#### Introducción a Redes Neuronales

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Diplomado Ciencia de Datos con Python

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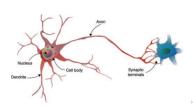
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#### Introduction

#### Redes Neuronales

Las redes neuronales artificiales son técnicas de Machine Learning que simulan el mecanismo de aprendizaje de los organismos biológicos. El sistema nervioso humano contiene células (neuronas), conectadas entre sí por axones y dendritas. Las regiones de conexión entre axones y dendritas se denominan sinapsis. La fuerza de las conexiones sinápticas cambia en respuesta a estímulos externos. Así es como se produce el aprendizaje en los organismos vivos.



#### El perceptrón

 El algoritmo Perceptrón (McCulloch-Pitts-Rosenblatt, 1943-1961) desempeñó un papel importante en la historia del ML. Fue simulado por primera vez en una computadora IBM 704 en 1957. A principios de los 60, se diseñó un hardware específico (Mark I perceptron) para implementar el algoritmo.



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 Fue criticado por Marvin Minsky, quien demostró las limitaciones del algoritmo cuando se trataba de un conjunto no linealmente separable.
 Esto provocó un vacío en la investigación de la computación neuronal que duró hasta mediados de los 80s.

#### Deep Learning

El aprendizaje profundo forma parte de una familia más amplia de métodos de ML, se basan en redes neuronales artificiales. El aprendizaje puede ser supervisado o no supervisado.

El adjetivo *deep* en deep learning hace referencia al uso de multiplies capas en una red, lo cual le da *profundidad*.

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Las arquitecturas profundas se componen de múltiples niveles de operaciones no lineales, como en las redes neuronales con muchas capas ocultas.

Las arquitecturas profundas son útiles para:

• Reducir la cantidad de elementos de cómputo en el cálculo de funciones complejas.

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- Generar representaciones distribuídas del espacio de entrada (embeddings).
- Producir modelos que permitan generalizar funciones con entradas de alta variabilidad.

Algunos de los usos de estas arquitecturas profundas son:

Reconocimiento automático del habla.

- Reconocimiento automático del habla.
- Reconocimiento de imágenes.

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Algunos tipos de Artificial neural networks:

• Perceptrones Multicapa (MLP) o Fully Connected Network.

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- Redes Convolucionales (CNN).

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- Self-Organizing Map (SOM).

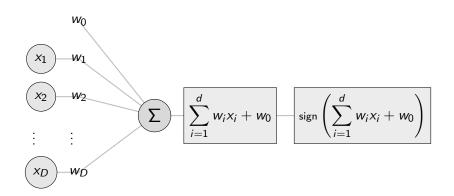
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- Transformadores: GPT, BERT, ...

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#### El perceptrón



- $\mathbf{w} = (w_0, w_1, ..., w_d)$  es el vector de pesos (matriz).
- Σ es una neurona.
- sign is the activation function.

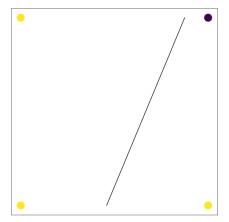
#### El algoritmo

Para cada época, el algoritmo es el siguiente:

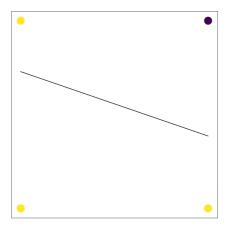
```
Data: X = \{x_1, ..., x_N\} \subset \mathbb{R}^{D+1}: puntos de entrenamiento,
         y = \{y_1, ..., y_N\} \subset \{-1, 1\}: etiquetas de entrenamiento,
        \eta > 0: tasa de aprendizaje.
Result: w: vector de pesos definiendo la frontera de decisión.
Function Perceptron(X, y, \eta):
     w = 0:
     converged = False;
     while converged == False do
          for i \in \{1, ..., N\} do
                if y_i \cdot \langle \mathbf{w}, x \rangle \leq 0 then
                 w = w + y_i \eta x_i;
converged = False
     return w:
```

