MACHINE LEARNING
MEI/1

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Linear Discriminants: Exercise

- Consider the following truth tables, corresponding to the classical “**AND**”, ‘’**OR**’’ and “**XOR**” problems:
  - Suppose we want to *learn* three **logistic regression** classifiers that appropriatelly discriminate between the ”0”|”1” classes

AND

X1	X2	Y
0	0	0
0	1	0
1	0	0
1	1	1

✓

OR

X1	X2	Y
0	0	0
0	1	1
1	0	1
1	1	1

✓

XOR

X1	X2	Y
0	0	0
0	1	1
1	0	1
1	1	0

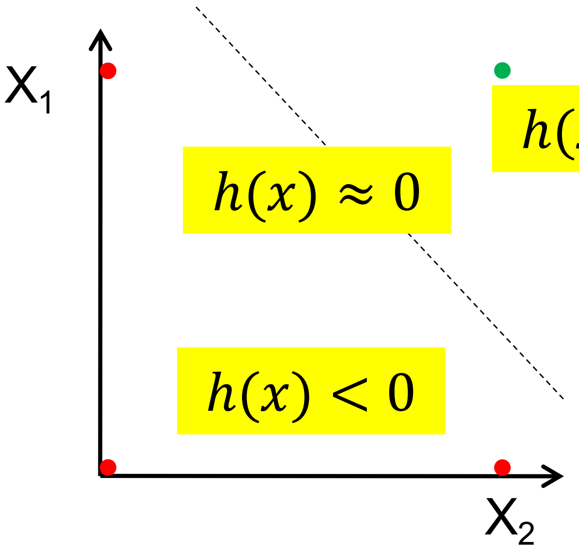
✗

Linear Discriminants: Exercise

- As we previously saw, the logistic regression is only able **to find hyperplanes (straight lines, in 2D data)** that separate the subspaces of each class, which happens in the "AND/OR" problems.

  - These are called **linear discriminants**

AND



$$g\big(h_\theta(\boldsymbol{x})\big) = g(\theta_1 x_1 + \theta_2 x_2 + \theta_0)$$

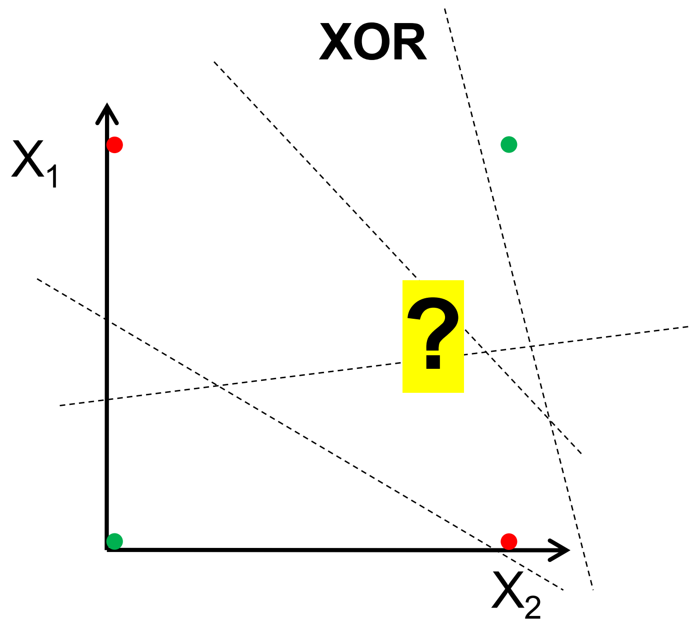
$$\frac{1}{1 + e^{-x}}$$

$$= \frac{1}{1+e^{-(\theta_1 x_1 + \theta_2 x_2 + \theta_0)}}$$

An appropriate "AND" solution could be:
$(\theta_1, \theta_2, \theta_0)$ = (0.8, 0.8, -1.5)

Linear Discriminants: Exercise

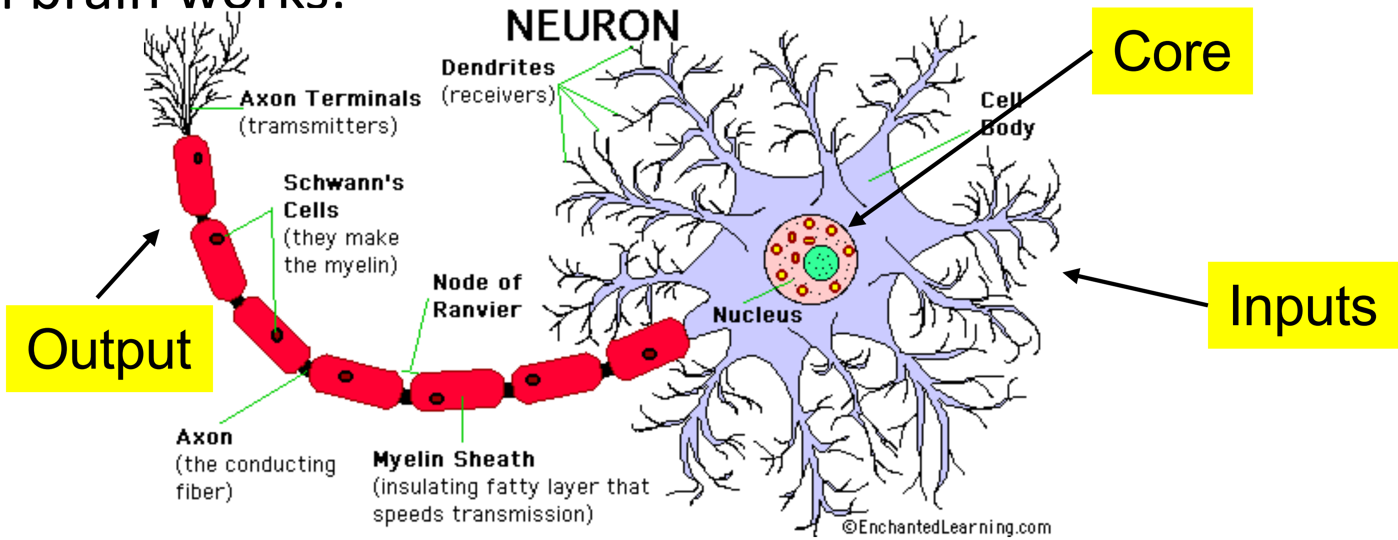
- However, for the "**XOR**" problem, there is no possible configurations for $\boldsymbol{\theta}$ that satisfy the requirements:



