# Introducción a Redes Neuronales

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Diplomado Ciencia de Datos con Python

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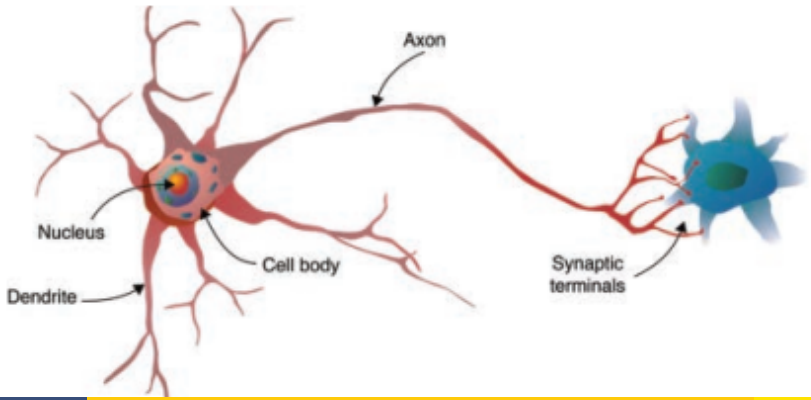
# Introduction

## Neural Networks

Artificial neural networks are machine learning techniques that simulate the mechanism of learning in biological organisms. The human nervous system contains cells, referred to as neurons. The neurons are connected to one another by of axons and dendrites, and the connecting regions between axons and dendrites are called synapses. The strengths of synaptic connections change in response to external stimuli. This change is how learning takes place in living organisms.



# El modelo lineal de clasificación

- The Perceptrón algorithm (Rosenblatt, 1961) played an important role in Machine Learning history. It was first simulated in a computer IBM 704 at Cornell in 1957. By the early 60s, a dedicated hardware was designed to implement the learning algorithm.

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- It was criticized by Marvin Minsky, who showed the limitations of the perceptron algorithm when dealing with a non linear separable set of points. This caused a void in the neural computation research lasting until the mid 80s.

# Deep Learning

## Deep Learning

Deep learning is part of a broader family of machine learning methods, which is based on artificial neural networks. Learning can be supervised, semi-supervised or unsupervised.
Deep learning processes machine learning by using a hierarchical level of artificial neural networks, built like the human brain, with neuron nodes connecting in a web.

The adjective *deep* in deep learning refers to the use of multiple layers in the network.

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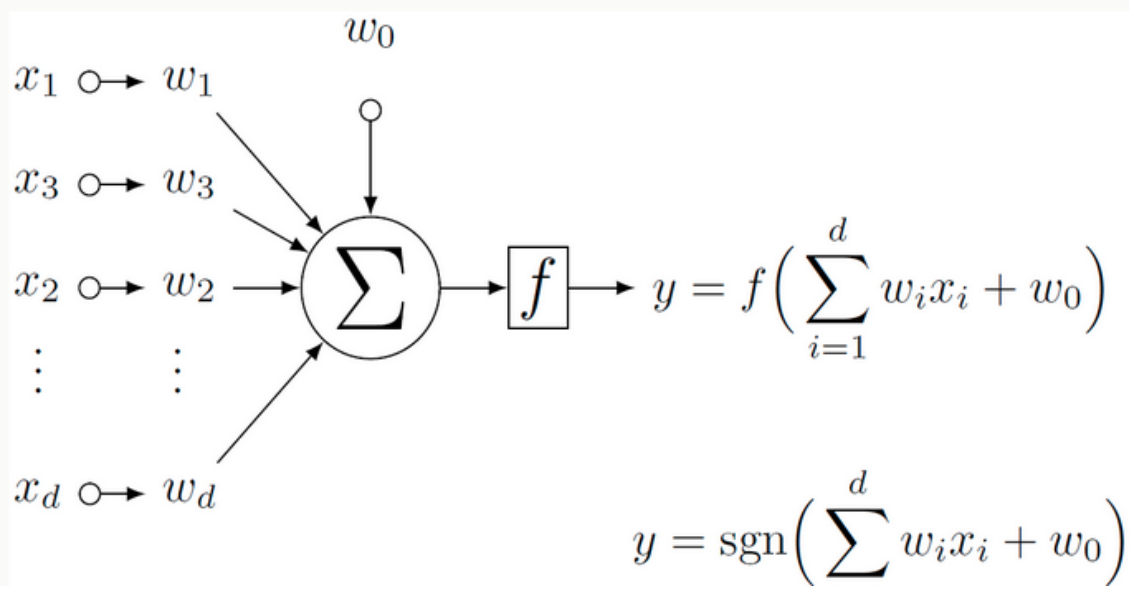
# The Rosenblatt Perceptron




- $\mathbf{w} = (w_0, w_1, ..., w_d)$ is the weights vector (matrix).
- $\Sigma$ is a neuron.
- sgn is the activation function.

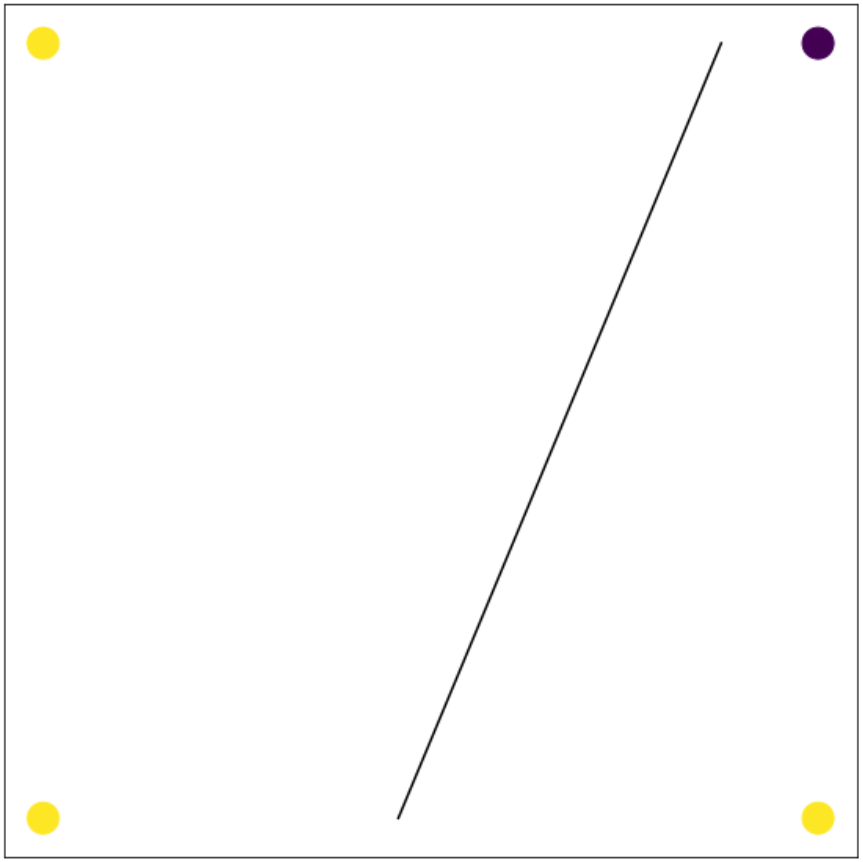
# The Algorithm

For each epoch, the algorithm is summarized as follows:

**Data:** $A$: training set of points, $X = \{x_1, ..., x_N\} \subset \mathbb{R}^{D+1}$,
$Y = \{y_1, ..., y_N\}$: set of labels
$\eta > 0$: learning rate.
**Result:** $\mathbf{w}$: weight vector defining the decision frontier.

```
Function Perceptron(X, y, η):
    w = 0;
    converged = False;
    while converged == False do
        for i ∈ {1, ..., N} do
            if y_i ⟨w, x⟩ ≤ 0 then
                w = w + y_i η x_i;
                converged = False
    return w;
```

# Example



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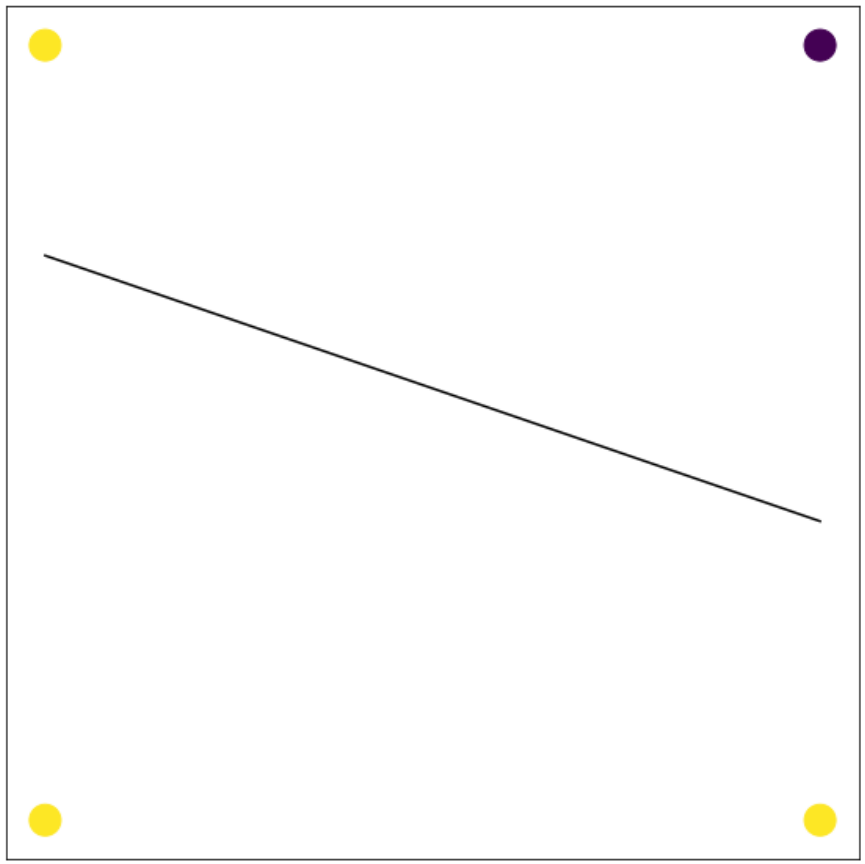