Detalles

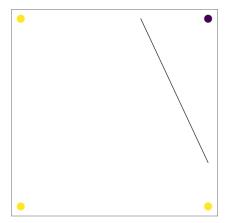
# Ejemplo

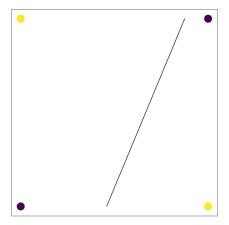


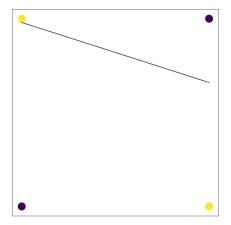
# Ejemplo

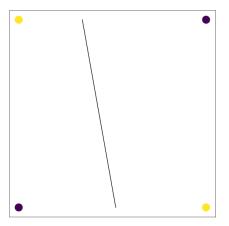


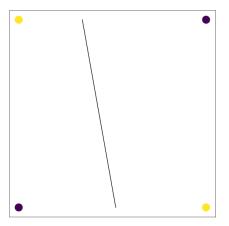
# Ejemplo

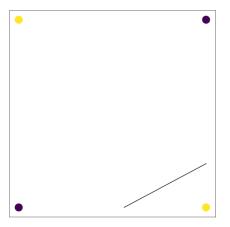


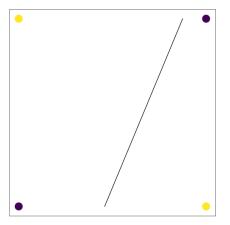












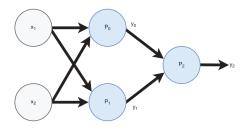
# Limitaciones del Perceptrón

¿Qué pasa si los datos no son linealmente separables?



#### Alternativas:

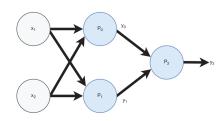
- Cambiar el modelo de una neurona.
- Combinar multiples neuronas.



Con esta arquitectura ya podemos resolver, de manera perfecta, este problema de clasificación

$$X = \begin{pmatrix} -1 & 1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{pmatrix}, \ y = \begin{pmatrix} -1 \\ +1 \\ +1 \\ -1 \end{pmatrix}$$



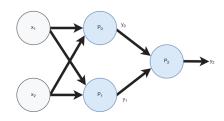


$$y_{0} = f_{0} \left( \left( \begin{array}{ccc} w_{0}^{(0)} & w_{1}^{(0)} & w_{2}^{(0)} \end{array} \right) \left( \begin{array}{c} 1 \\ x_{1} \\ x_{2} \end{array} \right) \right)$$

$$y_{1} = f_{1} \left( \left( \begin{array}{ccc} w_{0}^{(1)} & w_{1}^{(1)} & w_{2}^{(1)} \end{array} \right) \left( \begin{array}{c} 1 \\ x_{1} \\ x_{2} \end{array} \right) \right)$$

$$y_{2} = f_{2} \left( \left( \begin{array}{ccc} w_{0}^{(2)} & w_{1}^{(2)} & w_{2}^{(2)} \end{array} \right) \left( \begin{array}{c} 1 \\ y_{0} \\ y_{1} \end{array} \right) \right)$$



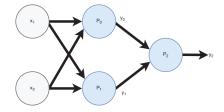


$$y_{0} = \begin{pmatrix} w_{0}^{(0)} & w_{1}^{(0)} & w_{2}^{(0)} \end{pmatrix} \begin{pmatrix} 1 \\ x_{1} \\ x_{2} \end{pmatrix}$$

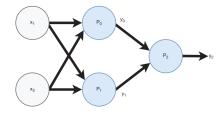
$$y_{1} = \begin{pmatrix} w_{0}^{(1)} & w_{1}^{(1)} & w_{2}^{(1)} \end{pmatrix} \begin{pmatrix} 1 \\ x_{1} \\ x_{2} \end{pmatrix}$$

$$y_{2} = \text{sign} \begin{pmatrix} \begin{pmatrix} w_{0}^{(2)} & w_{1}^{(2)} & w_{2}^{(2)} \end{pmatrix} \begin{pmatrix} 1 \\ y_{0} \\ y_{1} \end{pmatrix}$$

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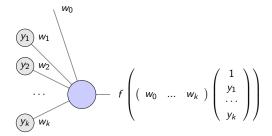
Este arreglo de perceptrones (neuronas) es uno de los ejemplos más sencillos de red Feed-Forward Fully Connected. Completamente conectada significa que la salida de cada neurona de una capa está conectada a todas las neuronas de la capa siguiente. Feed-forward significa que no hay conexiones hacia atrás. Una red neuronal multinivel tiene una capa de entrada, una o más capas ocultas y una capa de salida. La capa de entrada no contiene neuronas, sino sólo las propias entradas (features).