- **XOR** appears to be a very simple problem. However, Minksy and Papert (1969) showed that this was a big problem for neural network architectures of the 1960s, known as perceptrons.
  - The inefficiency of Perceptron networks to solve this problem caused the "*NN winter*" (period up to the early 90s, when NN were almost abandoned by the ML community)

Neural Networks

- Among the three classical approaches for machine learning (pattern recognition) models, this kind of methods aims at replicate the way the human brain works:



- In practice terms, this functioning model has remarkable similarities to the way our previous models were defined:
  - "*Mixing"* the values from a set of inputs, followed by one non-linear activation function".

Neural Networks

- A logistic regression classifier is defined by:

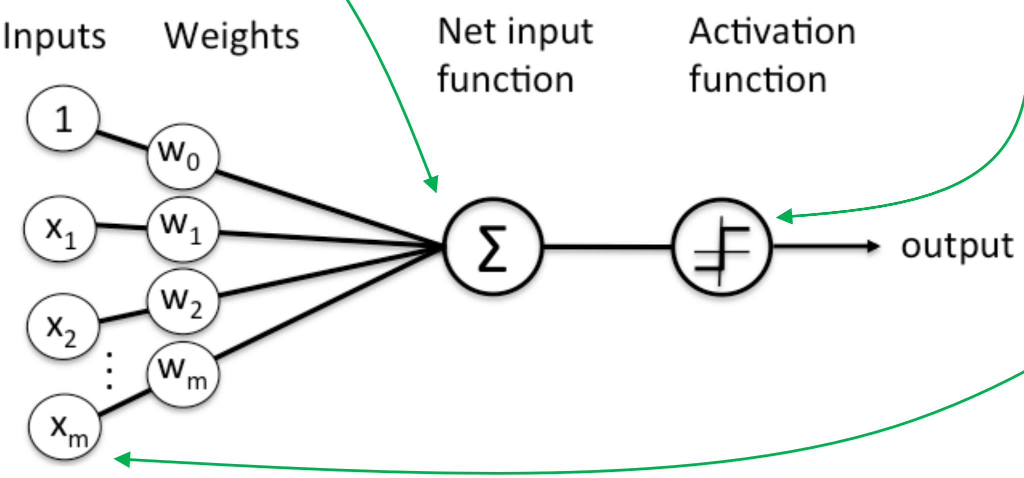
Inputs: x_1, x_2,...

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-(\theta_1 x_1 + \theta_2 x_2 + \theta_0)}}$$