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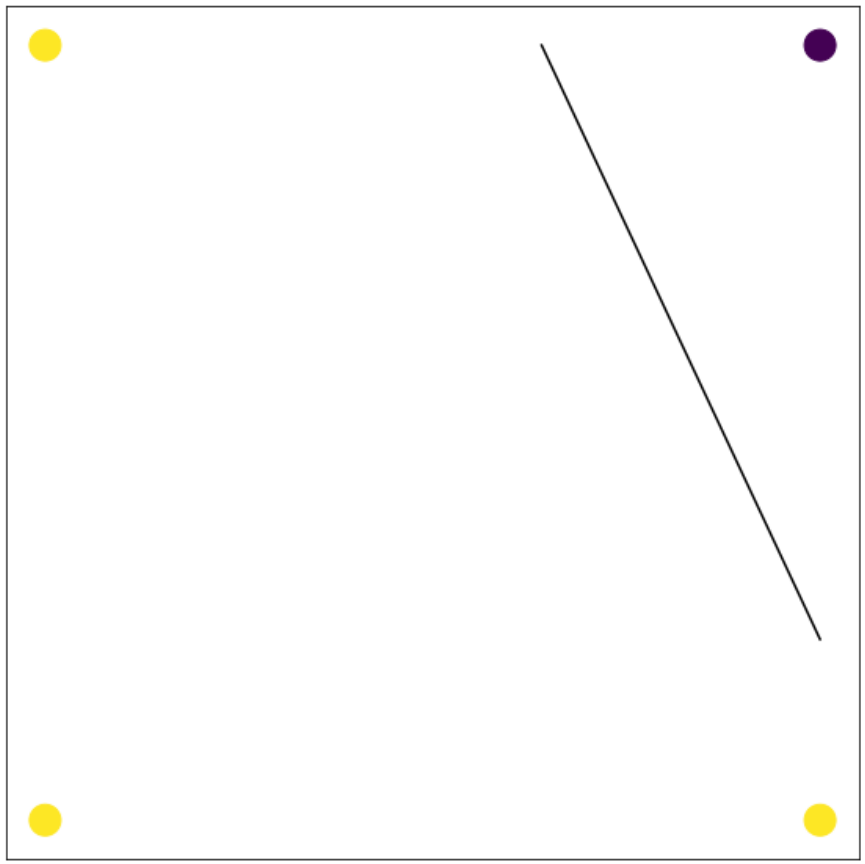

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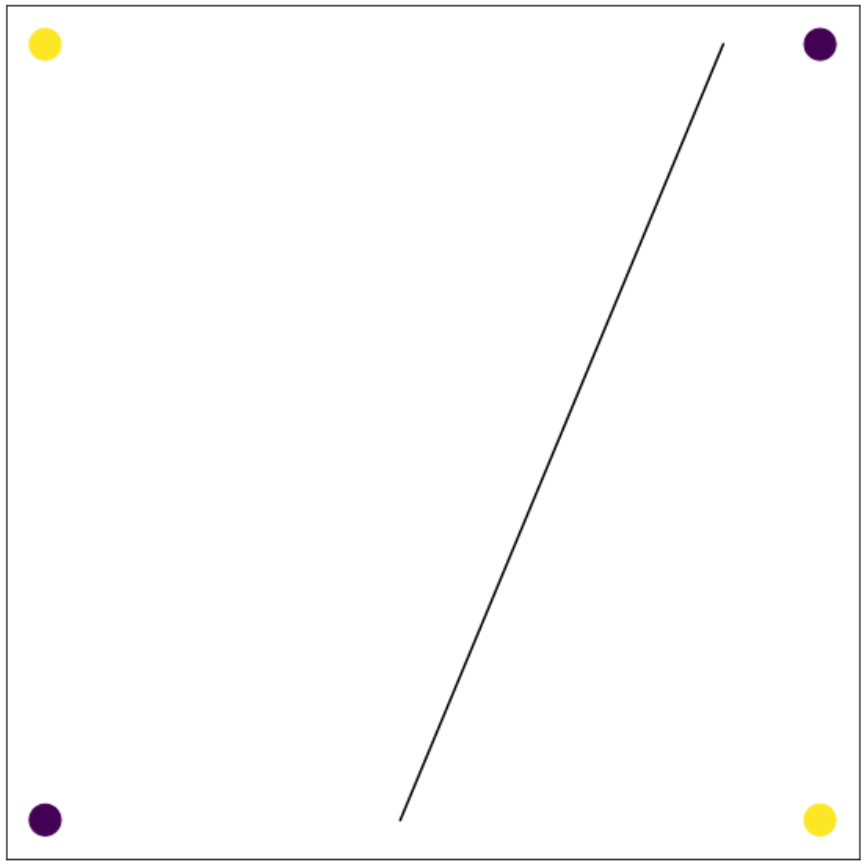
What happens if a straight line cannot separate the data points?



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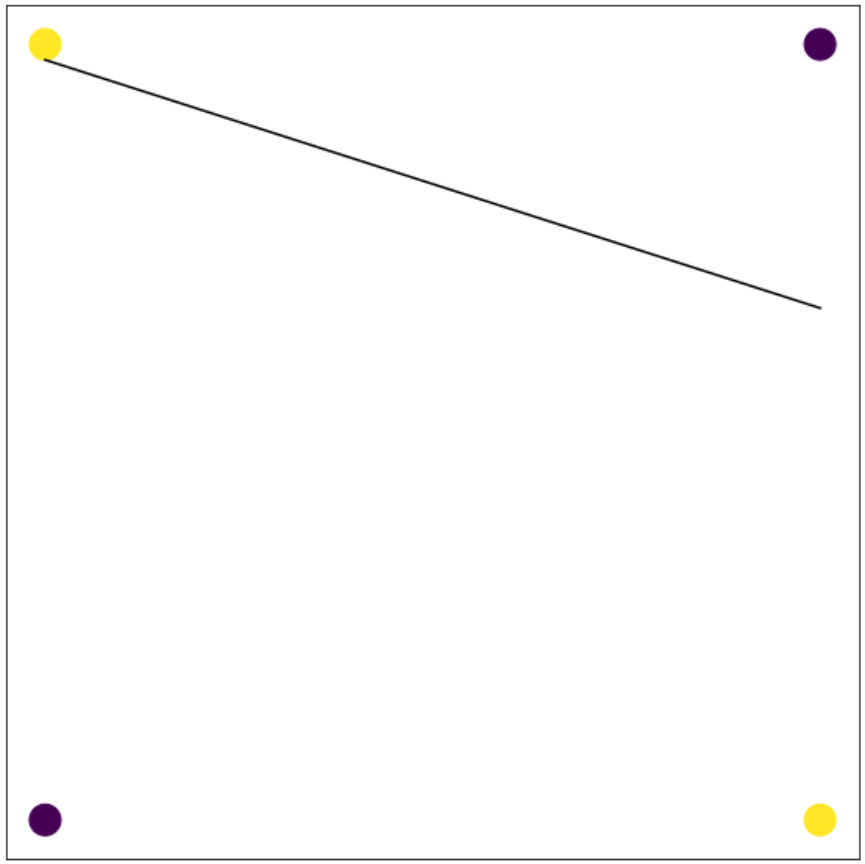

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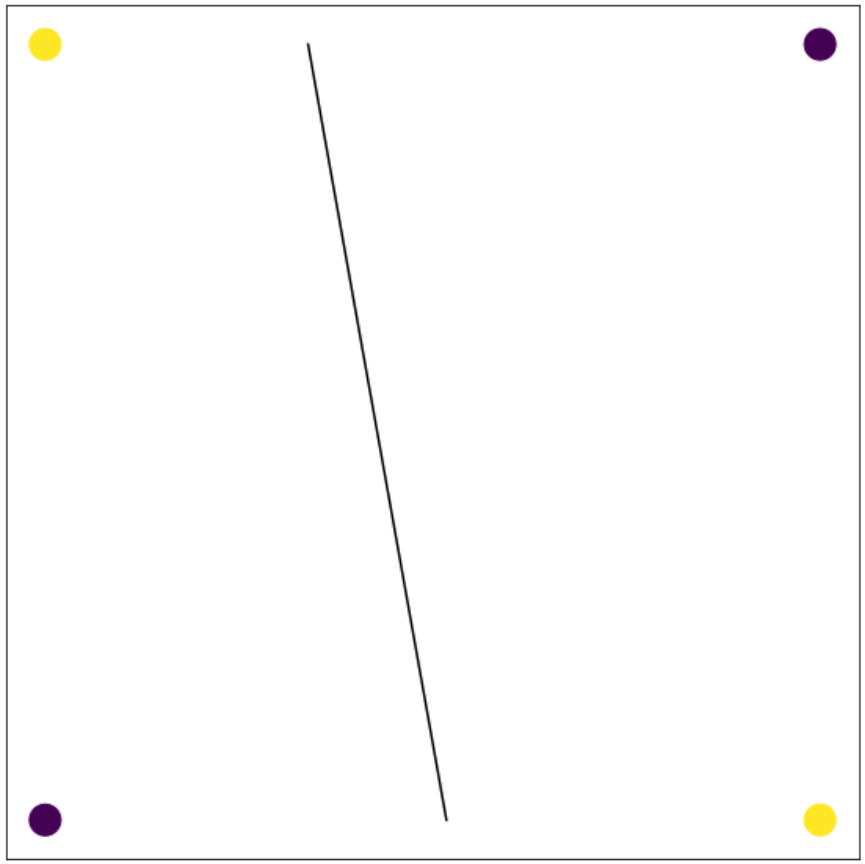