- Tenemos dos features (blanco).
- Tenemos dos capas de neuronas (azul).
  - La capa oculta tiene dos neuronas, sin activación.
  - La capa de salida tiene una neurona con activación sign.

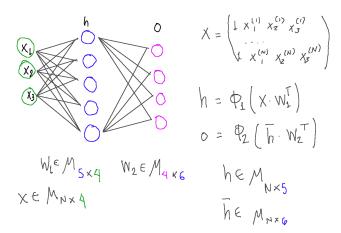
Entrenar esta red de perceptrones significa encontrar los mejores pesos (parámetros)  $w_i^{(k)}$ .

### El funcionamiento de una neurona



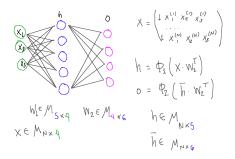
La capa previa tiene k neuronas, la función de activación es f.

### El output de una red neuronal



Los valores en las neuronas de salida dependen de la función de activación  $\Phi_2$ .

### El output de una red neuronal



Los valores de salida se comparan con las etiquetas del dataset y el error se mide con una función de perdida.

El aprendizaje de una red neuronal consiste en determinar los valores de las matrices  $W_i$  que minimicen el error total de salida.

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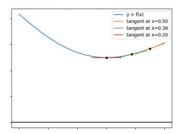


### ¿Cómo encontramos el mínimo de una función?

• Sea f(x) una función, queremos encontrar el mínimo de f.

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- La derivada en el punto x que minimiza el valor de f es 0.



### Descenso de gradiente

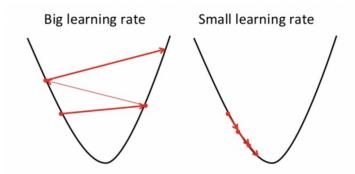
- A partir de un valor inicial x queremos encontrar un valor que minimiza f.
- El signo de f'(x) nos indica la dirección en la cual *mover* x para reducir el valor de f(x).
- La magnitud de f'(x) nos indica que tanto ajustar x. Usamos un peso  $\eta$ , llamado learning rate,

$$x_{n+1} = x_n - \eta f'(x_n).$$

- Si  $\eta$  es muy grande, el método puede *pasarse* de la solución y no converger.
- El algoritmo no garantiza encontrar el mínimo global, puede quedarse atorado en un mínimo local.

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# Learning Rate

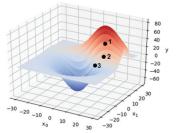


### El caso de dimensión alta

• Consideremos la función  $f(x_0, x_1)$ .

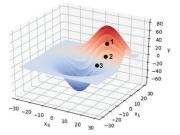
### El caso de dimensión alta

- Consideremos la función  $f(x_0, x_1)$ .
- El gradiente es un vector que consta de las derivadas e indica la dirección en el espacio de features en la que se produce el ascenso más pronunciado en el valor de f.



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• Si estamos en el punto  $\mathbf{x_n} = \left(x_0^{(n)}, x_1^{(n)}\right)$  y queremos minimizar f, ajustamos el punto de la siguiente forma

$$\mathbf{x}_{\mathsf{n}+1} = \mathbf{x}_{\mathsf{n}} - \eta \nabla f(\mathbf{x}_{\mathsf{n}})$$

Al aplicar descenso de gradiente a nuestra red neuronal, consideramos las features  $\mathbf{x}$  como constantes, el objetivo es encontrar los pesos  $\mathbf{w}$  de tal forma que minimicemos el error.

• ¿Qué función queremos minimizar? Una función de perdida.

