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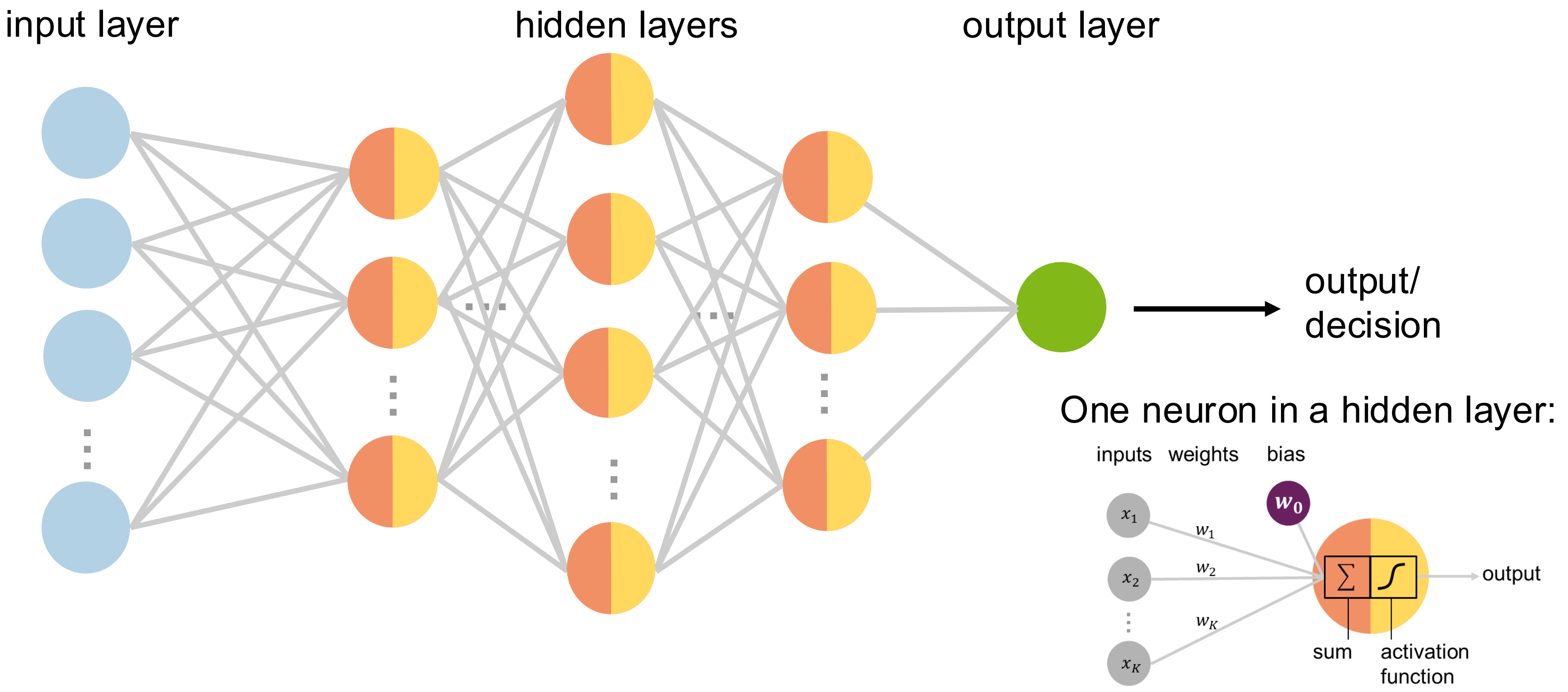
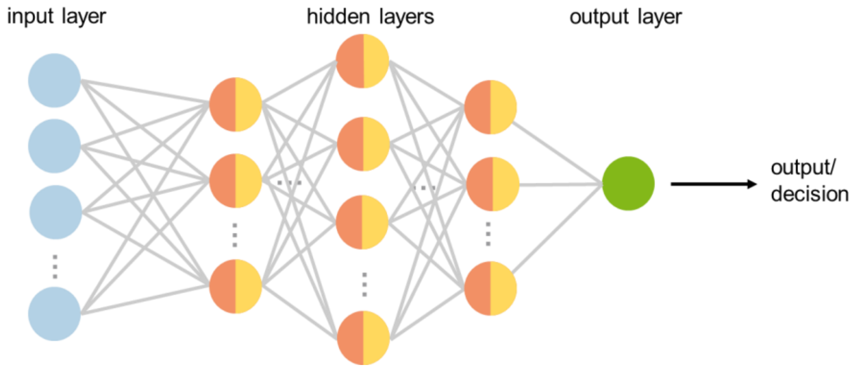
Feed-forward neural networks

A Neural Network has an Input Layer, one or several Hidden Layers and an Output Layer