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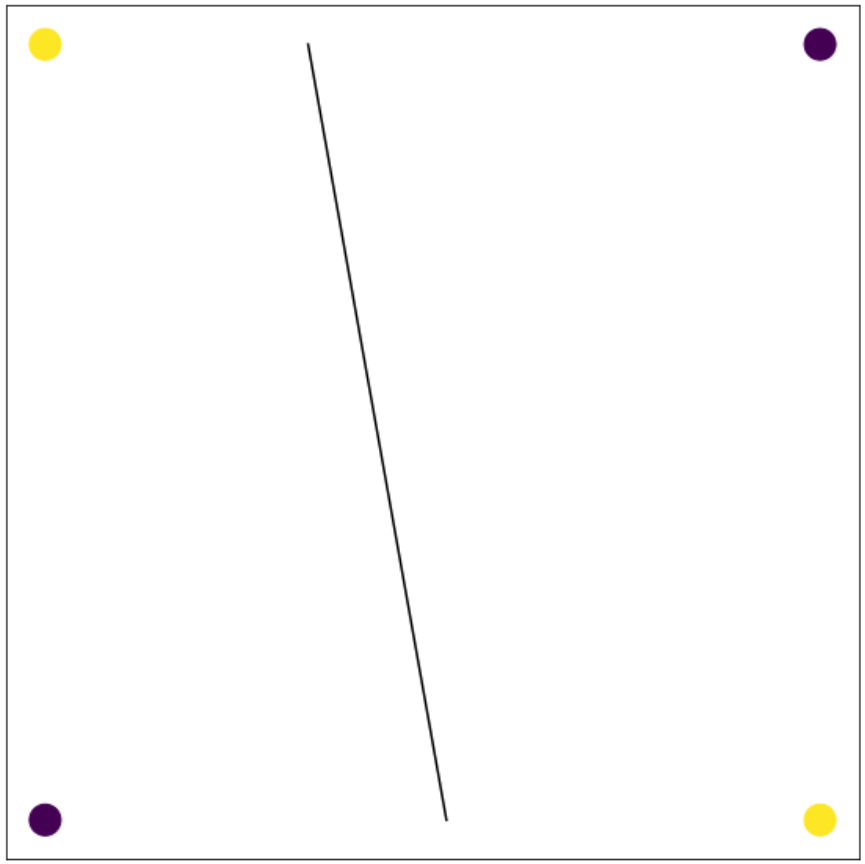

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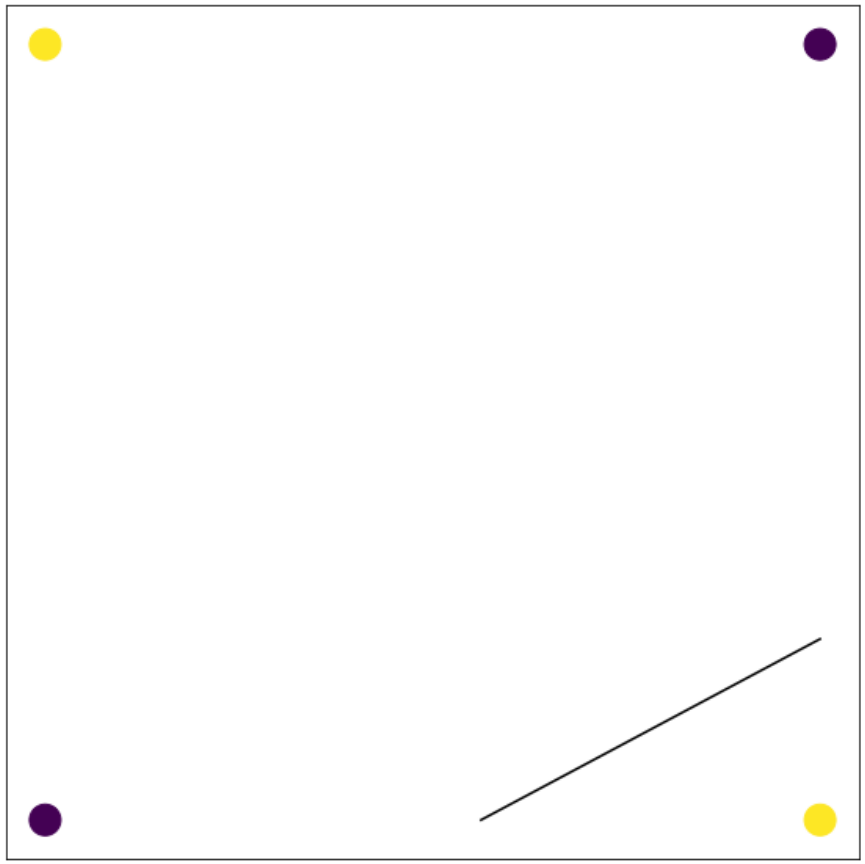

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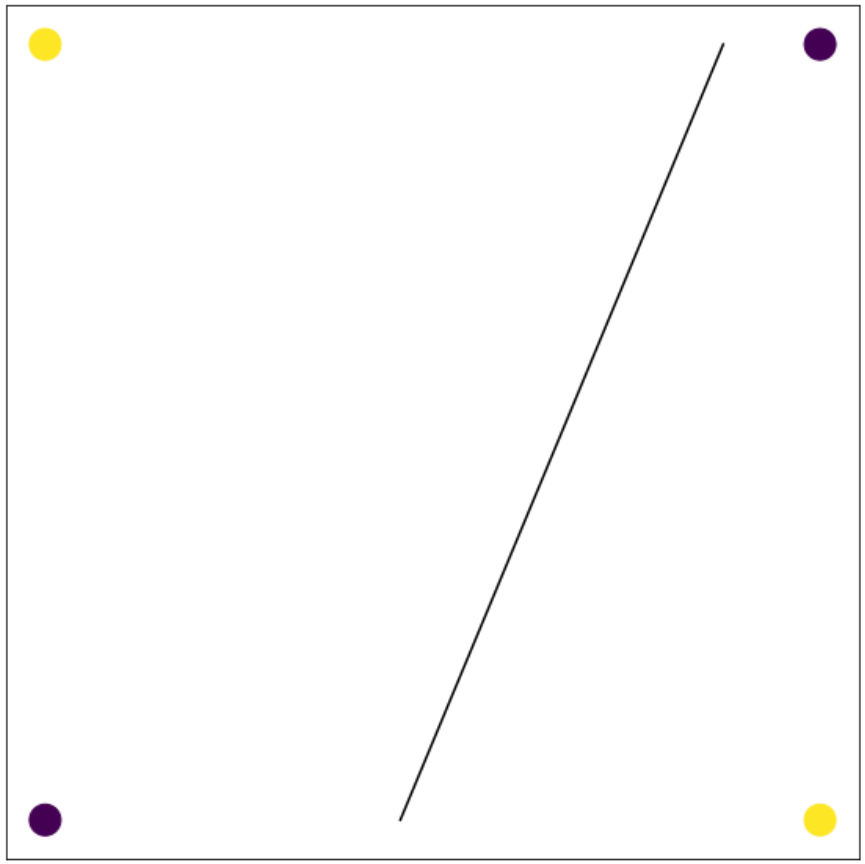

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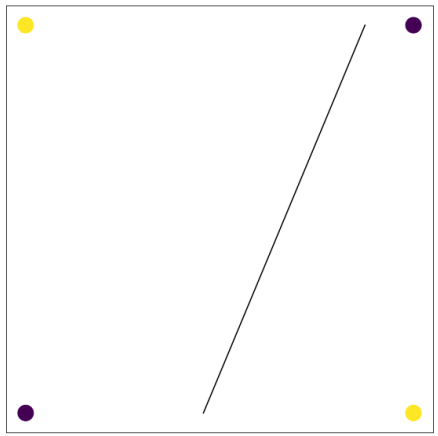
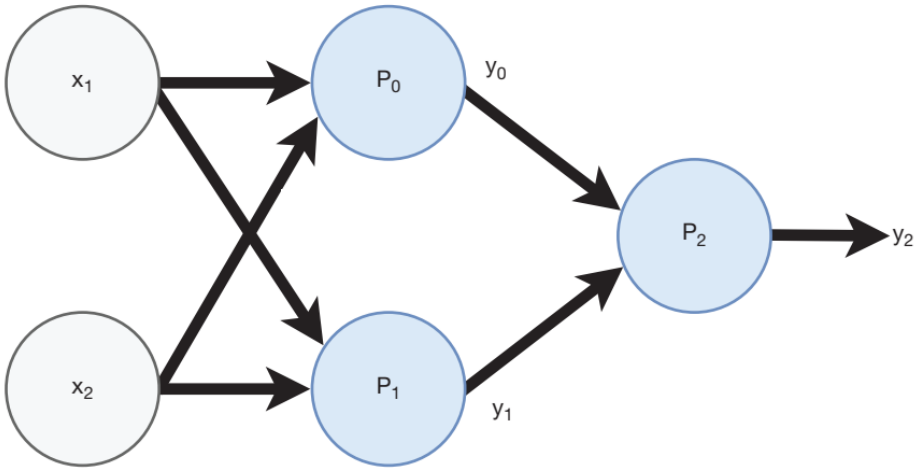


Alternatives:

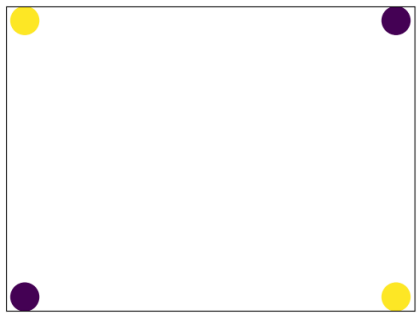
- We change the model of a neuron or
- We combine multiple of them to solve this limitation.