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- ¿Qué función queremos minimizar? Una función de perdida.
- En el contexto de optimización, la función que evalua una solución candidata se le llama función objectivo. En las redes neuronales, la función objetivo se le llama función costo o perdida (loss function).

In the case of the Perceptron, the loss function is given by

$$L^{(0/1)}(\mathbf{w}) = (y_i - \operatorname{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle)^2$$

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$$L^{(0/1)}(\mathbf{w}) = \frac{1}{2}(y_i - \operatorname{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle)^2 = 1 - y_i \operatorname{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle$$

This function is not smooth, we use the smooth surrogate loss function

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Applying gradient descent

$$\mathbf{w}_{n+1} = \mathbf{w}_n - \eta \nabla L(\mathbf{w})$$

$$= \begin{cases} \mathbf{w}_n + \eta y_i \mathbf{x}_i, & \text{well classified} \\ \mathbf{w}_n, & \text{misclassified} \end{cases}$$

### Loss Functions

Other examples of loss functions

▶ Keras Losses

### Loss Functions: MSE

Mean Square Error (MSE)

$$L(y,t)=(t-y)^2.$$

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- L2 loss.
- Good for regression tasks.
- Trivial derivative for gradient descent.

### Loss Functions: MAE

### Mean Absolute Error (MAE)

$$L=|t-y|.$$

- I 1 loss.
- More robust to outliers than mse.
- Good for regression tasks.
- Discontinuity in its derivative.

## Loss Functions: Hinge

#### Hinge Loss

$$L = \max\{-y_i \hat{y}_i, 0\}.$$

- Used in SVMs and Perceptron.
- Penalizes errors, but also correct predictions of low confidence (probabilities).
- Good for binary classification tasks.

# Loss Functions: Categorical cross entropy

#### Categorical cross entropy

$$L = \sum_{i}^{n} y_{i} \log \left(\hat{y}_{i}\right).$$

- Good for multi-class classification problems.
- Considers y to be a one-hot encoding vector in *n* classes.

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#### Advantages:

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#### Disadvantages:

- May trap at local minima.
- Weights are changed after calculating gradient on the whole dataset.
   May take a long time to converge.
- Requires large memory to calculate gradient on the whole dataset.

## **Optimizers**

We can use other optimizing strategies:

- Gradient Descent
- Stochastic Gradient Descent
- Stochastic Gradient Descent with momentum
- Mini-Batch Gradient Descent
- Adagrad
- RMSProp
- AdaDelta
- Adam

► Keras Optimizers



### Stochastic Gradient Descent

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- Due to an increase in the number of iterations, the overall computation time increases. Still, the computation cost is still less than that of the gradient descent optimizer.
- If the data is enormous and computational time is an essential factor, stochastic gradient descent should be preferred over batch gradient descent algorithm.

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- The benefit of using Adagrad is that it abolishes the need to modify the learning rate manually. It is more reliable than gradient descent algorithmss, as it reaches convergence at a higher speed.
- One downside of AdaGrad optimizer is that it decreases the learning rate aggressively and monotonically. There might be a point when the learning rate becomes extremely small.

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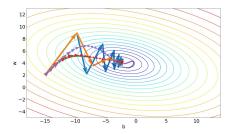
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- It is often used as a default optimization algorithm. It has faster running time, low memory requirements, and requires less tuning than any other optimization algorithm.
- It tends to focus on faster computation time, it might not generalize the data well enough.



# Different Optimizers



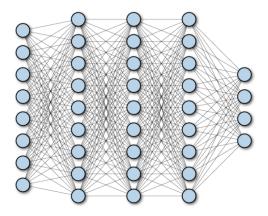
Visualizaciones, Several optimizers

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# Fully Connected Networks



A fully connected neural network consists of a series of fully connected layers that connect every neuron in one layer to every neuron in the other layer.

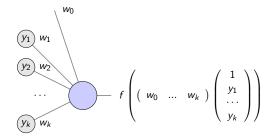
# Advantages and Disadvantages

• The major advantage of fully connected networks is that they are no special assumptions needed to be made about the input.

