MACHINE LEARNING

MEI/1

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Machine Learning

[04]

Syllabus

- Non-Linear Discrimination
- Multi-layer Perceptrons

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

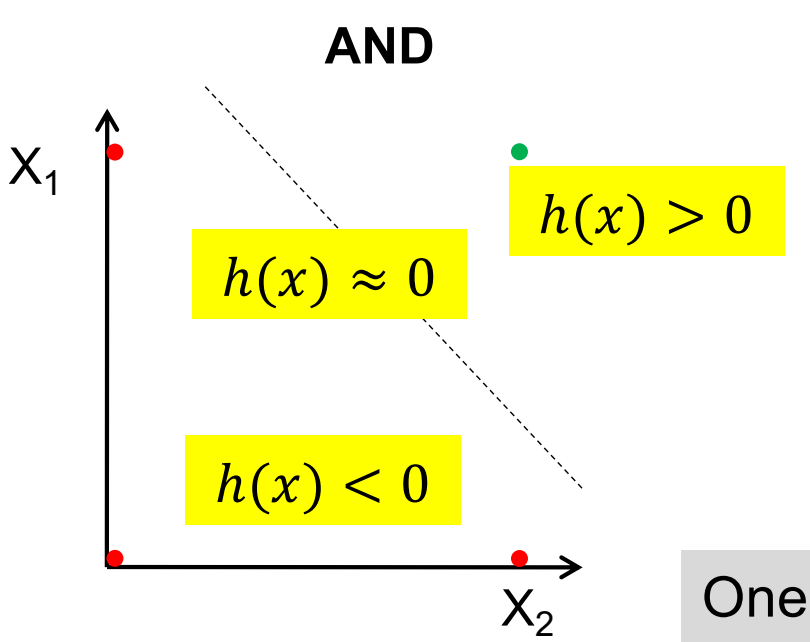
XOR

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**



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

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

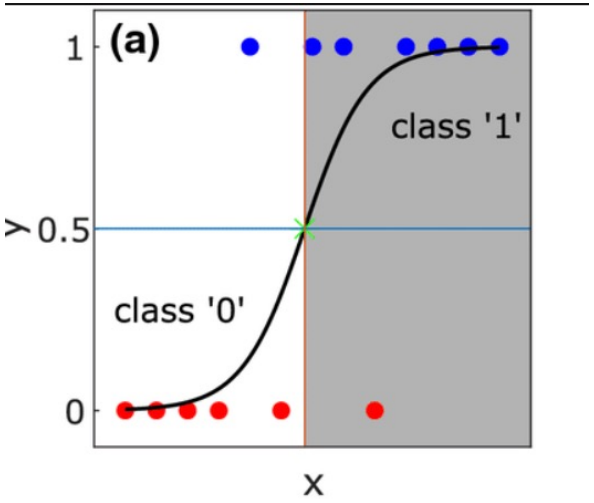
$$= \frac{1}{1+e^{-(\theta_1 x_1 + \theta_2 x_2 + \theta_0)}}$$

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

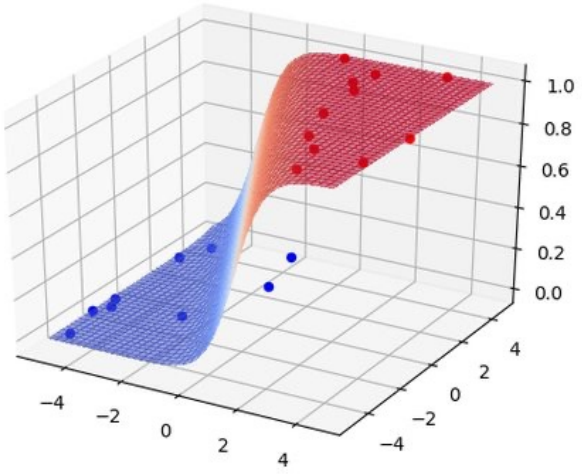
Linear Discriminants: Summary

- In short, one logistic regression model is effective only in linearly separable problems, where there **is a hyperplane** that **appropriately separates** the feature space.