Phase 1:
Convolution
between **x** and $\boldsymbol{\theta}$

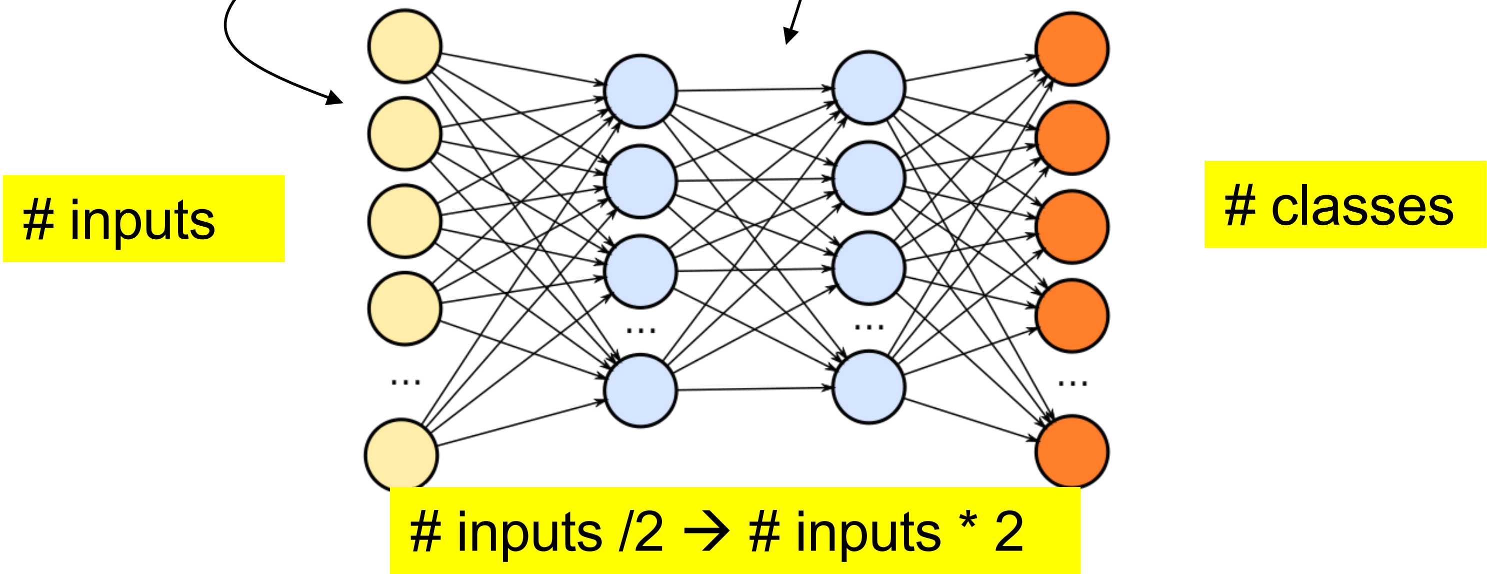
Phase 2: Non-linearity

- A Rosenblatt's perceptron is defined as:



Neural Networks: MLP Architecture

- The key concept of the most classical kind of neural networks (**feed-forward**) is to define **multiple layers**, in which neurons of one layer receive the input of all neurons in the previous layer.
  - These are called neurons in hidden layers
  - Neurons in the first layer receive the **x** input
    - They are called neurons in the input layer
  - Neurons in the last layer provide the result of the model
    - They are called neurons in the output layer



Machine Learning: Python **MLP**

- Let’s start by the easiest part:
  - How can I create one “Multi-Layer Perceptron” (MLP) network in Python and apply it to my problem?
  - **Step 1**: Import the corresponding library:

```
from sklearn.neural_network import MLPClassifier
```

  - **Step 2**: Have a **X** data set with shape (n, 2) and **y** with shape (n,)
    - In practice, **X** will be a “list of lists” and **y** will be a list.

```
X = [[0., 0.], [1., 1.]]
y = [0, 1]
```

  - **Step 3**: Create the network:

```
clf = MLPClassifier(solver='lbfgs', alpha=1e-5,
        hidden_layer_sizes=(5, 2), random_state=1)
```

  - **Step 4**: Start learning:

```
clf.fit(X, y)
```

  - **Step 5**: Use it, to predict on new instances:

```
clf.predict([[2., 2.], [-1., -2.]])
```

Neural Networks

- When designing a neural network, there are different parameterizations that have to be chosen, with might determine the system effectiveness:
  - The number of neurons in the input/output layers result directly of the problem considered:
    - **Input Layer = Dimension of the Feature Space**
    - **Output Layer = Number of classes** (hot encoded)

1	⇨	**0 0 1**
2		**0 1 0**
3		**1 0 0**

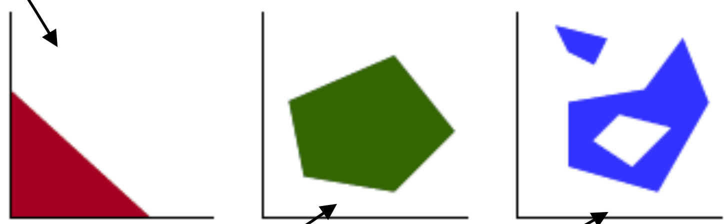
- In the hidden layers, the number of neurons can vary:
  - A too short number might not be enough to model the decision surface desired;
  - A too high value might lead to overfitting
  - In practice, values between half and the double of the number of neurons in the input layer are tested

- Regarding the number of hidden layers:

  Networks with one layer have the ability to approximate any linear decision surface

  Networks with two layers approximate any continuous decision surface

  Networks with three layers approximate any decision surface

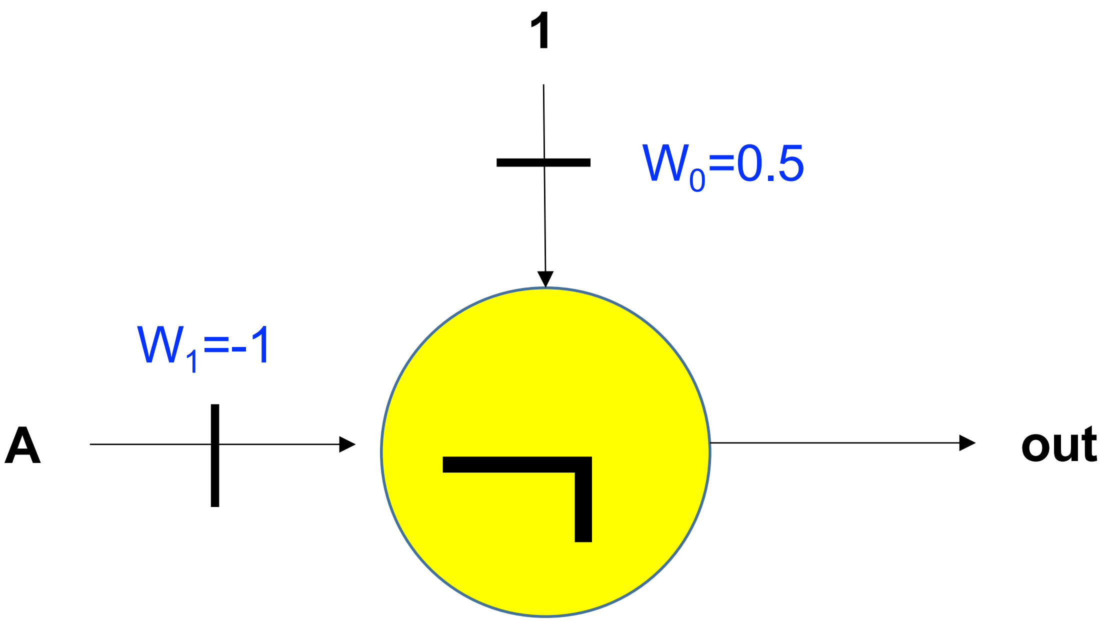


Machine Learning: NN Exercise

- Considering that:

$$A \bigotimes B = \neg\,(\,(A \bigwedge B) \vee (\neg A \bigwedge \neg B)\,)$$

- For example, how to infer the weights for a “NOT” neuron, i.e., a neuron that replicates the functioning of a logical “NOT” operation.
  - In this simple case, there are various weight configurations that will work