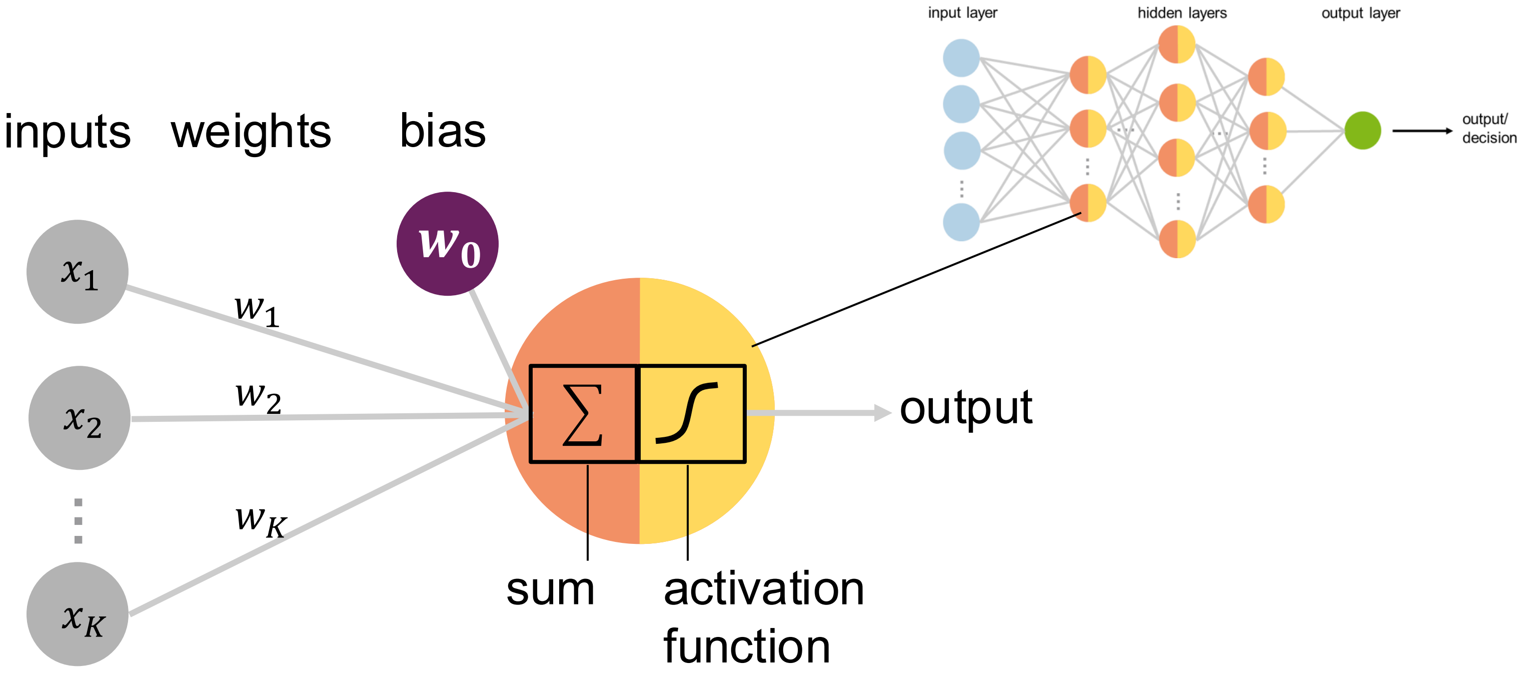
Feedforward Neural Network



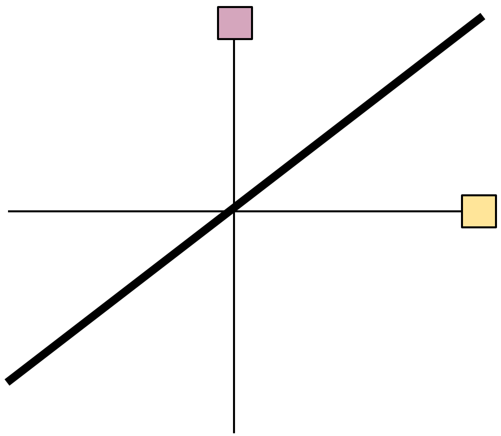
- The information moves in only **one direction:** forward from the input nodes, through the hidden nodes (if any) to the output nodes.
- Each neuron in one layer has directed connections to the neurons of the subsequent layer
- **No connections** between nodes within the **same layer**
- There are no cycles or loops in the network
- Vanilla Neural Network Structure: Subsequent layers are **fully connected**
- **Trainable Parameters:** Weights connecting the nodes and biases