1D



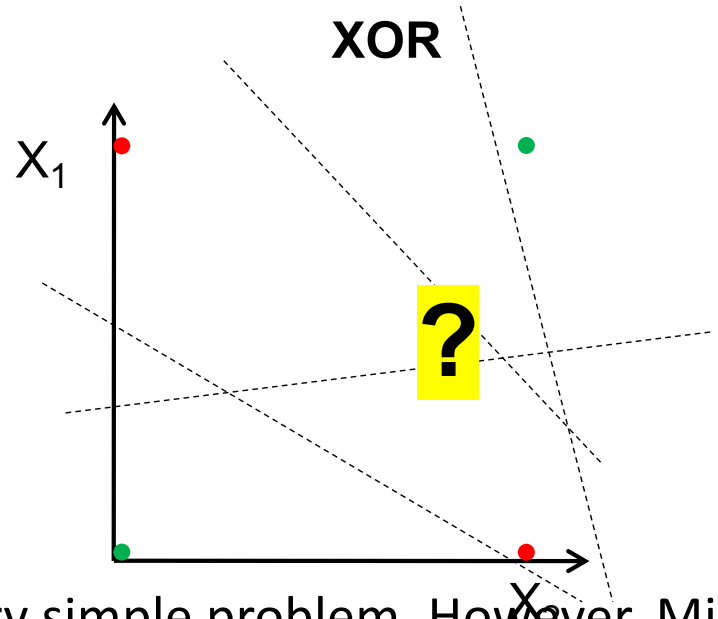
2D



…nD

Linear Discriminants: Exercise

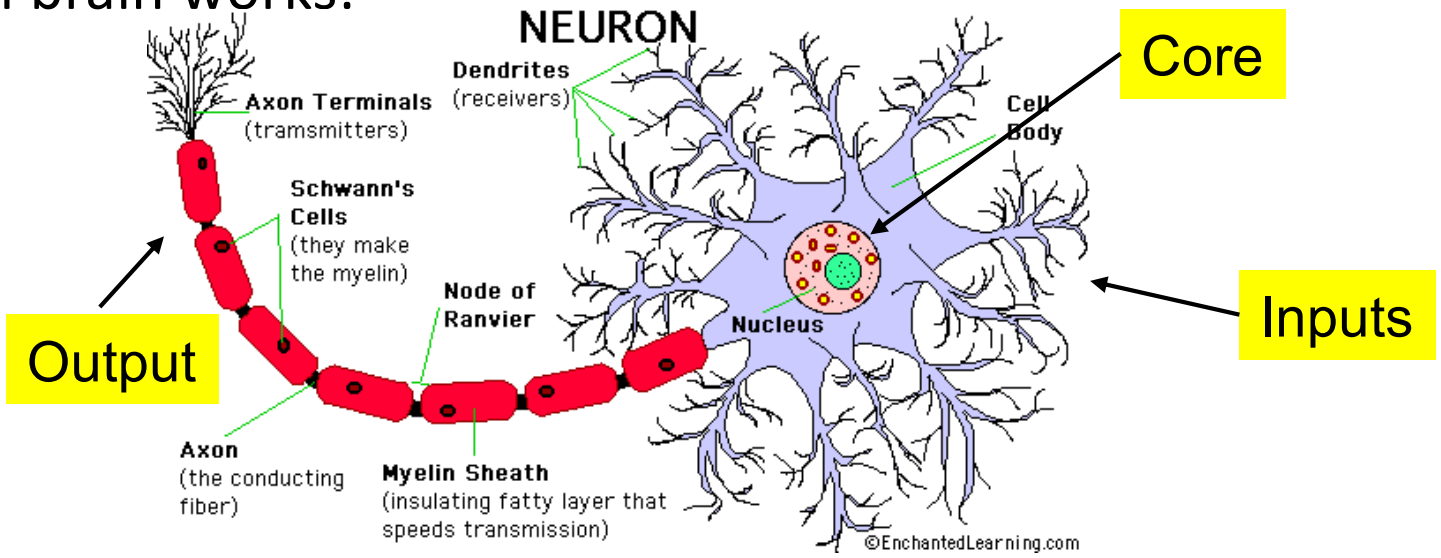
- However, for the "**XOR**" problem, there is no possible configurations for $\boldsymbol{\theta}$ that satisfy the requirements:



- **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:

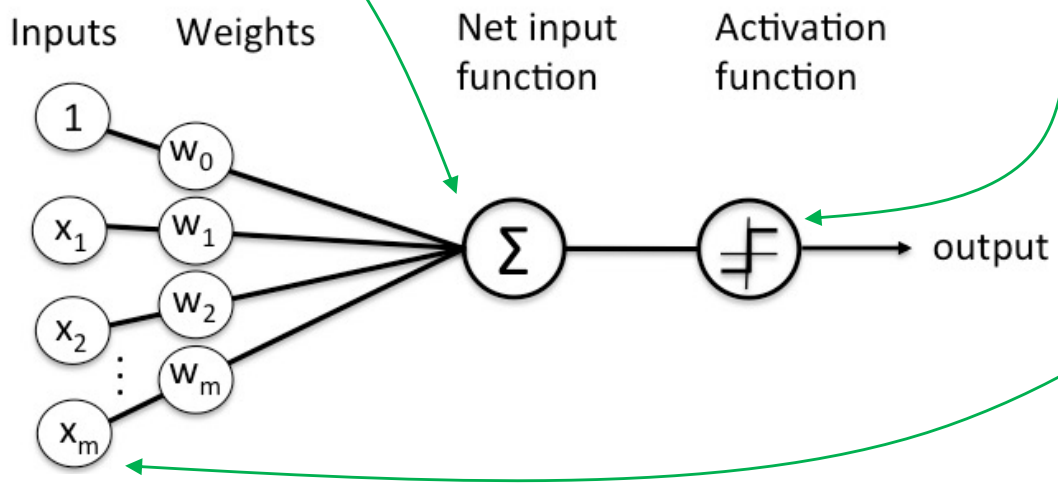
$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-(\theta_1 x_1 + \theta_2 x_2 + \theta_0)}}$$

Inputs: x_1, x_2,...

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

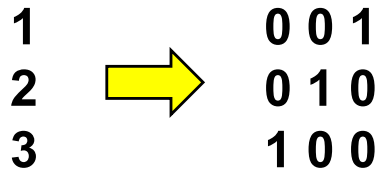
Phase 2: Non-linearity

- A Rosenblatt's perceptron is defined as:



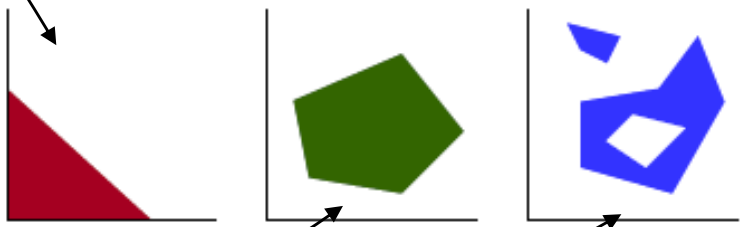
Neural Networks

- 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)



- 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

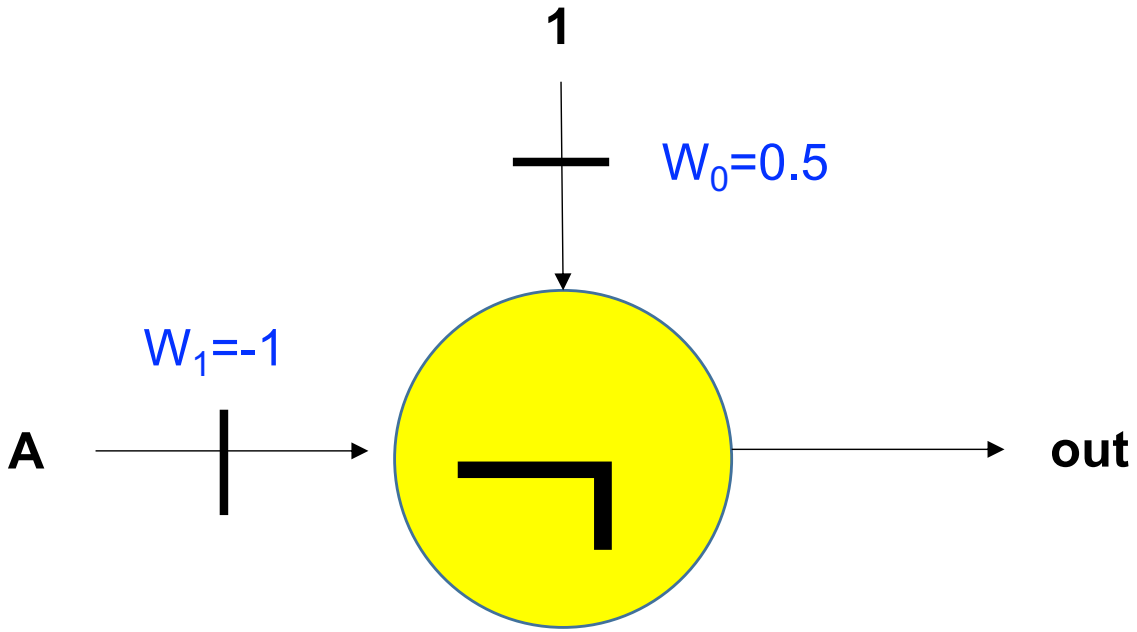


Machine Learning: NN Exercise

- Considering that:

$$A \otimes B = \neg\,(\,(A \wedge B)\ \mathrm{V}\ (\neg A \wedge \neg B)\,)$$

- 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

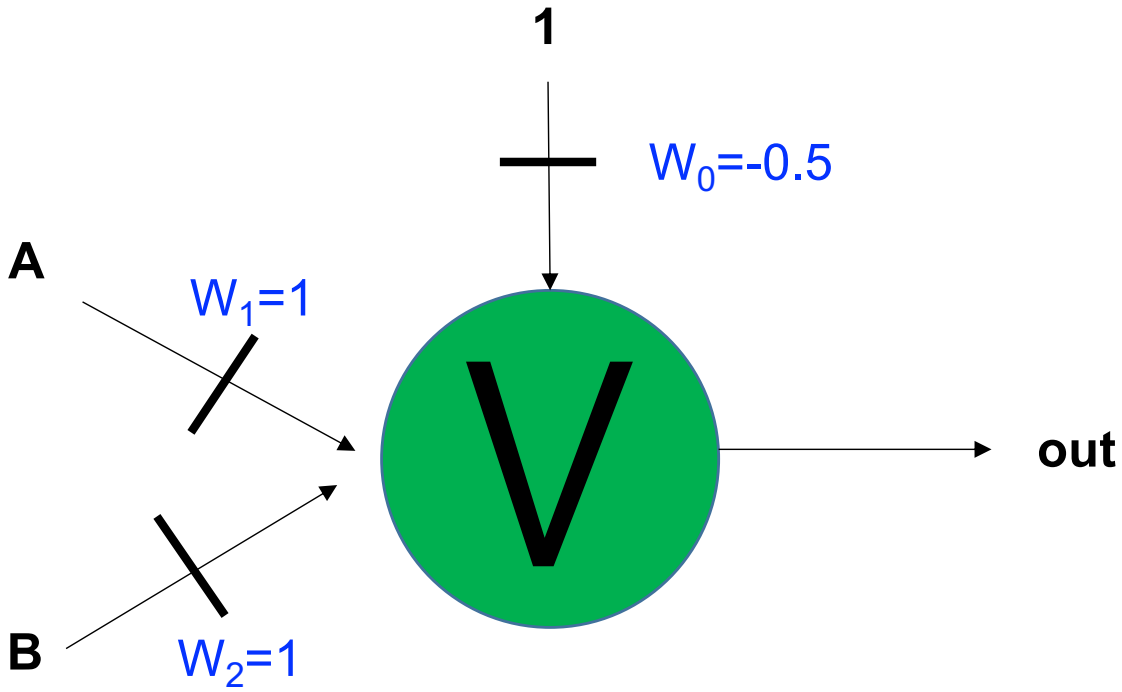


Machine Learning: NN Example

- Considering that:

$$A \otimes B = \neg\,(\,(A \bigwedge B)\ \mathrm{V}\ (\neg A \bigwedge \neg B)\,)$$

- 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:

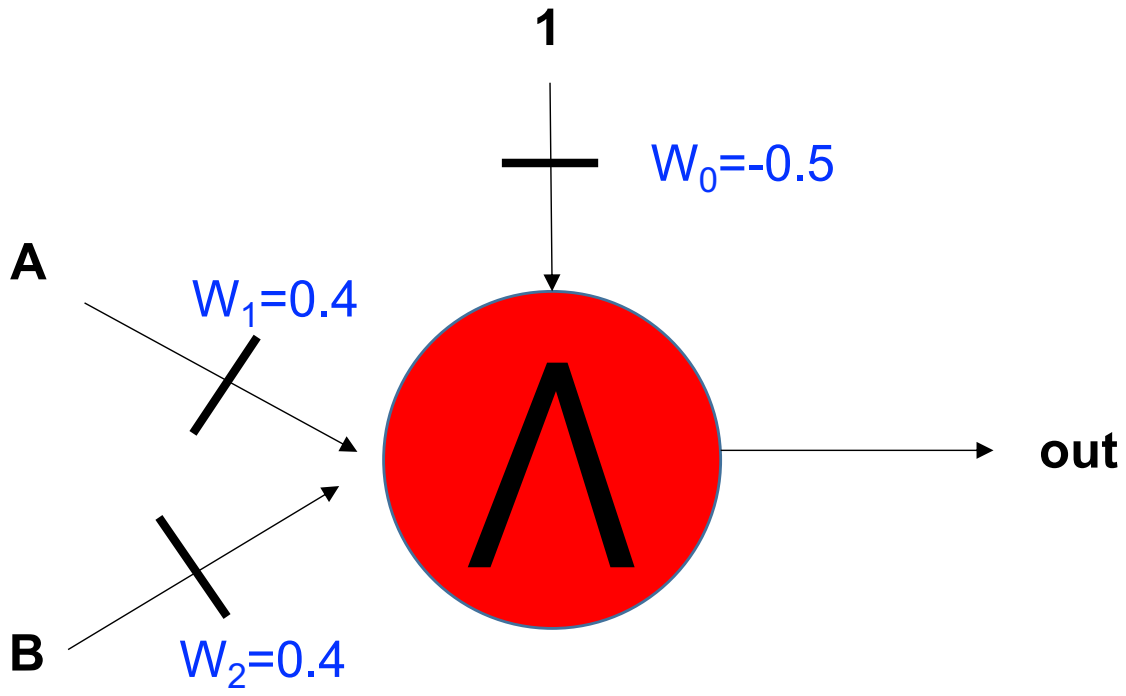


Machine Learning: NN Example

- Considering that:

$$A \otimes B = \neg\,(\,(A \wedge B)\ \mathrm{V}\ (\neg A \wedge \neg B)\,)$$

- 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:

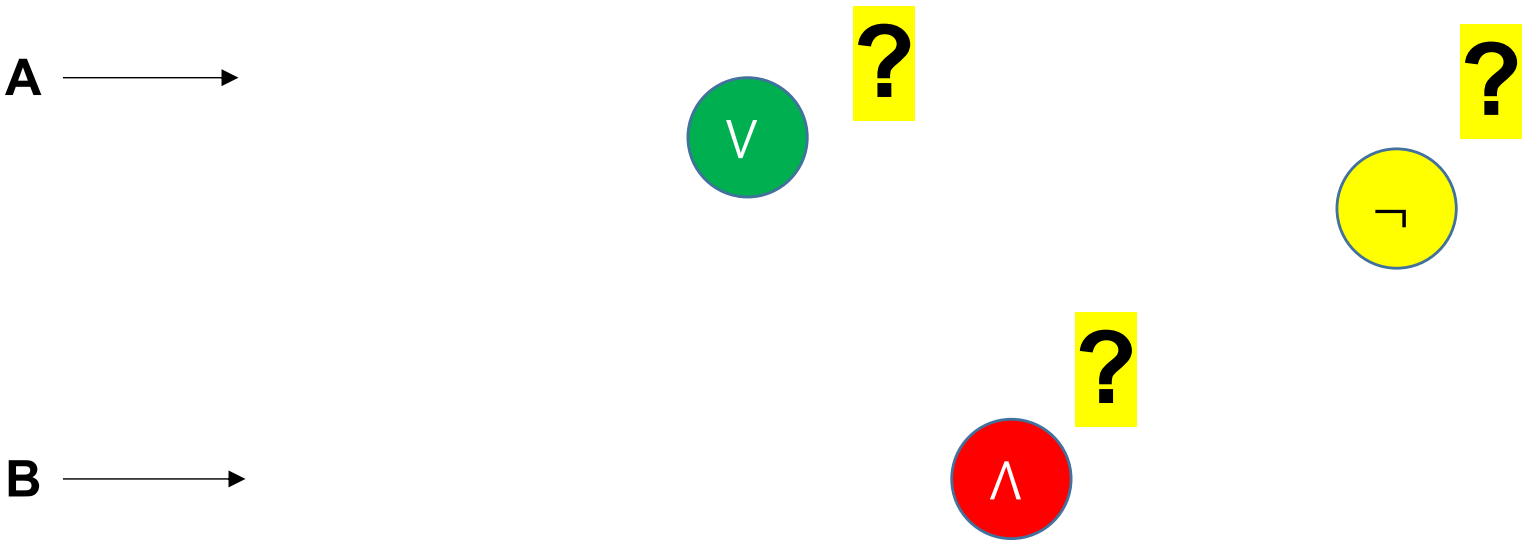


Machine Learning: NN Exercise

- Considering that:

$$A \otimes B = \neg\,(\,(A \bigwedge B)\,\mathrm{V}\,(\neg A \bigwedge \neg B)\,)$$