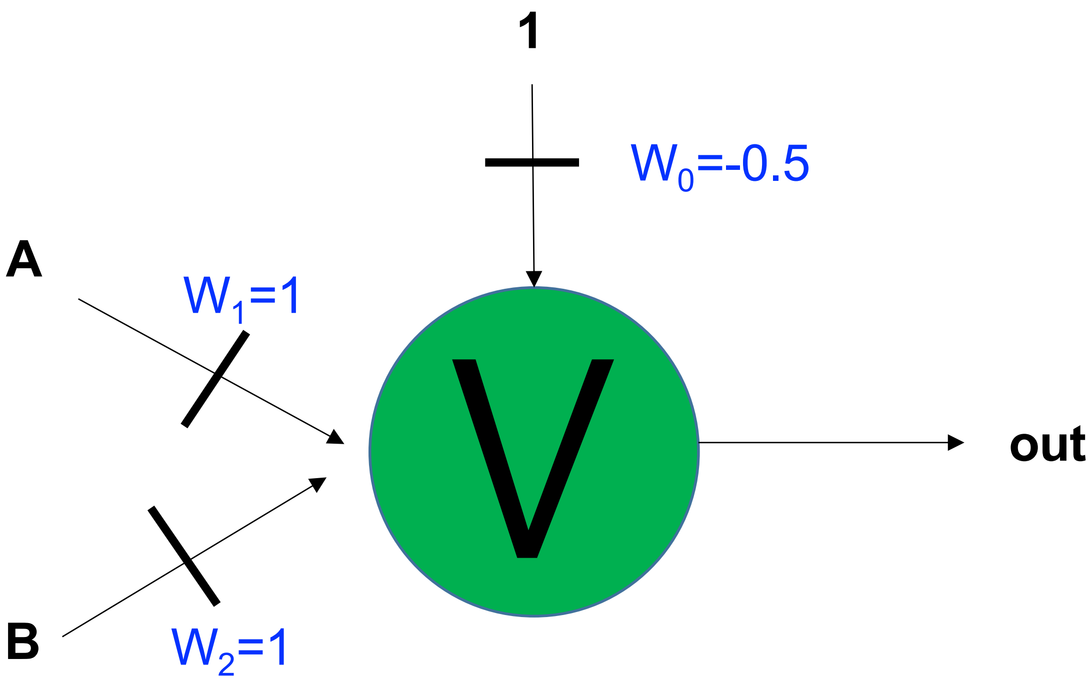


Machine Learning: NN Example

- Considering that:

$$A \bigotimes B = \neg\,(\,(A \bigwedge B) \vee (\neg A \bigwedge \neg B)\,)$$

- Now, how to infer the weights for a "OR" neuron, i.e., a neuron that replicates the functioning of a logical "OR" operation.
  - Again, there are various weight configurations that will work:

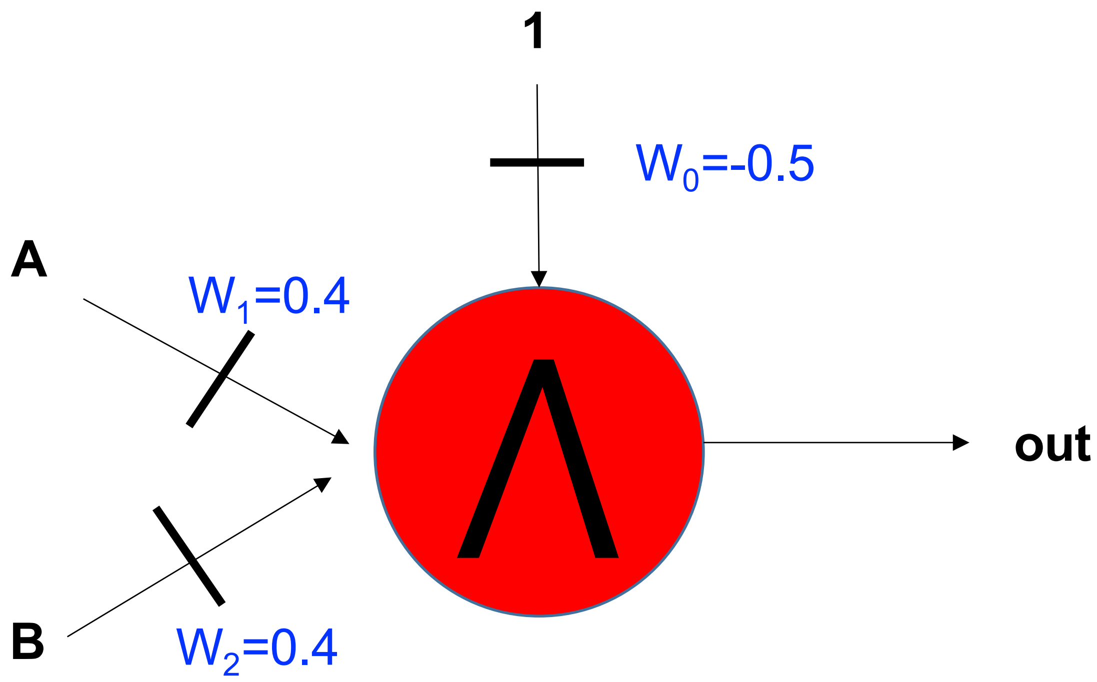


Machine Learning: NN Example

- Considering that:

$$A \bigotimes B = \neg\,(\,(A \bigwedge B) \vee (\neg A \bigwedge \neg B)\,)$$

- Next, in a similar way, if we want to infer the weights for a "AND" neuron, i.e., a neuron that replicates the functioning of a logical "AND" operation.
  - As in the previous cases, there are various weight configurations that will work:

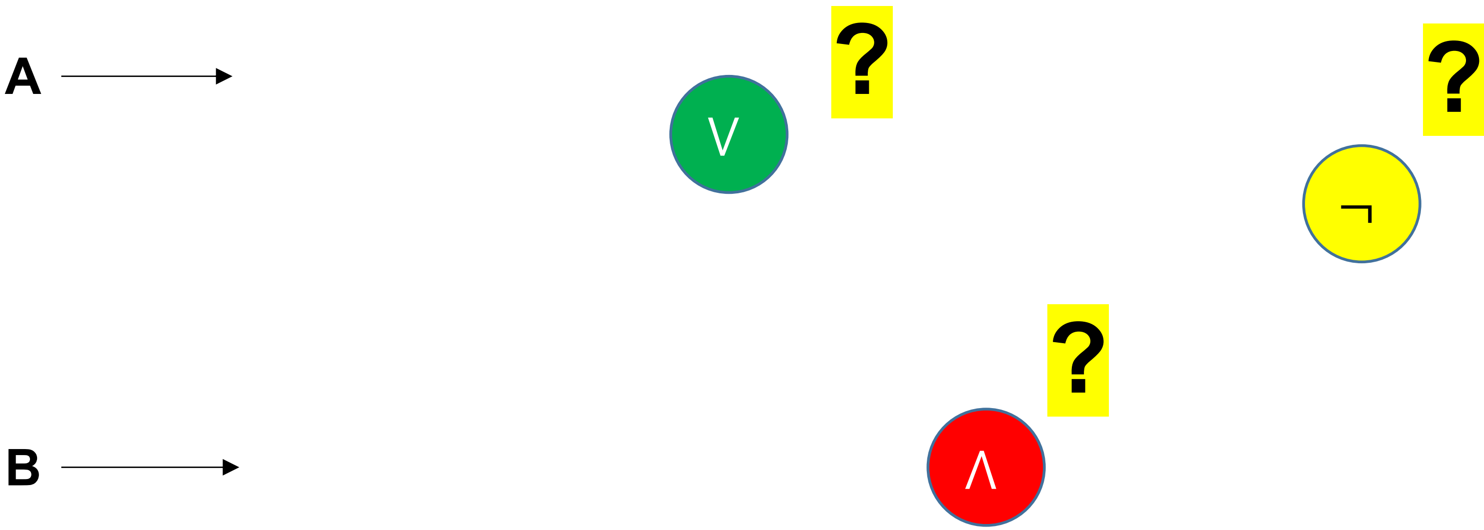


Machine Learning: NN Exercise

- Considering that:

$$A \bigotimes B = \neg\,(\,(A \bigwedge B) \vee (\neg A \bigwedge \neg B)\,)$$

- Design a multi-layer network, with the corresponding weights $\boldsymbol{\theta}$, able to solve the "**XOR**" problem.