# Combining Perceptrons




Now, we can solve the classification problem

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



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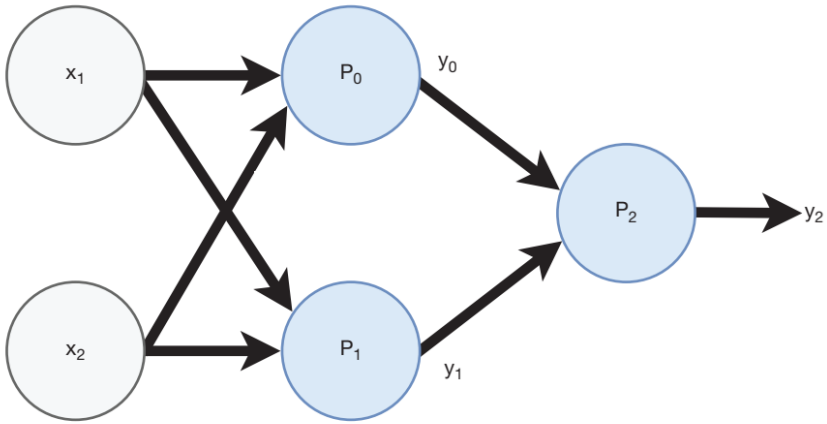


$$y_0 = f_0\left(\begin{pmatrix} w_0^{(0)} & w_1^{(0)} & w_2^{(0)} \end{pmatrix}\begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix}\right)$$

$$y_1 = f_1\left(\begin{pmatrix} w_0^{(1)} & w_1^{(1)} & w_2^{(1)} \end{pmatrix}\begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix}\right)$$

$$y_2 = f_2\left(\begin{pmatrix} w_0^{(2)} & w_1^{(2)} & w_2^{(2)} \end{pmatrix}\begin{pmatrix} 1 \\ y_1 \\ y_2 \end{pmatrix}\right)$$

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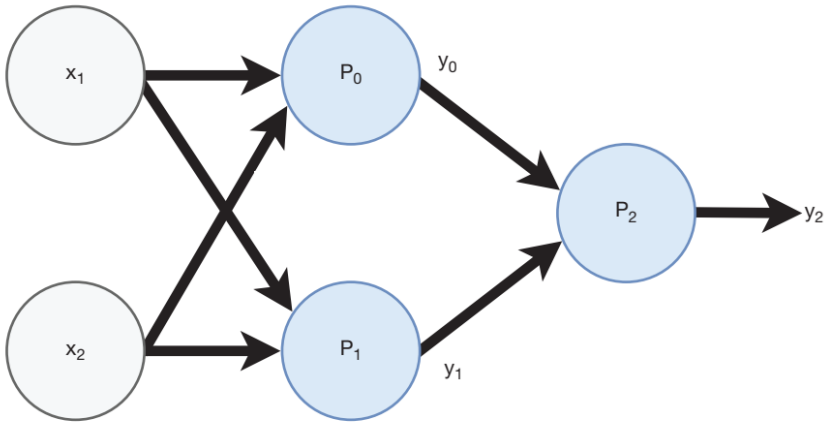


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$$y_2 = \text{sgn}\left( \begin{pmatrix} w_0^{(2)} & w_1^{(2)} & w_2^{(2)} \end{pmatrix} \begin{pmatrix} 1 \\ y_1 \\ y_2 \end{pmatrix} \right)$$

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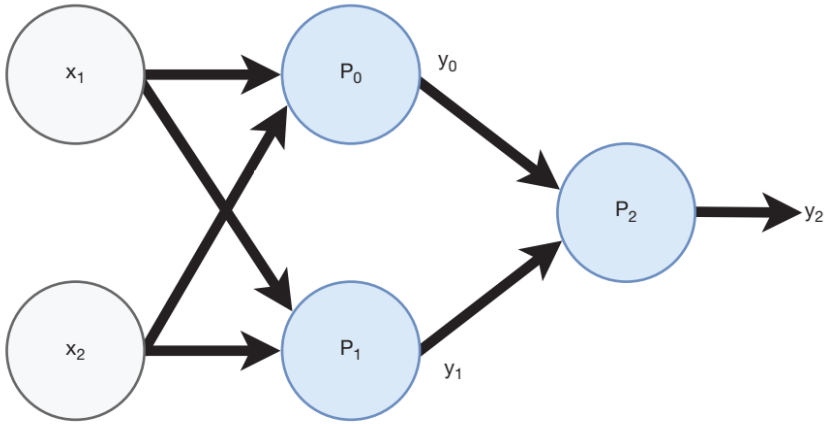
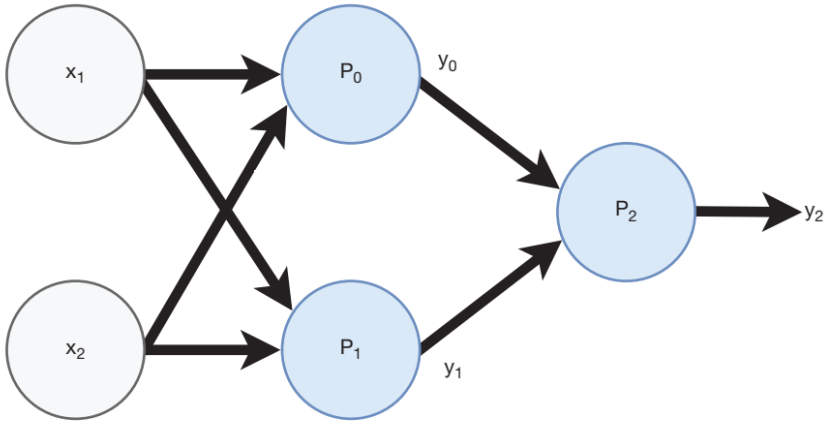



This neural network is one of the simplest examples of a fully connected feedforward network. Fully connected means that the output of each neuron in one layer is connected to all neurons in the next layer. Feedforward means that there are no backward connections. A multilevel neural network has an input layer, one or more hidden layers, and an output layer. The input layer does not contain neurons but contains only the inputs themselves.

# Combining Perceptrons




- We have two features (white).
- We have two layers of neurons (blue).
- The hidden layer has two neurons, with no activation function.
- The output layer has one neuron with activation function sgn.

To train this network of perceptrons means to find the best parameters $w_i^{(k)}$.

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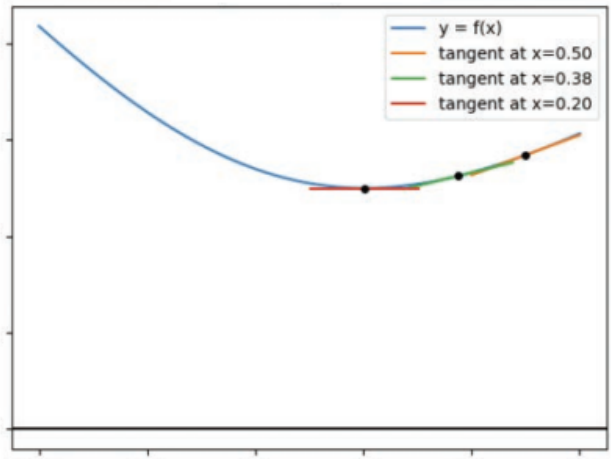

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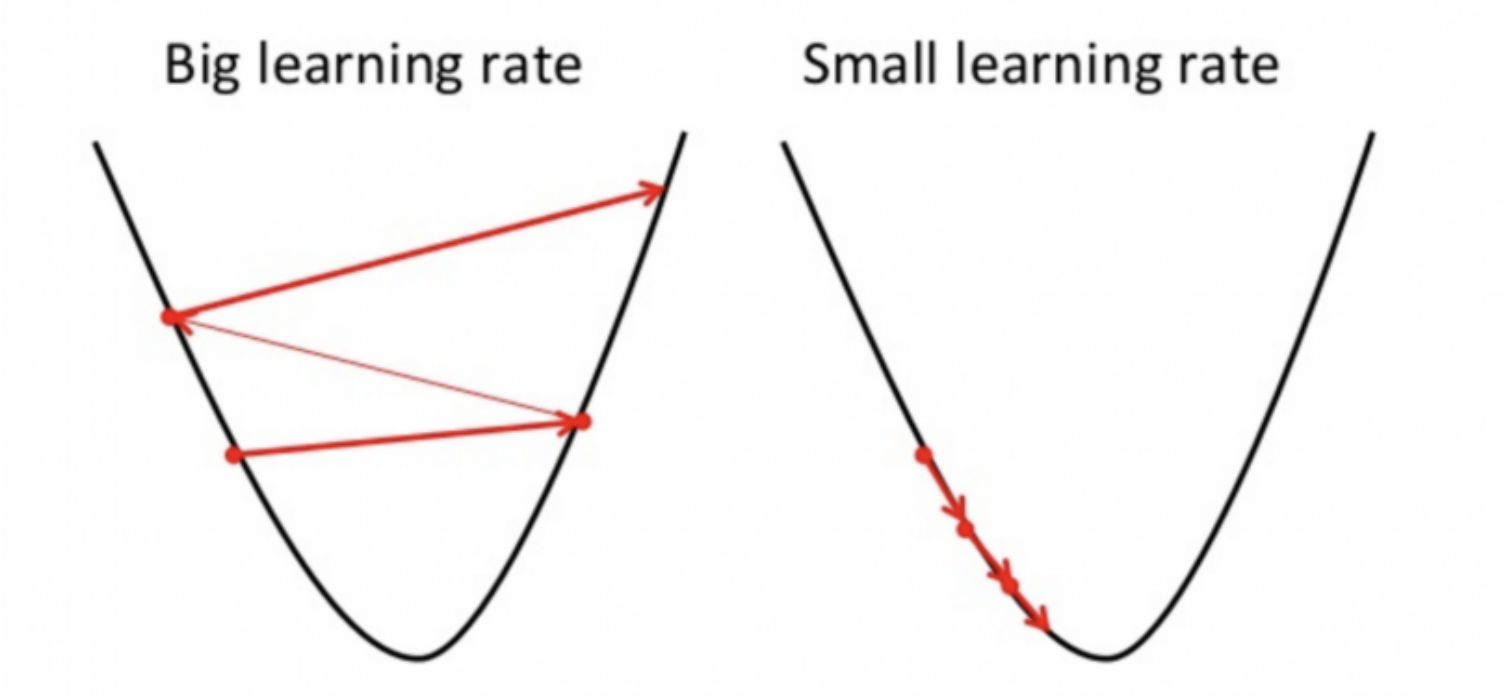
- If the learning rate $\eta$ is to too large, gradient descent can overshoot the solution and fail to converge.
- The algorithm is not guaranteed to find the global minimum because it can get stuck in a local minimum.