- 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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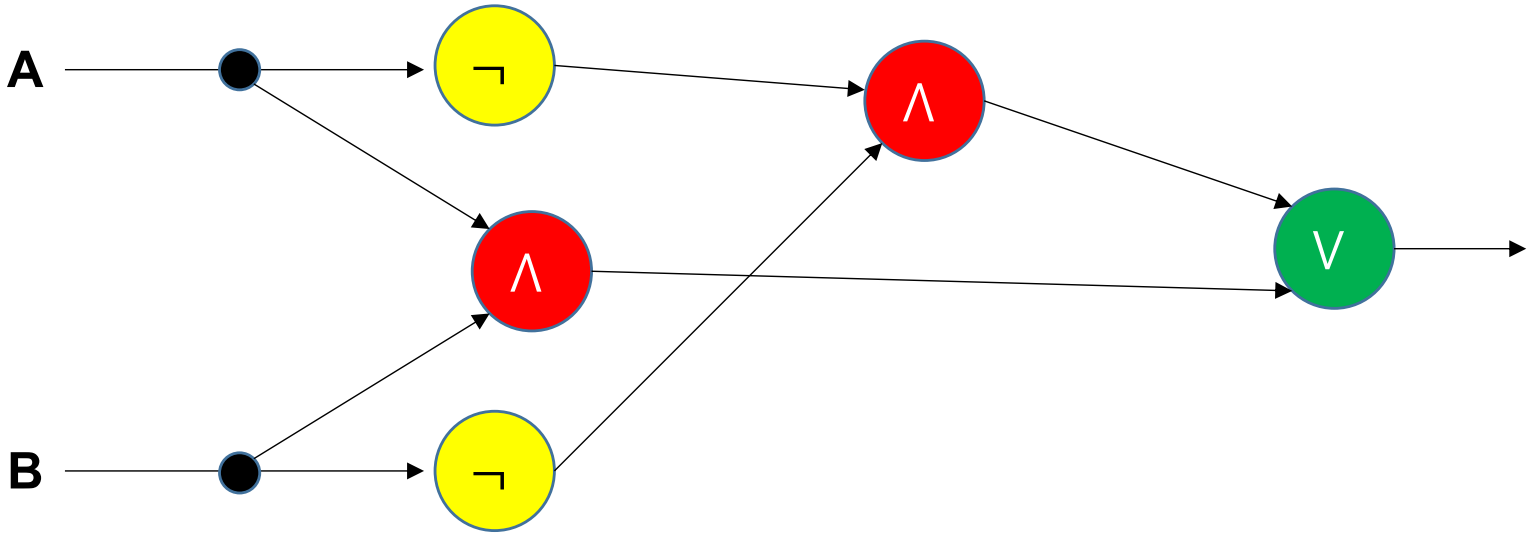
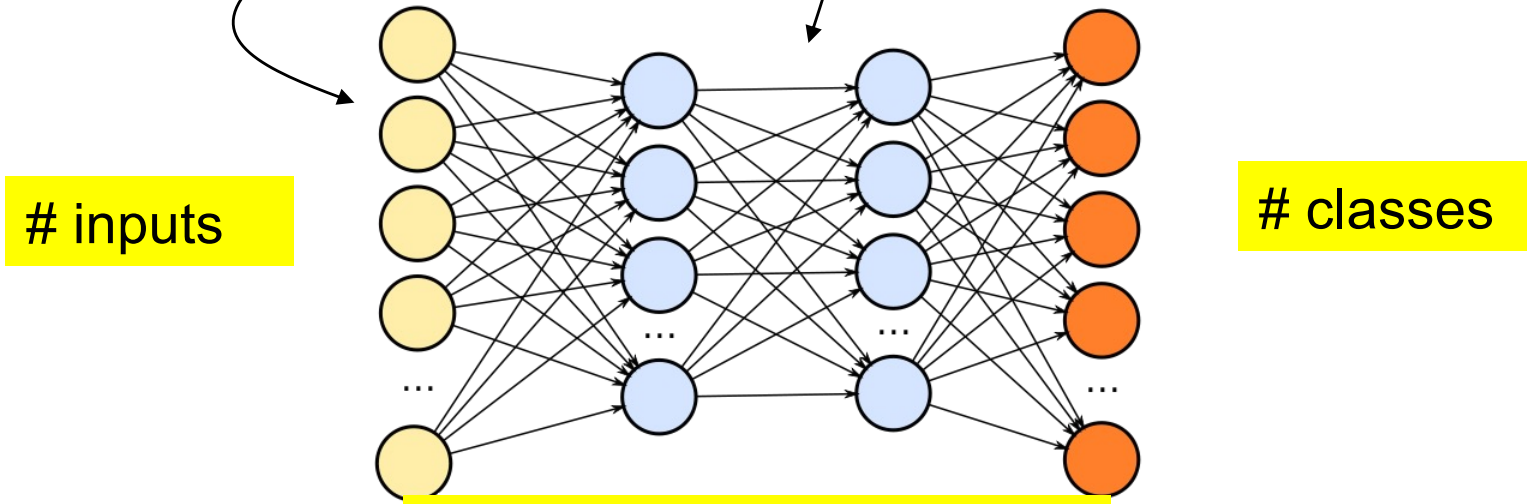