Machine Learning: NN Exercise

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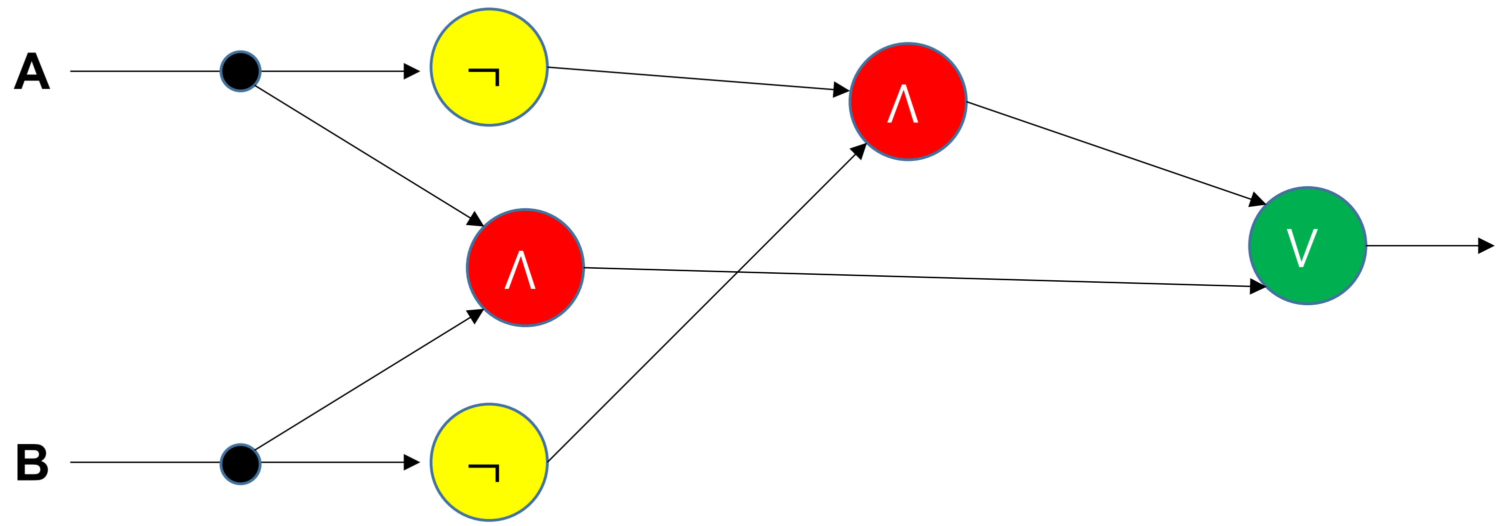
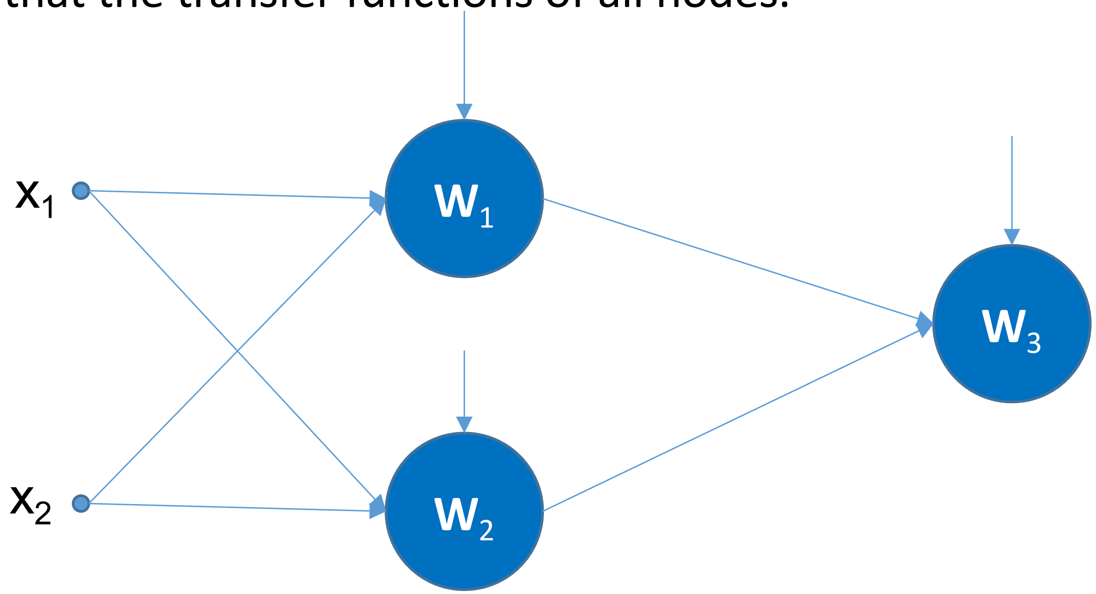


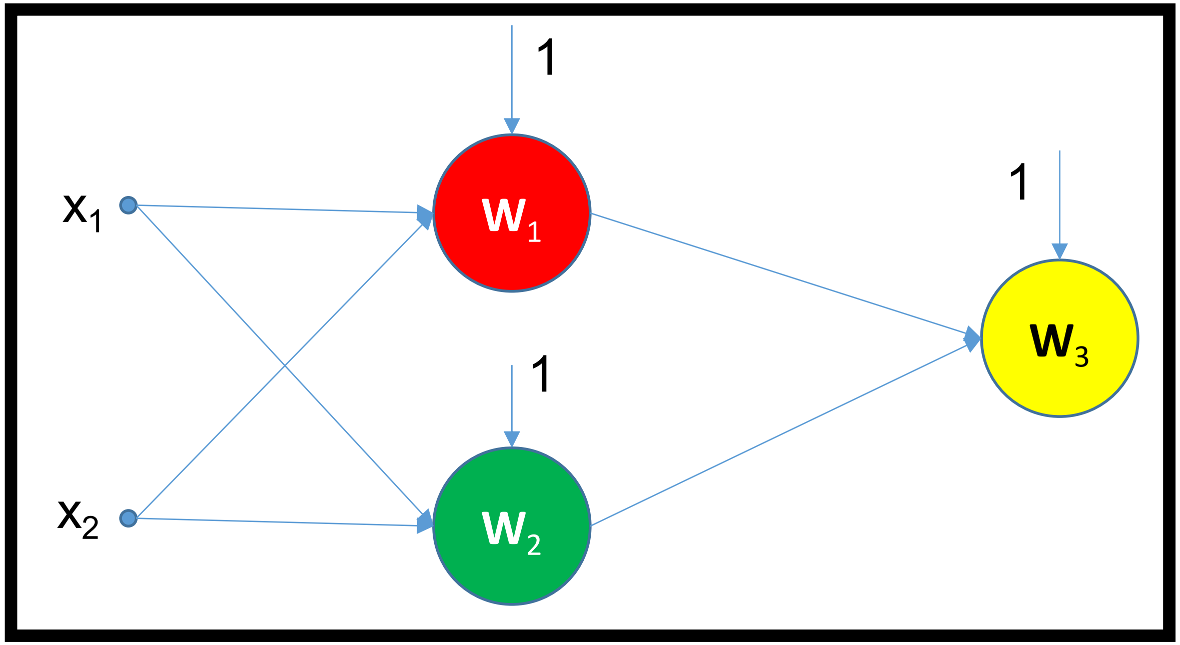
- <u>This will be a network "specific" to reproduce this function.</u>
- <u>However, the big question remains: **How to automatically obtain the $\boldsymbol{\theta}$ values?**</u>

Neural Networks: Learning

- In case of multilayered networks, the closed-form equation for the whole network, the cost function and the corresponding derivatives might not be easy to obtain.
- **Exercise**:
  - Obtain the function that describes the functioning of the following network, considering that the transfer functions of all nodes.