# Learning Rate



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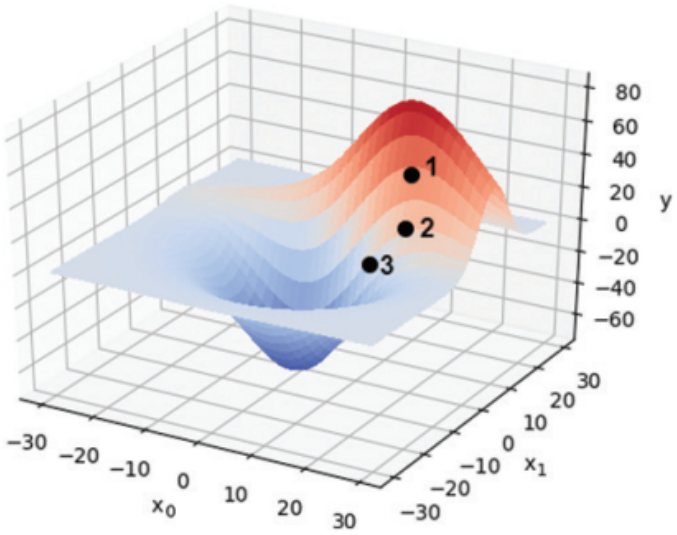

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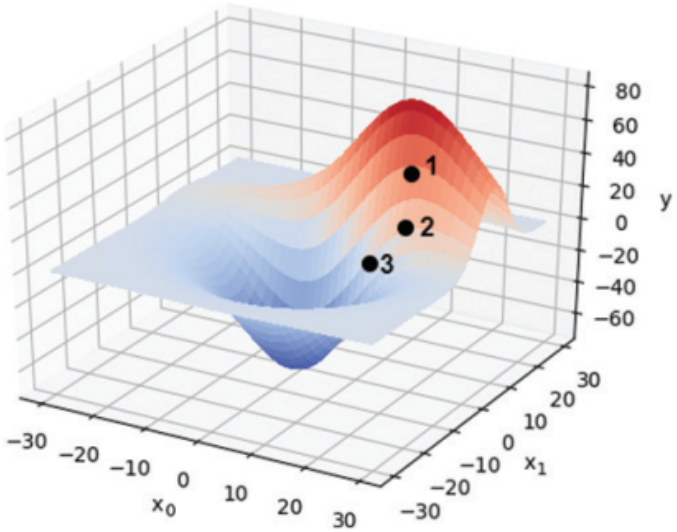


- If we are at the point $\mathbf{x_n} = (x_0^{(n)}, x_1^{(n)})$ and want to minimize y, then we choose our next point as

$$\mathbf{x_{n+1}} = \mathbf{x_n} - \eta \nabla f(\mathbf{x_n})$$

# Gradient-based Learning

When applying gradient descent to our neural network, we consider input values $\mathbf{x}$ to be constants, with our goal being to adjust the weights $\mathbf{w}$.

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When applying gradient descent to our neural network, we consider input values $\mathbf{x}$ to be constants, with our goal being to adjust the weights $\mathbf{w}$.

- Which function we want to minimize? A loss function.
- In the context of an optimization algorithm, the function used to evaluate a candidate solution is referred to as the objective function. With neural networks, we seek to minimize the error. As such, the objective function is often referred to as a cost function or a loss function.

# Gradient-based Learning

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

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

# Gradient-based Learning

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

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

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

$$L(\mathbf{w}) = \max\{-y_i \text{sign}\langle \mathbf{w}, \mathbf{x}_i \rangle, 0\}.$$

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- Applying gradient descent

$$\begin{aligned} \mathbf{w}_{n+1} &= \mathbf{w}_n - \eta \nabla L(\mathbf{w}) \\ &= \begin{cases} \mathbf{w}_n + \eta y_i \mathbf{x}_i, & \text{well classified} \\ \mathbf{w}_n, & \text{misclassified} \end{cases} \end{aligned}$$

# 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)

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

- L1 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.

# Optimizers: Gradient Descent

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Gradient descent is the most basic but most used optimization algorithm. It's used heavily in linear regression and classification algorithms. Gradient descent is a first-order optimization algorithm which is dependent on the first order derivative of a loss function.

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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

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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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- 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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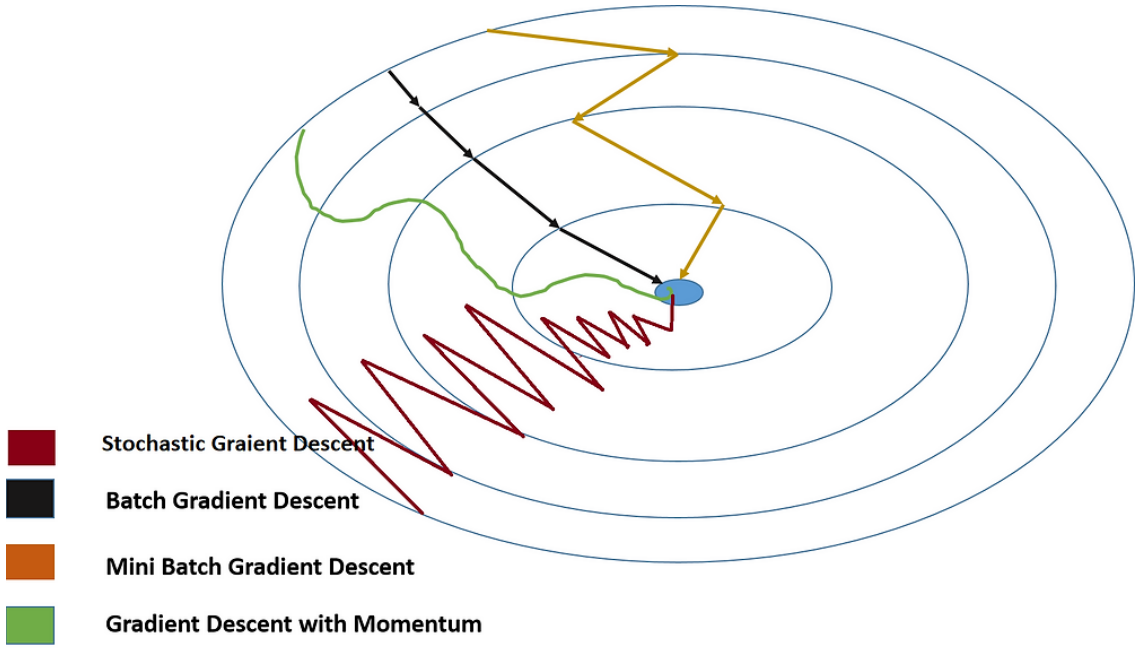
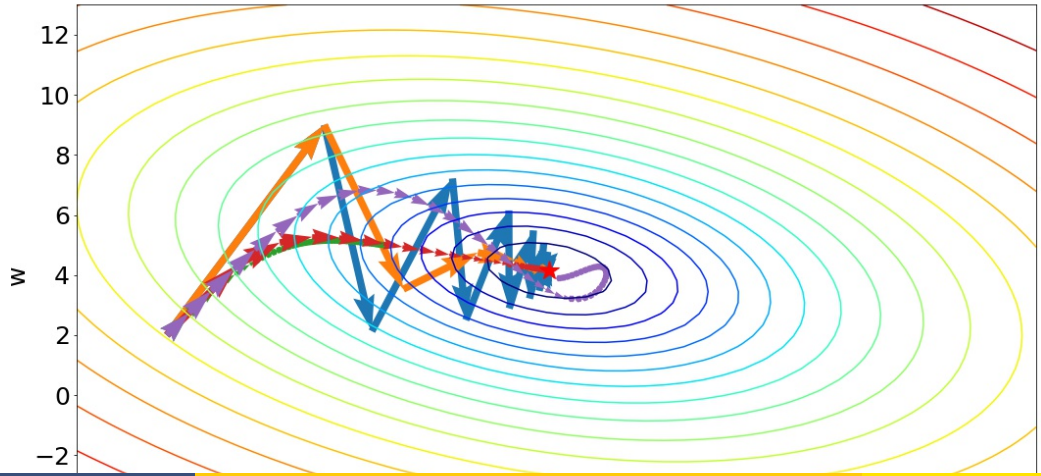
- It tends to focus on faster computation time, it might not generalize the data well enough.

