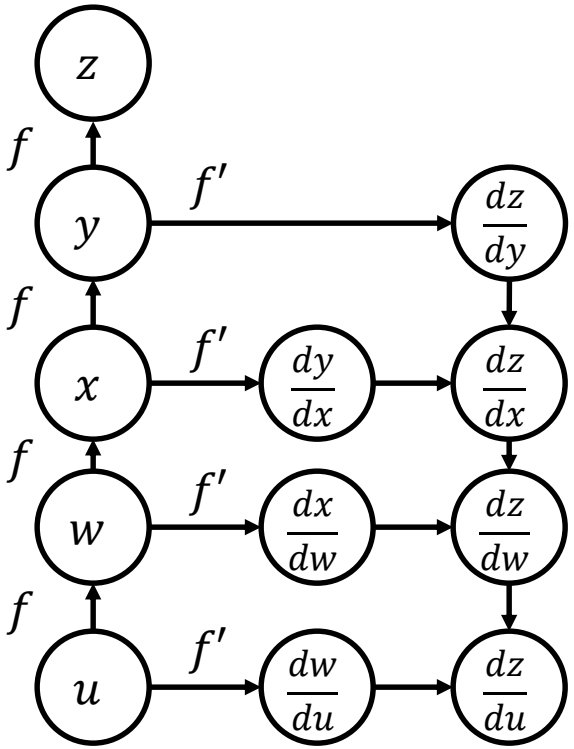
- Forward propagation
  - the initial information propagates up to the hidden units at each layer and finally produces output
- Backpropagation
  - allows the information from the cost to flow backwards through the network in order to compute the gradients



Backpropagation

- Chain Rule
  - Computing the derivative of the composition of functions
    - $f\big(g(x)\big)' = f'\big(g(x)\big)g'(x)$
    - $\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$
    - $\frac{dz}{dw} = \left(\frac{dz}{dy} \cdot \frac{dy}{dx}\right) \cdot \frac{dx}{dw}$
    - $\frac{dz}{du} = \left(\frac{dz}{dy} \cdot \frac{dy}{dx} \cdot \frac{dx}{dw}\right) \cdot \frac{dw}{du}$

- Backpropagation
  - Update weights recursively



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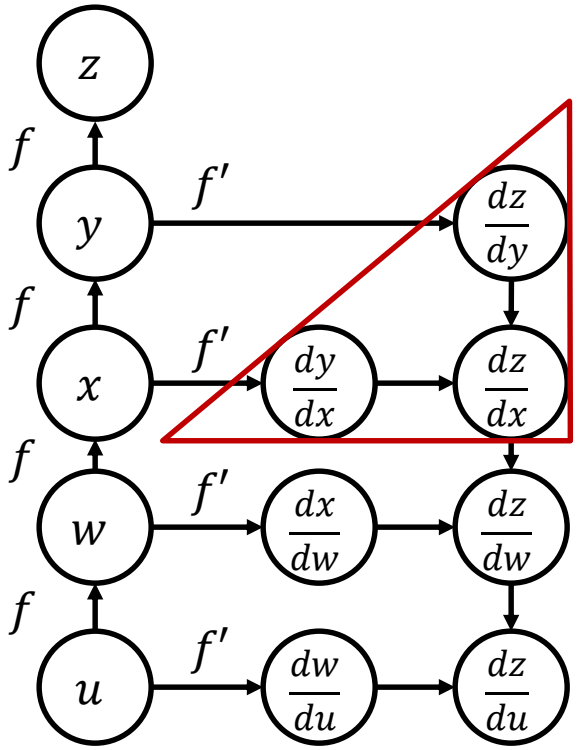

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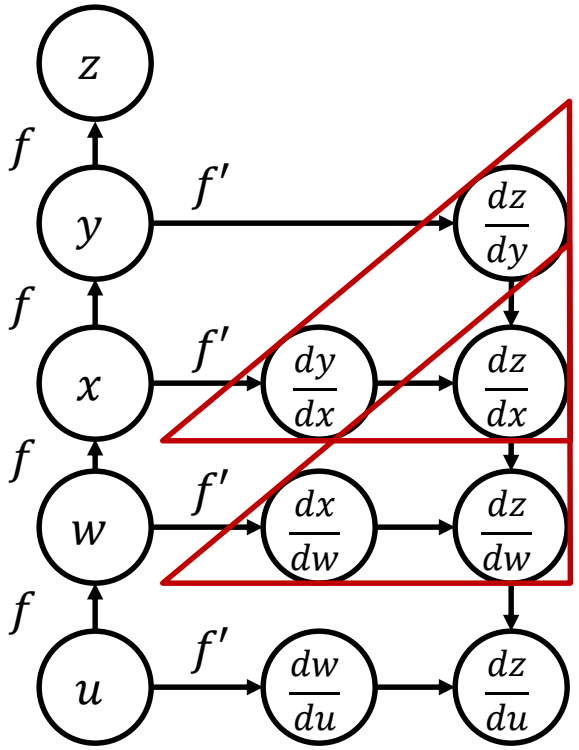
- Backpropagation
  - Update weights recursively