Backpropagation



$$t_1 = \frac{1}{1 + e^{-w_{1,0} - w_{1,1}x_1 - w_{1,2}x_2}}$$

$$t_2 = \frac{1}{1 + e^{-w_{2,0} - w_{2,1}x_1 - w_{2,2}x_2}}$$

$$\mathrm{NN} = \frac{1}{1 + e^{-w_{3,0} - w_{3,1}t_1 - w_{2,2}t_2}}$$

$$\mathrm{NN} = \frac{1}{1 + e^{-w_{3,0} - w_{3,1}\frac{1}{1+e^{-w_{1,0} - w_{1,1}x_1 - w_{1,2}x_2}} - w_{3,2}\frac{1}{1+e^{-w_{2,0} - w_{2,1}x_1 - w_{2,2}x_2}}}}$$

Backpropagation

$$\mathrm{NN} = \frac{1}{1+e^{-w_{3,0}-w_{3,1}\frac{1}{1+e^{-w_{1,0}-w_{1,1}x_1-w_{1,2}x_2}}-w_{3,2}\frac{1}{1+e^{-w_{2,0}-w_{2,1}x_1-w_{2,2}x_2}}}}$$

$$J(\mathbf{w}) = \frac{1}{N}\sum Cost(NN\left(\omega, x^{(i)}, y^{(i)}\right))$$

- $Cost\left(NN(\mathbf{w}, x^{(i)}), y^{(i)}\right) = \begin{cases} -\log\left(NN(\mathbf{w}, x^{(i)})\right), \text{ if } y^{(i)}=1 \\ -\log\left(1 - NN(\mathbf{w}, x^{(i)})\right), \text{ if } y^{(i)}=0 \end{cases}$

- Therefore, as we did before for the logistic regression classifier, the cost function is combined in a single function:

$$J(\mathbf{w}) = -\frac{1}{N}\sum_i y^{(i)} \log\left(NN(\mathbf{w}, x^{(i)})\right) + (1-y^{(i)}) \log\left(1 - NN(\mathbf{w}, x^{(i)})\right)$$

Backpropagation

- Using the gradient descent (delta rule) learning strategy previously described, it will be required to obtain:

$$\frac{\partial}{\partial w_{1,0}} =? \qquad \frac{\partial}{\partial w_{2,0}} =? \qquad \frac{\partial}{\partial w_{3,0}} =?$$

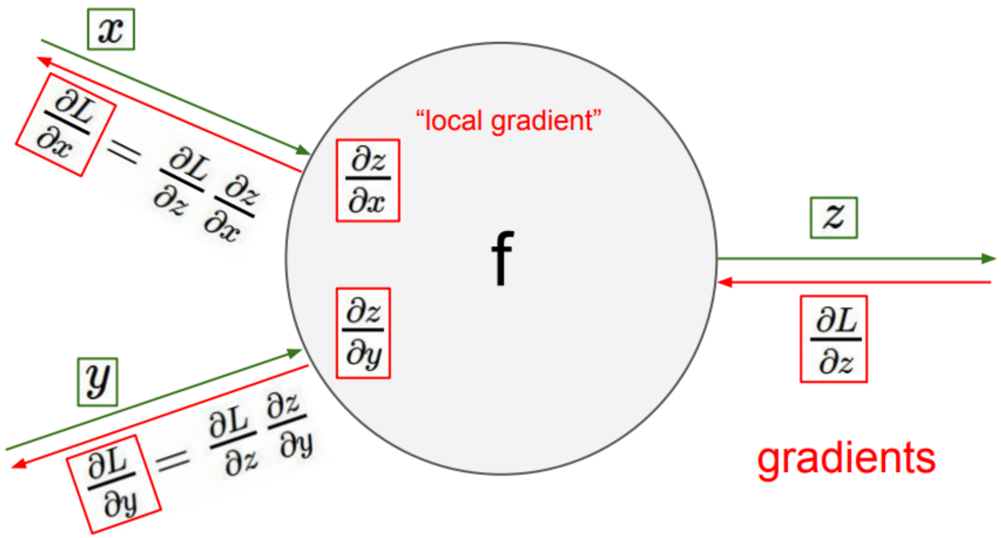
$$\frac{\partial}{\partial w_{1,1}} =? \qquad \frac{\partial}{\partial w_{2,1}} =? \qquad \frac{\partial}{\partial w_{3,1}} =?$$