# Optimizers


Stochastic Graient Descent
Batch Gradient Descent
Mini Batch Gradient Descent
Gradient Descent with Momentum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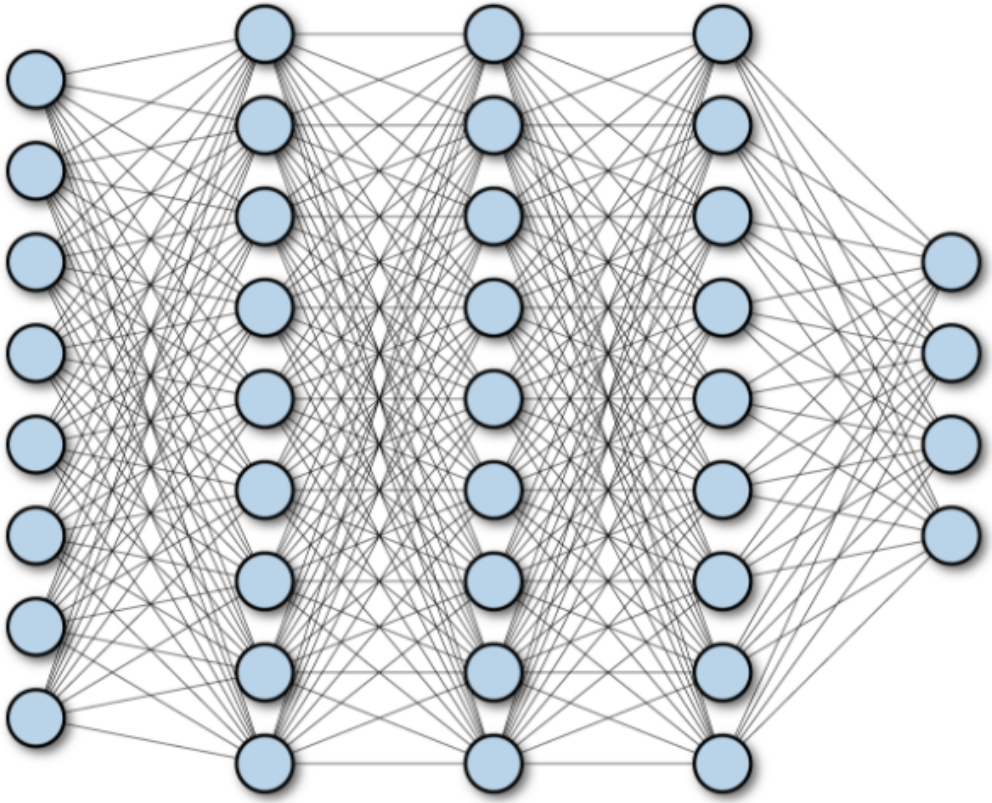
# Fully Connected Networks



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.

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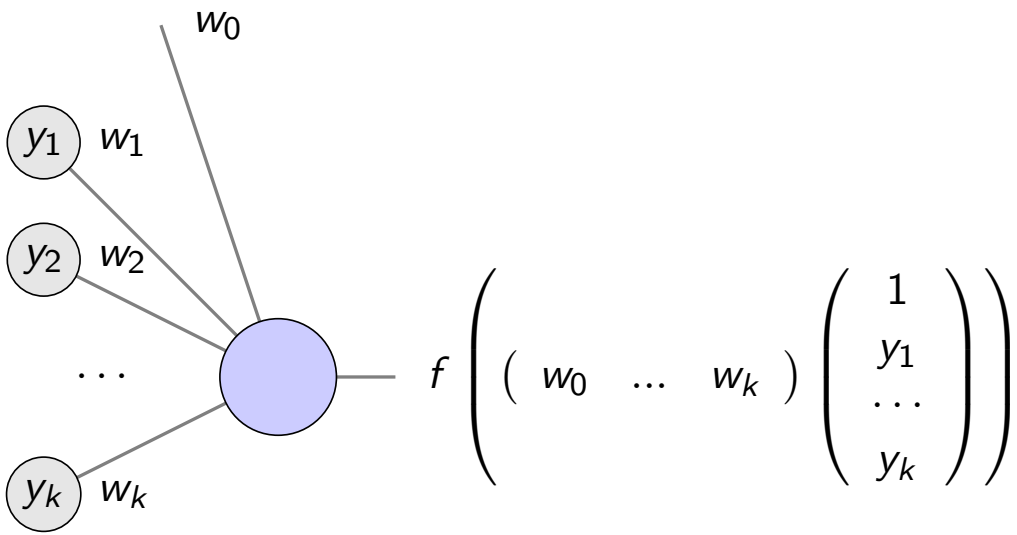
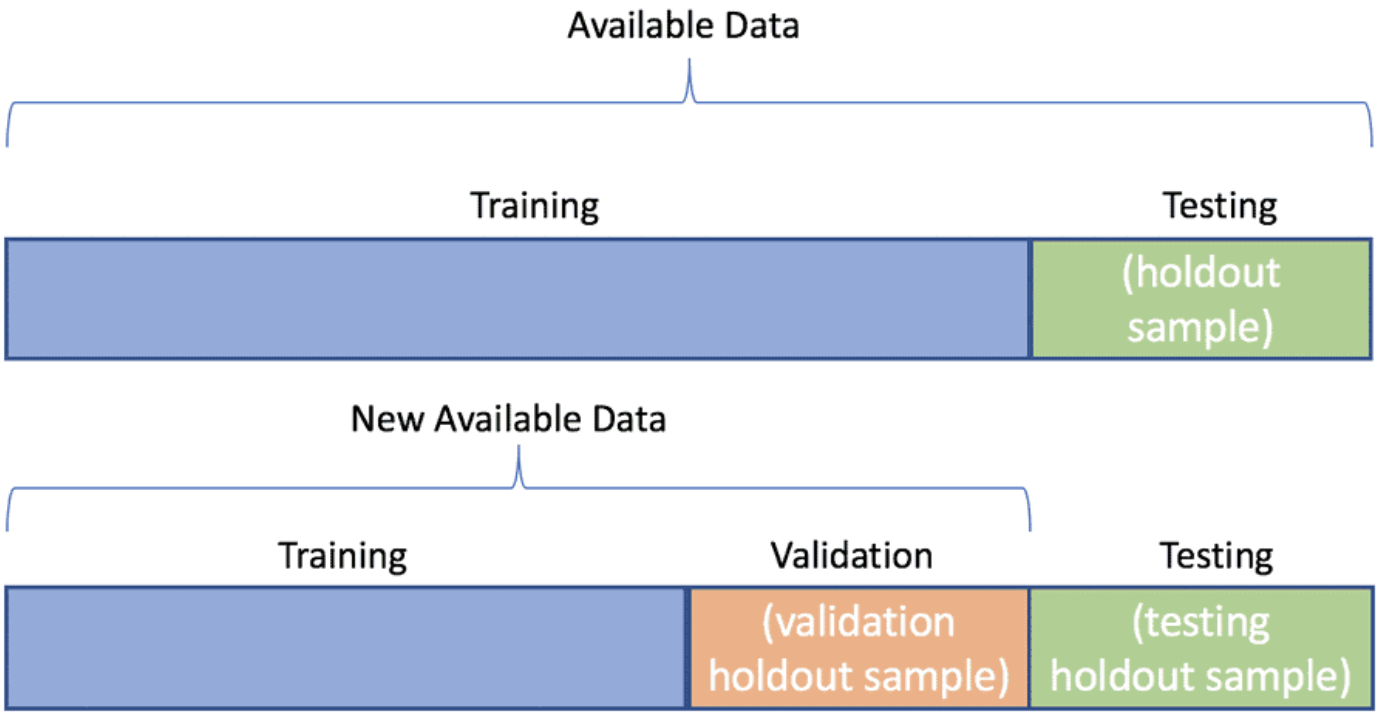
- The major advantage of fully connected networks is that they are no special assumptions needed to be made about the input.
- While being structure agnostic makes fully connected networks very broadly applicable, such networks do tend to have weaker performance than special-purpose networks tuned to 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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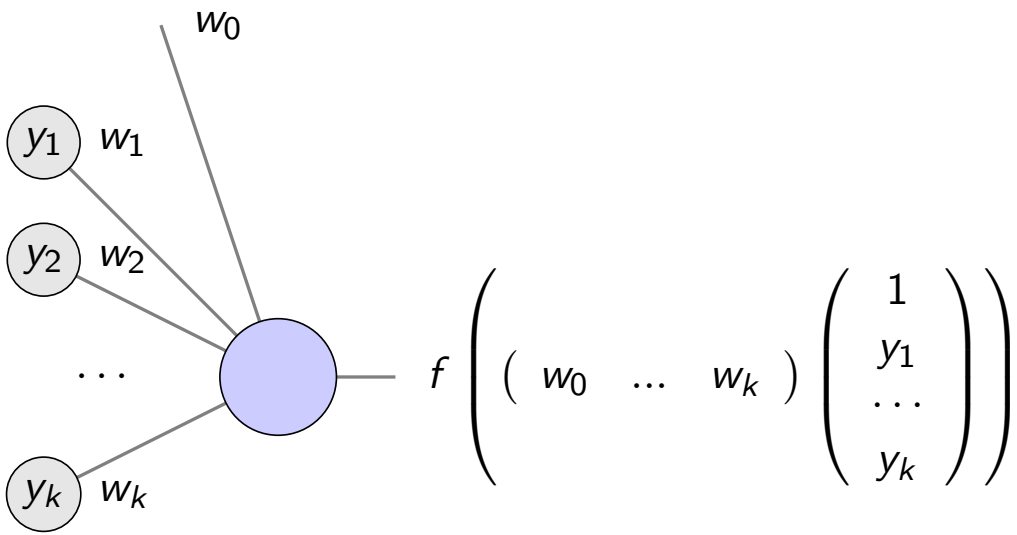
- First, present one or more training examples to the neural network: Feed-Forward.
- Second, compare the output of the neural network to the desired value: Loss function.
- Finally, adjust the weights to make the output get closer to the desired value using gradient descent: Back propagation.