- This will be a network "specific" to reproduce this function.
- However, the big question remains: **How to automatically obtain the θ values?**

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: (implementation)
  - 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.]])
```

Machine Learning: Keras **MLP**

- And, using Keras...

```
import keras as K
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Activation, Softmax

tot_classes = 5

model = Sequential()
model.add(Dense(7, input_shape=(X.shape[1],)))
model.add(Activation('sigmoid'))
model.add(Dense(6))
model.add(Activation('sigmoid'))
model.add(Dense(tot_classes))
model.add(Softmax())

def J(y_true, y_pred):
        squared_difference = K.square(y_true - y_pred)
        return K.mean(squared_difference, axis=-1)

model.compile(optimizer='adam', loss=J, metrics=['accuracy'])

model.fit(X_train, y_train, epochs=100, batch_size=8, verbose=1)
```

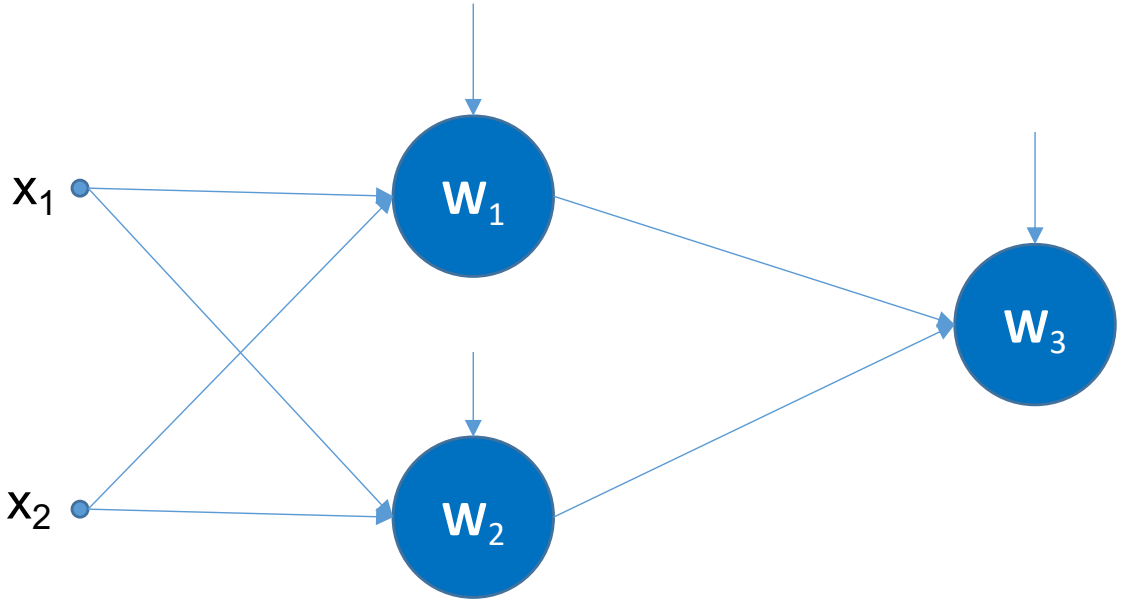
 # neurons Input Layer

 # neurons Hidden Layer

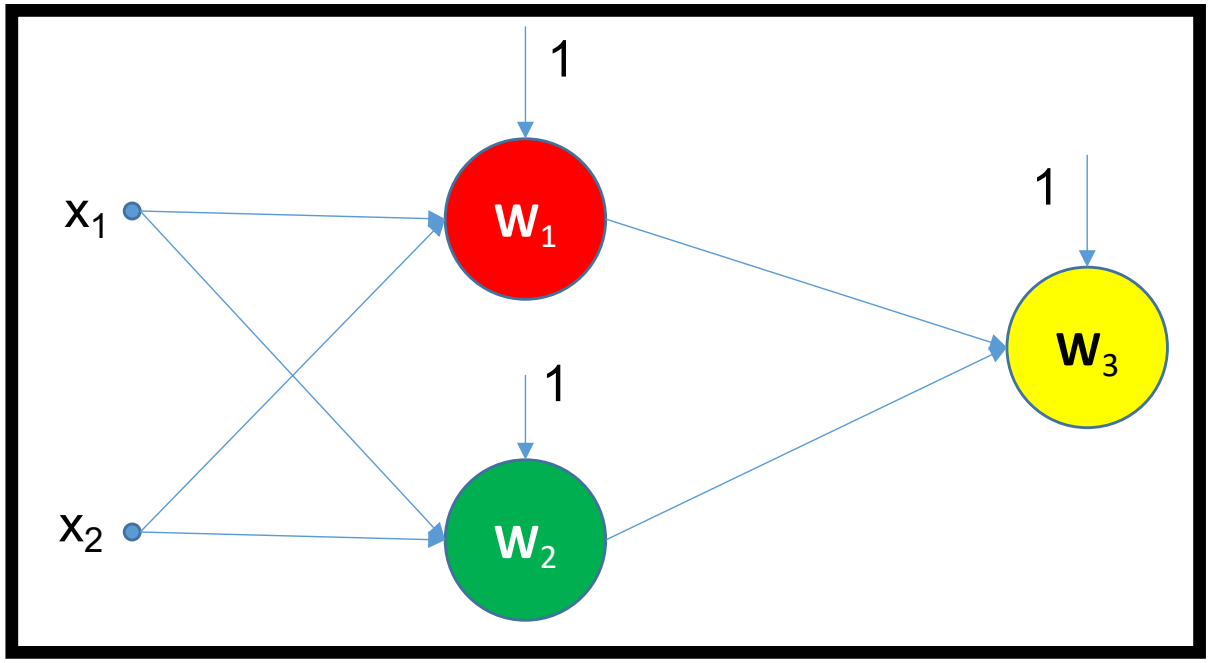
 # neurons Output Layer

Neural Networks: Learning