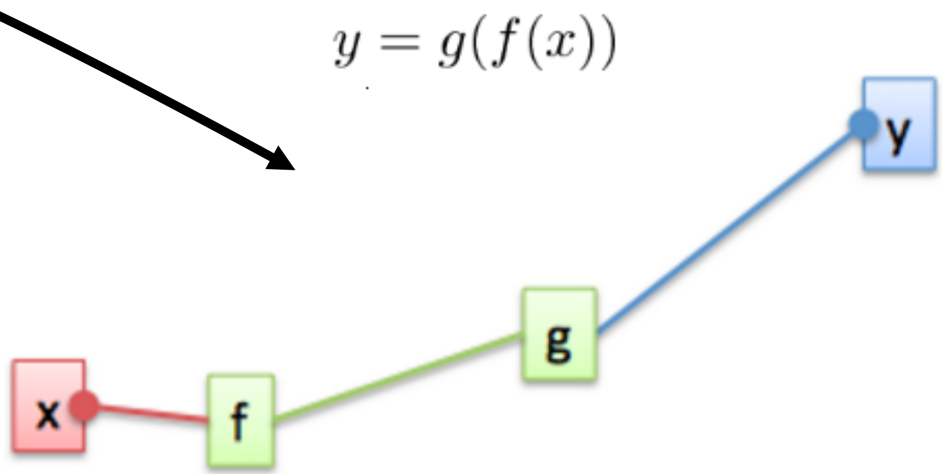
$$\frac{\partial}{\partial w_{1,2}} =? \qquad \frac{\partial}{\partial w_{2,2}} =? \qquad \frac{\partial}{\partial w_{3,2}} =?$$

…and this is a tiny network...

Backpropagation and the Chain Rule

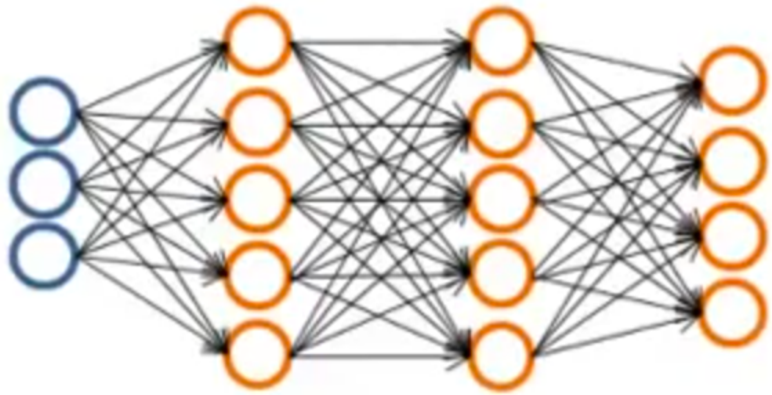
- "**Backpropagation**" is the short name for "backward propagation of errors"
- It is an algorithm for supervised learning of multi-layer artificial neural networks, based in gradient descent
- The key concept is the **chain rule**:
  - **δg/δx = δg/δf . δf/δx**
- Calculates the gradient of the error function with respect to the neural network's weights;
- It is a **generalization** of the delta rule for perceptrons to multilayer feed-forward neural networks.





Backpropagation: Forward Pass

- Forward Pass:
  - Let $p^{(i,j)}$ denote the "inner product" between the inputs and the weights of the j^{th} neuron of the i^{th} layer of the network;
  - Let s() denote the sigmoid transfer function;
  - Hence, the output of one neuron is given by $s^{(i,j)}(p^{(i,j)})$
  - We consider that at the input layer the output is simply given by the network inputs, i.e., $s(p^{(0,*)})=\mathbf{x}$
  - $p^{(1,*)} = w^{(1,*)}\, s^{(0,*)}$
  - $s^{(1,*)} = s(p^{(1,*)})$
  - $p^{(2,*)} = w^{(2,*)}\, s^{(1,*)}$
  - …



$$p^{(i,*)} = w^{(i,*)}\, s^{(i-1,*)}$$

$$s^{(i,*)} = s(p^{(i,*)})$$

Backpropagation: Backward Pass

- We start by obtaining the error at the output layer $e^{(last)}$
- Use this value to obtain the error at the previous layer ($e^{(last-1)}$) and so on...
- $e^{(last,*)} = s^{(last,*)} - y$
- $e^{(last-1,*)} = w^{(last-1,*)T} . e^{(last)} .* [s(p^{(last-1)})]'$
- Note that $[s(p^{(last-1)})]' = s^{(last-1)} .*(1-s^{(last-1)})$

$$e^{(i,*)} = w^{(i,*)T} . e^{(i+1)} .* [s(p^{(i)})]'$$

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

$$\frac{d\sigma(x)}{d(x)} = \sigma(x) \cdot (1 - \sigma(x))$$

Backpropagation Algorithm

- Having a learning set $\{(x^{(1)}, y^{(1)}),\dots (x^{(n)},y^{(n)})\}$, and a NN with "L" layers.

$u^{(l,i,j)}=0$ //update factor for the l^{th} layer, i^{th} neuron, j^{th} weight

For i=1..n

$s^{(1)}=x^{(i)}$ //input layer

Perform forward propagation to obtain $s^{(l)}$, l=1,..L

Use $y^{(i)}$ to obtain $e_i^{(L)}$

Obtain $e^{(L-1)},\dots,e^{(2)}$

$u^{(l,i,j)} = u^{(l,i,j)} + s^{(l,j)}\, e_i^{(l+1)}$

$$\boxed{\frac{\partial J}{\partial w_{l,i,j}} = D^{(l,i,j)}}$$

$D^{(l,i,j)} = 1/n\ u^{(l,i,j)} + \text{STEP}\ w^{(l,i,j)}$ for "non-bias" neurons

$D^{(l,i,j)} = 1/n\ u^{(l,i,j)}$ for "bias" neurons