# Advantages and Disadvantages

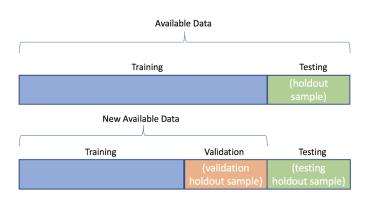
- The major advantage of fully connected networks is that they are no special assumptions needed to be made about the input.
- While being structure agnostic makes fully connected networks very broadly applicable, such networks do tend to have weaker performance than special-purpose networks tuned to the structure of a problem space.

### How each neuron works?



The previous layer has k neurons, the activation function is f.

#### Division of the dataset



### The Algorithm

The algorithm consists of three steps:

• First, present one or more training examples to the neural network: Feed-Forward.

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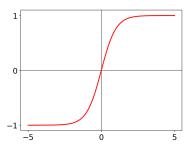
## The Algorithm

#### The algorithm consists of three steps:

- First, present one or more training examples to the neural network: Feed-Forward.
- Second, compare the output of the neural network to the desired value: Loss function.
- Finally, adjust the weights to make the output get closer to the desired value using gradient descent: Back propagation.

# Other Activation Functions: Hyperbolic Tangent

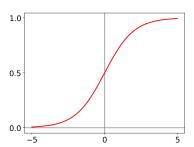
$$tanh(x) = \frac{e^{2x} - 1}{e^{2x} + 1} \in (-1, 1)$$
 $tanh'(x) = 1 - tanh^2(x)$ 



It is often used in the hidden layer. It can also be used if the predicted value of a regression task has values in (-1,1).

# Other Activation Functions: The Sigmoid

$$S(x) = \frac{1}{1 + e^{-x}} \in (0, 1)$$
$$S'(x) = S(x)(1 - S(x))$$



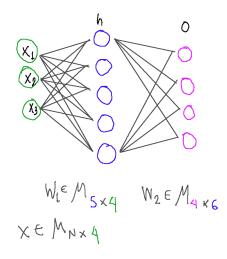
It is used when we need the output to be in (0,1). For example, in binary classification.

### Choice of Activation Functions

There exist a large number of activation functions. Two popular choices are tanh and the logistic sigmoid function. When picking between the two, choose tanh for hidden layers and logistic sigmoid for the output layer.

▶ Keras Activation Functions

# Feed-Forward: An Example



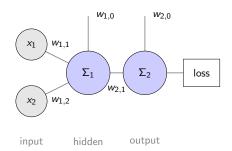
$$X = \begin{pmatrix} \downarrow & \chi_{1}^{(1)} & \chi_{2}^{(1)} & \chi_{3}^{(1)} \\ \downarrow & \chi_{1}^{(N)} & \chi_{2}^{(N)} & \chi_{3}^{(N)} \end{pmatrix}$$

$$h = \oint_{I} \left( \chi \cdot W_{I}^{T} \right)$$

$$0 = \oint_{Z} \left( \overline{h} \cdot W_{Z}^{T} \right)$$

$$h \in \mathcal{M}_{N \times 5}$$

$$\overline{h} \in \mathcal{M}_{N \times 6}$$



This neural network implements

$$f = S(w_{2,0} + w_{2,1} \tanh(w_{1,0} + w_{1,1}x_1 + w_{1,2}x_2))$$

We use the MSE loss:

$$e(f) = \frac{1}{2}(y - f)^2.$$



The error is given by

$$e(\mathbf{w}) = \frac{1}{2} \left( y - S \left( w_{2,0} + w_{2,1} \mathsf{tanh} (w_{1,0} + w_{1,1} x_1 + w_{1,2} x_2) \right) \right)^2$$
 where  $\mathbf{w} = \left( w_{1,0}, w_{1,1}, w_{1,2}, w_{2,0}, w_{2,1} \right)$ 