- In case of multilayered networks, the closed-form equation for the whole network cost function and its 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.



NN Learning



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

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

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

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

Backpropagation

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

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

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

- 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:

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

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

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

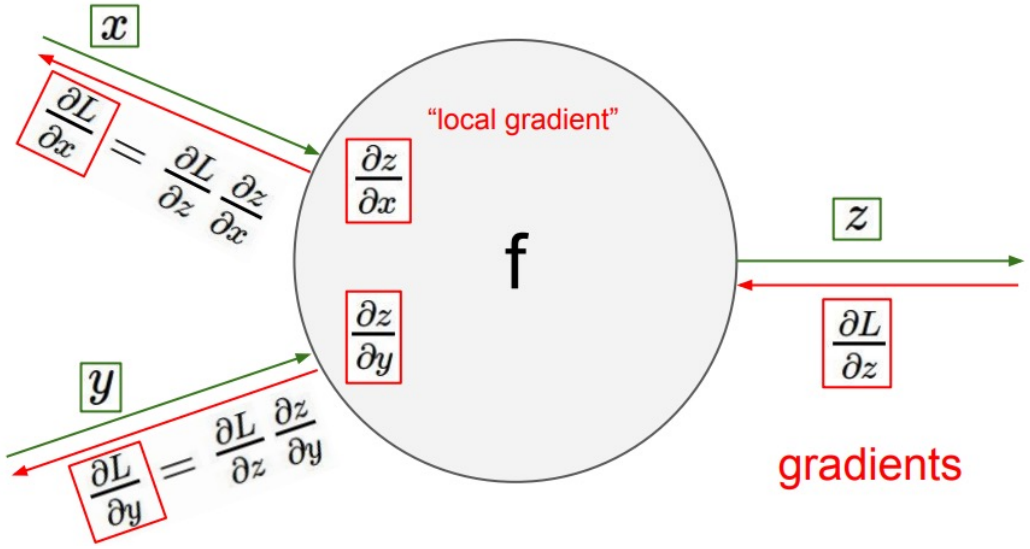
…and this is a tiny network...

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**:

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial g} \cdot \frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial x}$$

- 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.



$$y = g(f(x))$$