# Feed-Forward

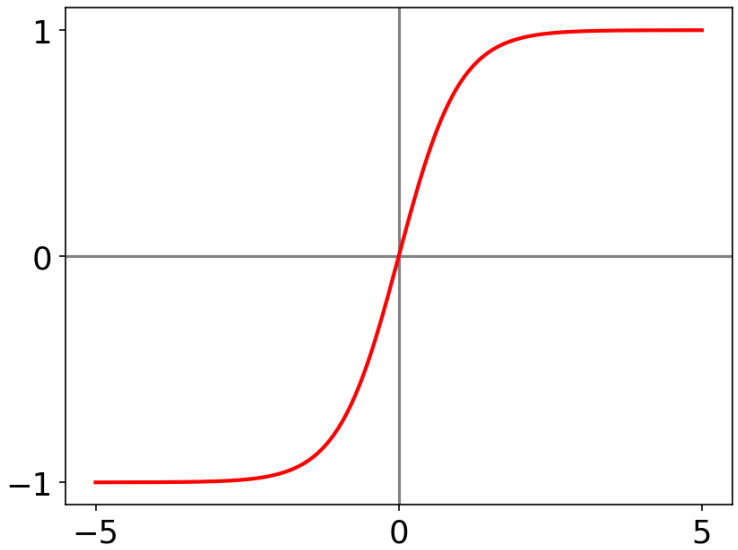



The previous layer has $k$ neurons, the activation function is $f$.

# Other Activation Functions

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

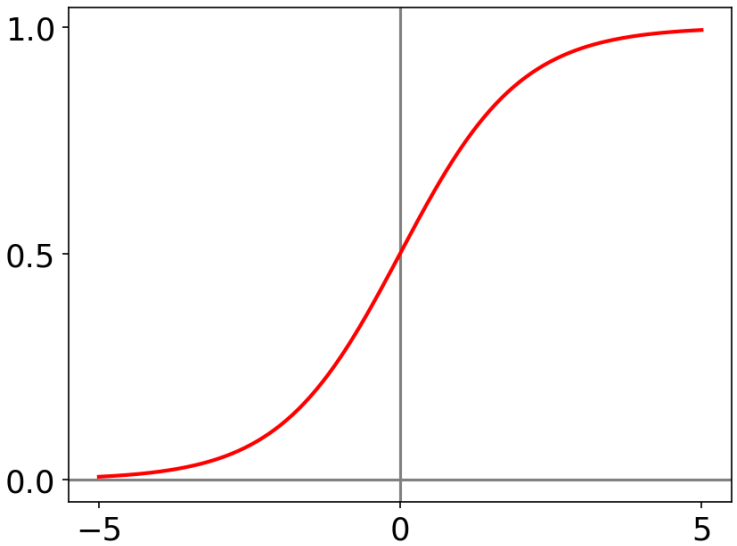
$$\tanh'(x) = 1 - \tanh^2(x)$$




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

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



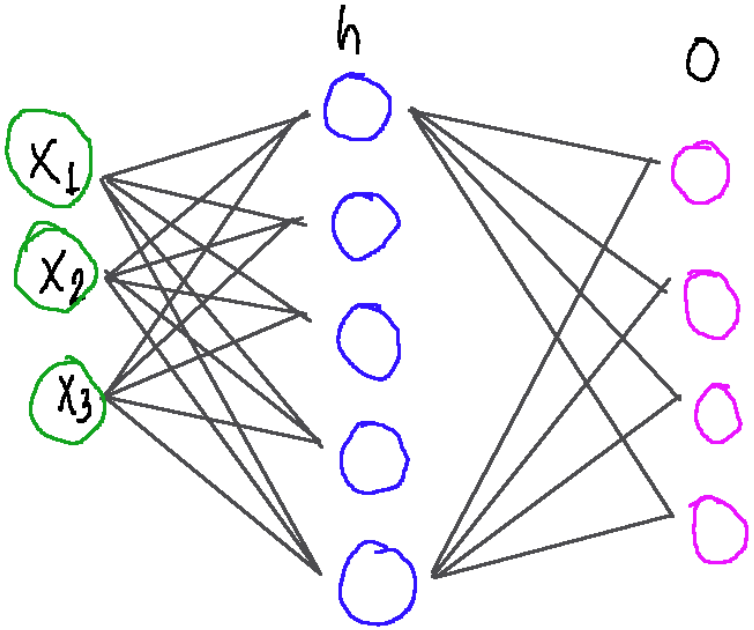

It is used when we need the output to be in $(0, 1)$. For example, in binary classification.

# 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




$$X = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & x_3^{(1)} \\ & \cdots & & \\ 1 & x_1^{(N)} & x_2^{(N)} & x_3^{(N)} \end{pmatrix}$$

$$h = \Phi_1\left(X \cdot W_1^T\right)$$

$$o = \Phi_2\left(\bar{h} \cdot W_2^T\right)$$

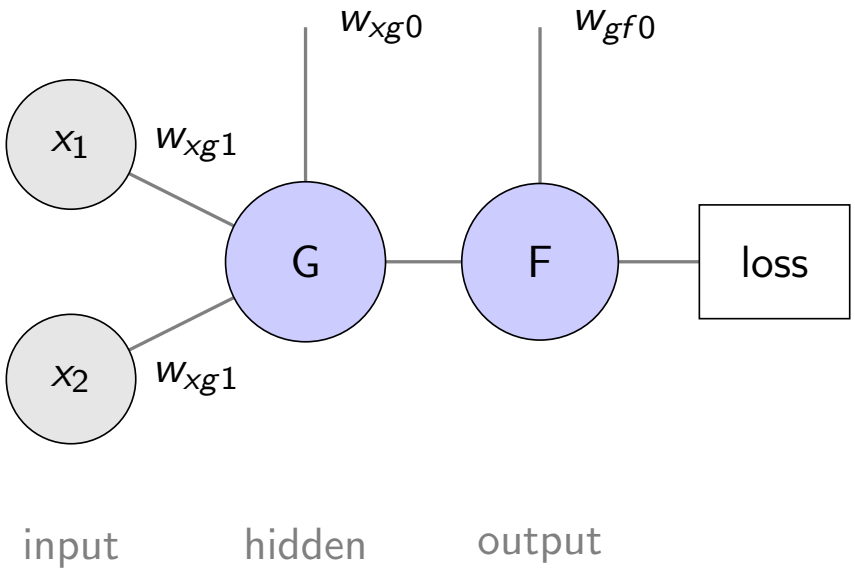
$W_1 \in M_{5\times 4}$ $\quad W_2 \in M_{4\times 6}$

$X \in M_{N\times 4}$

$h \in M_{N\times 5}$

$\bar{h} \in M_{N\times 6}$

# Example: Back-propagation




This neural network implements

$$\hat{y} = S\left(w_{gf0} + w_{gf1}\tanh(w_{xg0} + w_{xg1}x_1 + w_{xg2}x_2)\right)$$

We use the MSE loss:

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

# Example: Back-propagation

- The error is given by

$$\text{Error} = \frac{1}{2}\left(y - S\left(w_{gf0} + w_{gf1}\tanh(w_{xg0} + w_{xg1}x_1 + w_{xg2}x_2)\right)\right)^2$$

- We write it as:

$$\begin{aligned} e(f) &= \frac{1}{2}(y - f)^2 \\ f(z_f) &= S(z_f) \\ z_f(w_{gf0}, w_{gf1}, g) &= w_{gf0} + w_{gf1}g \\ g(z_g) &= \tanh(z_g) \\ z_g(w_{xg0}, w_{xg1}, w_{xg2}) &= w_{xg0} + w_{xg1}x_1 + w_{xg2}x_2 \end{aligned}$$

# Example: Back-propagation

Compute the partial derivatives

$$\frac{\partial}{\partial w_{gf0}} e = -(y - f) S'(z_f)$$

$$\frac{\partial}{\partial w_{gf1}} e = -(y - f) S'(z_f) g$$

$$\frac{\partial}{\partial w_{xg0}} e = -(y - f) S'(z_f) w_{gf1} \tanh'(z_g)$$

$$\frac{\partial}{\partial w_{xg1}} e = -(y - f) S'(z_f) w_{gf1} \tanh'(z_g) x_1$$

$$\frac{\partial}{\partial w_{xg2}} e = -(y - f) S'(z_f) w_{gf1} \tanh'(z_g) x_2$$