• We write it as:

$$e(f) = \frac{1}{2}(y - f)^{2}$$

$$f(z_{f}) = S(z_{f})$$

$$z_{f}(w_{2,0}, w_{2,1}, g) = w_{2,0} + w_{2,1}g$$

$$g(z_{g}) = \tanh(z_{g})$$

$$z_{g}(w_{1,0}, w_{1,1}, w_{1,2}) = w_{1,0} + w_{1,1}x_{1} + w_{1,2}x_{2}$$

### Compute the partial derivatives

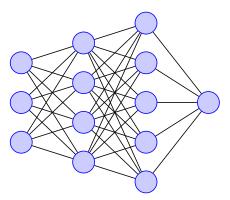
$$\begin{split} &\frac{\partial}{\partial w_{2,0}}e = -(y-f)S'(z_f)\\ &\frac{\partial}{\partial w_{2,1}}e = -(y-f)S'(z_f)g\\ &\frac{\partial}{\partial w_{1,0}}e = -(y-f)S'(z_f)w_{2,1}\tanh'(z_g)\\ &\frac{\partial}{\partial w_{1,1}}e = -(y-f)S'(z_f)w_{2,1}\tanh'(z_g)x_1\\ &\frac{\partial}{\partial w_{1,2}}e = -(y-f)S'(z_f)w_{2,1}\tanh'(z_g)x_2 \end{split}$$

Finally, we update the weights, via gradient descent

$$\begin{aligned} w_{2,0} &\leftarrow w_{2,0} - \eta \frac{\partial e}{\partial w_{2,0}} \\ w_{2,1} &\leftarrow w_{2,1} - \eta \frac{\partial e}{\partial w_{2,1}} \\ w_{1,0} &\leftarrow w_{1,0} - \eta \frac{\partial e}{\partial w_{1,0}} \\ w_{1,1} &\leftarrow w_{1,1} - \eta \frac{\partial e}{\partial w_{1,1}} \\ w_{1,2} &\leftarrow w_{1,2} - \eta \frac{\partial e}{\partial w_{1,2}} \end{aligned}$$

## Regression

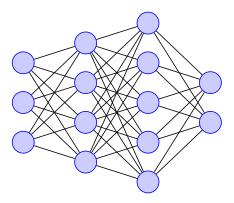
Si tenemos tres variables independientes y una variable dependiente



La función de activación en la capa de salida es *usualmente* None (la función identidad).

# Multivariate Regression

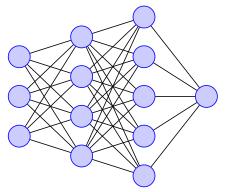
If we have three independent variables and two dependent variable



La función de activación en la capa de salida es *usualmente* None (la función identidad).

# **Binary Classification**

If we have three independent variables and two classes



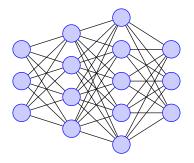
La función de activación en la capa de salida es la sigmoide

$$\sigma(x) = \frac{1}{1 + e^{-x}} \in (0, 1)$$

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### Multi-class Classification

Si tenemos tres, o más, clases



La función de activación en la capa de salida es softmax

$$\sigma(j;(x_1,...,x_n)) = \frac{e^{x_j}}{\sum_{i=1}^n e^{x_i}} \in (0,1)$$

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# Deep Learning Libraries





Tensorflow

Pytorch

# Deep Learning Libraries

	Keras	Tensorflow	Pytorch
API Level	High	High and low	Low
Architecture	Simple, read- able	Not easy to use	Complex, less readable
Datasets	Smaller datasets	Large datasets	Large datasets
Debugging	Debugging is not often needed	Good	Difficult
Written in	Python	C++, CUDA, Python	Lua
Trained models	Yes	Yes	Yes
Speed	Slow, low per- formance	Fast, high- performance	Fast, high- performance

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6 Appendix

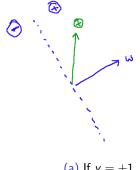


# Casos del perceptron

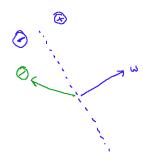
We iterate over the training set

$$(x_1, y_1), (x_2, y_2) \cdots, (x_N, y_N).$$

If the point is well classified:



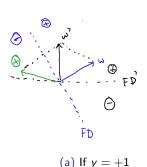
(a) If 
$$y = +1$$

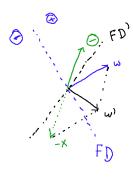


(b) If 
$$y = -1$$

# Casos del perceptron

If the point is not well classified:





(b) If 
$$y = -1$$

We update the vector w with w + yx