Backpropagation

- Chain Rule
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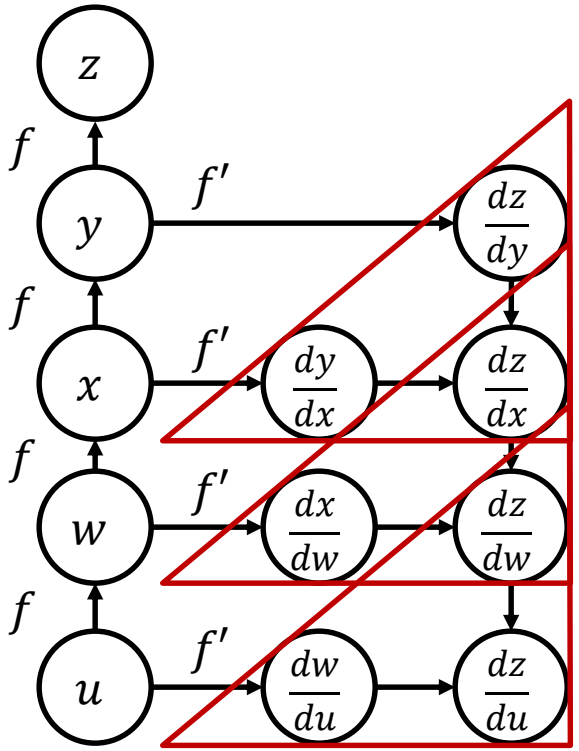
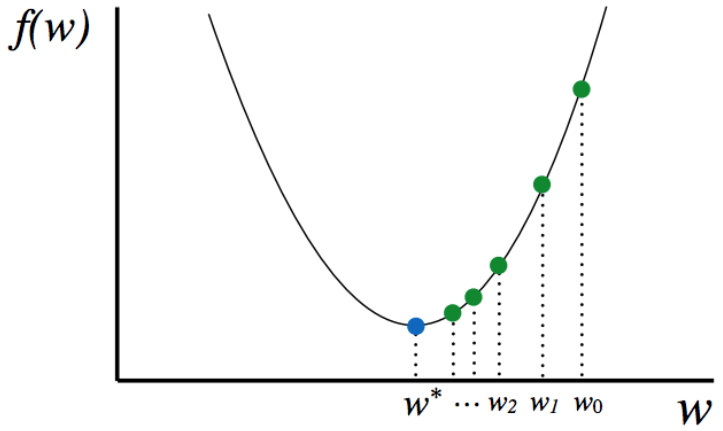
- Backpropagation
  - Update weights recursively



Training Neural Networks

- Optimization procedure

Start at a random point
Repeat
    Determine a descent direction
    Choose a step size
    Update
Until stopping criterion is satisfied

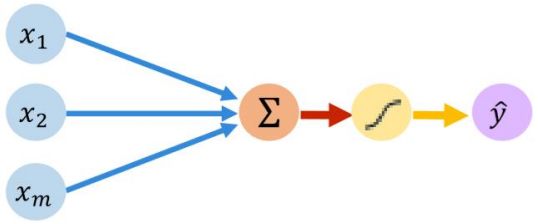


- It is not easy to numerically compute gradients in network in general.
  - The good news: people have already done all the "hard work" of developing numerical solvers (or libraries)
  - There are a wide range of tools

Core Foundation Review

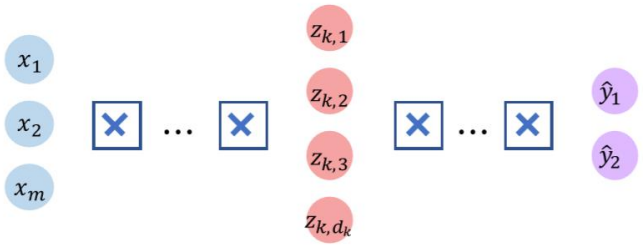
The Perceptron

- Structural building blocks
- Nonlinear activation functions



Neural Networks

- Stacking Perceptrons to form neural networks
- Optimization through backpropagation



Training in Practice

- Adaptive learning
- Batching
- Regularization