# Example: Back-propagation

Finally, we update the weights, via gradient descent

$$w_{gf0} \leftarrow w_{gf0} - \eta \frac{\partial e}{\partial w_{gf0}}$$

$$w_{gf1} \leftarrow w_{gf1} - \eta \frac{\partial e}{\partial w_{gf1}}$$

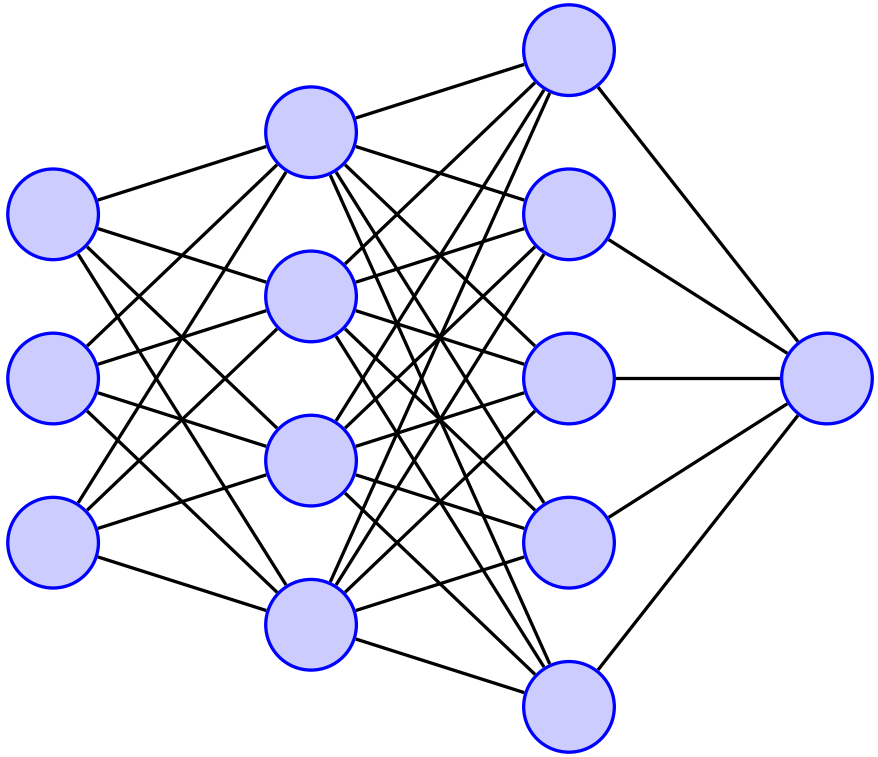
$$w_{xg0} \leftarrow w_{xg0} - \eta \frac{\partial e}{\partial w_{xg0}}$$

$$w_{xg1} \leftarrow w_{xg1} - \eta \frac{\partial e}{\partial w_{xg1}}$$

$$w_{xg2} \leftarrow w_{xg2} - \eta \frac{\partial e}{\partial w_{xg2}}$$

# Regression

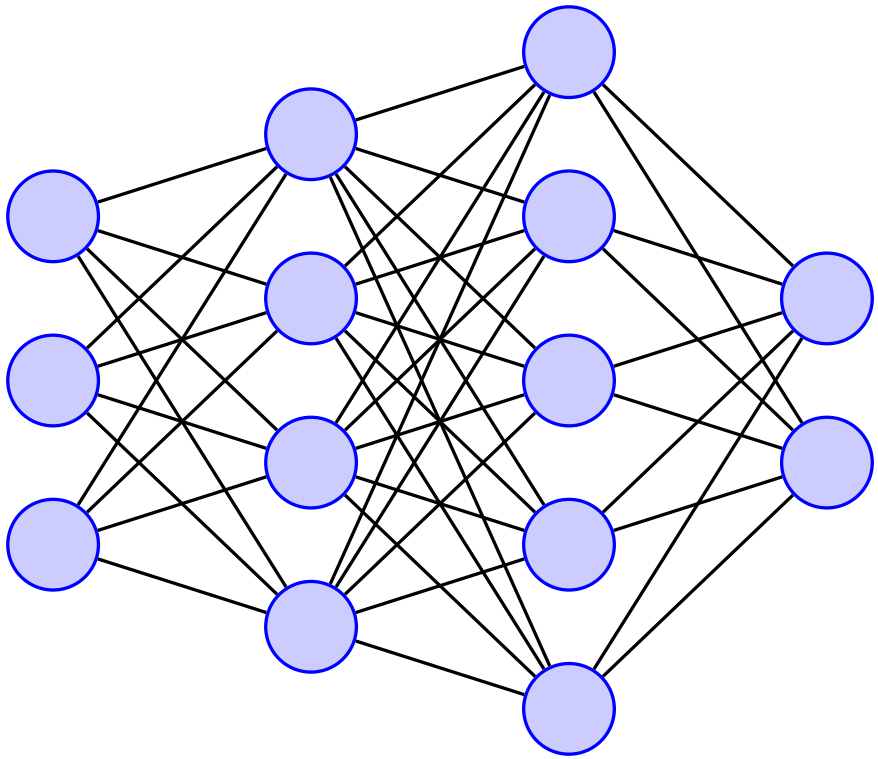
If we have three independent variables and one dependent variables



The activation in the output layer is *usually* `None` (the identity).

# Multivariate Regression

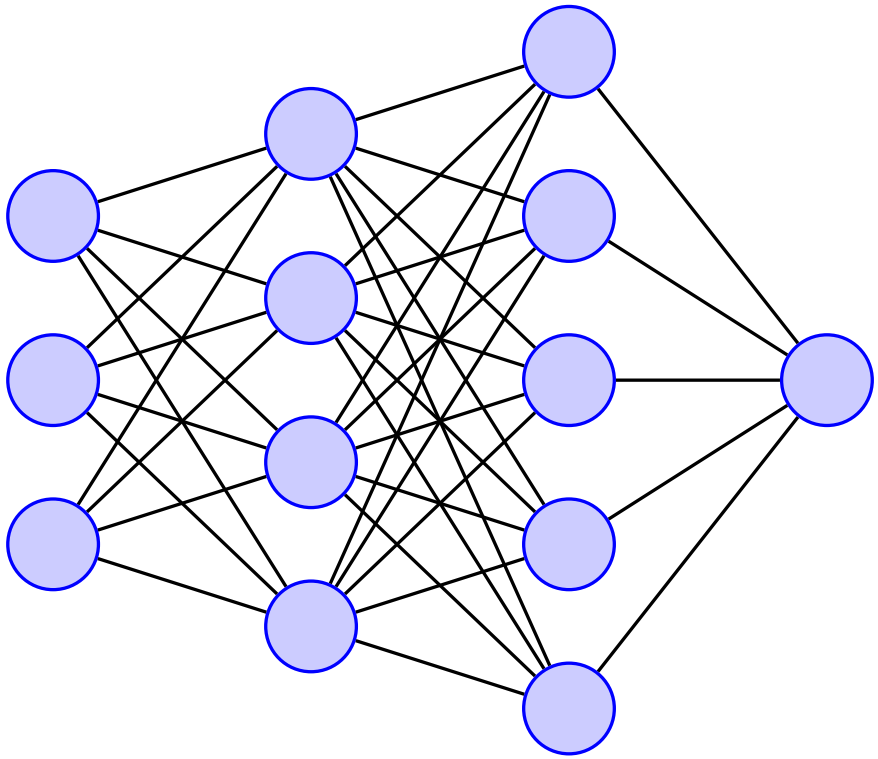
If we have three independent variables and two dependent variable



The activation in the output layer is *usually* `None` (the identity).

# Binary Classification

If we have three independent variables and two classes

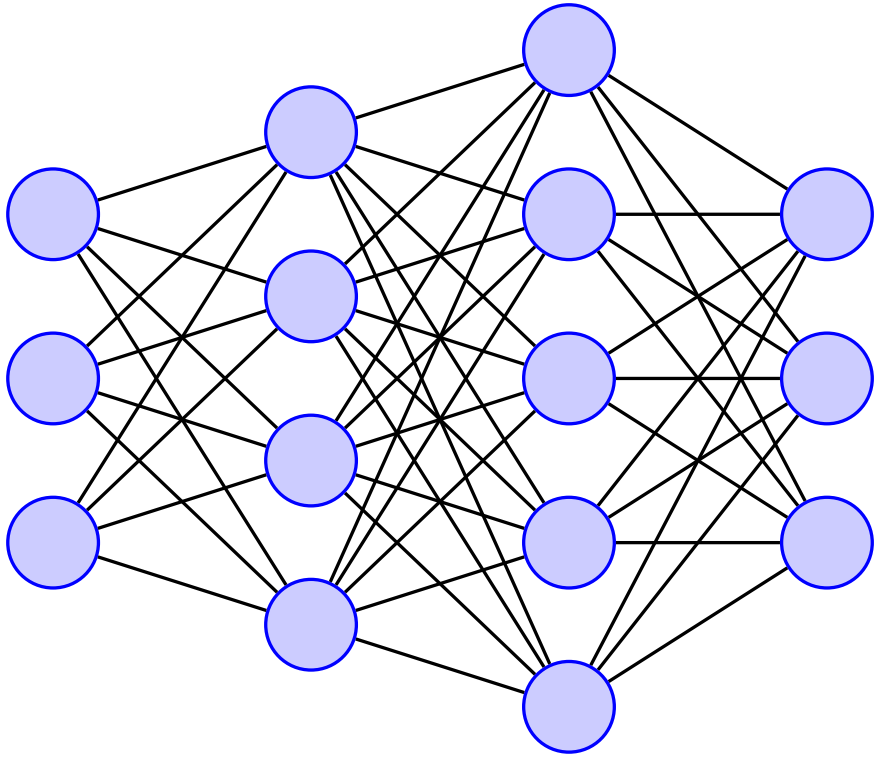


The activation function in the output layer is the sigmoid

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

# Multi-class Classification

If we have three classes



The activation function in the output layer is softmax

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

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# Deep Learning Libraries


**Tensorflow**


**Pytorch**

# Deep Learning Libraries

| | **Keras** | **Tensorflow** | **Pytorch** |
|---|---|---|---|
| API Level | High | High and low | Low |
| Architecture | Simple, readable | 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 performance | Fast, high-performance | Fast, high-performance |