A neuron

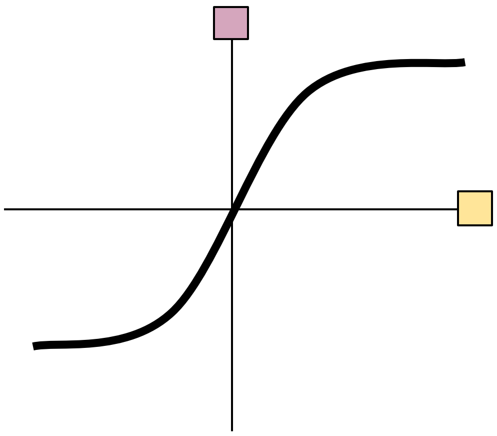
… applies an activation function to the weighted sum of its inputs



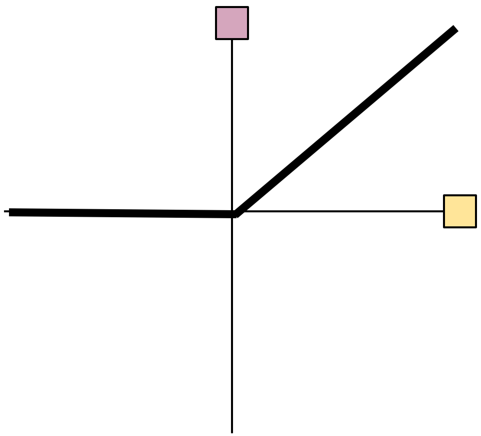
Activation functions



LINEAR
like linear regression
(only used in output
layer)

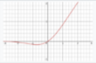
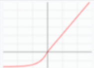
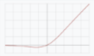
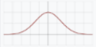


LOGISTIC /
SIGMOIDAL / TANH
Smooth, differentiable,
saturating functions



RECTIFIED
LINEAR (ReLU)
Cheap to
compute, popular
lately

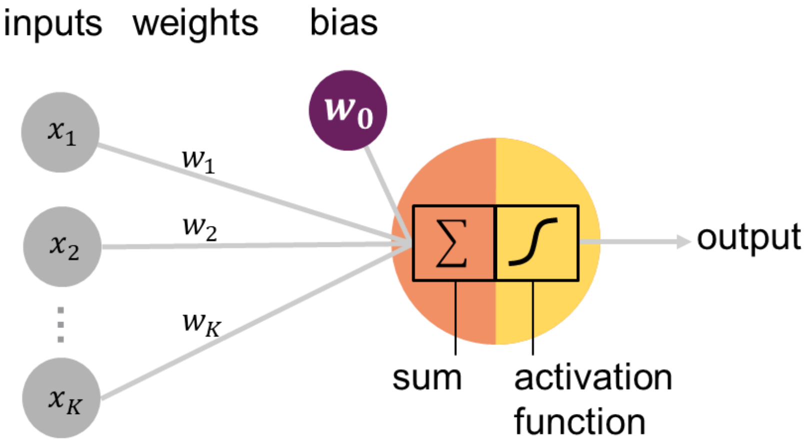
Activation functions

Name	Plot	Function, $g(x)$	Derivative of g, $g'(x)$	Range	Order of continuity
Identity		x	1	$(-\infty, \infty)$	C^∞
Binary step		$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$\begin{cases} 0 & \text{if } x \neq 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$\{0, 1\}$	C^{-1}
Logistic, sigmoid, or soft step		$\sigma(x) \doteq \frac{1}{1+e^{-x}}$	$g(x)(1-g(x))$	$(0, 1)$	C^∞
Hyperbolic tangent (tanh)		$\tanh(x) \doteq \frac{e^x - e^{-x}}{e^x + e^{-x}}$	$1 - g(x)^2$	$(-1, 1)$	C^∞
Rectified linear unit (ReLU)[8]		$(x)^+ \doteq \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases} = \max(0, x) = x\mathbf{1}_{x>0}$	$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$[0, \infty)$	C^0
Gaussian Error Linear Unit (GELU)[5]		$\frac{1}{2}x\left(1 + \text{erf}\left(\frac{x}{\sqrt{2}}\right)\right) = x\Phi(x)$	$\Phi(x) + x\phi(x)$	$(-0.17\ldots, \infty)$	C^∞
Softplus[9]		$\ln(1 + e^x)$	$\frac{1}{1+e^{-x}}$	$(0, \infty)$	C^∞
Exponential linear unit (ELU)[10]		$\begin{cases} \alpha(e^x - 1) & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$ with parameter α	$\begin{cases} \alpha e^x & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ 1 & \text{if } x = 0 \text{ and } \alpha = 1 \end{cases}$	$(-\alpha, \infty)$	$\begin{cases} C^1 & \text{if } \alpha = 1 \\ C^0 & \text{otherwise} \end{cases}$
Scaled exponential linear unit (SELU)[11]		$\lambda\begin{cases} \alpha(e^x - 1) & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$ with parameters $\lambda = 1.0507$ and $\alpha = 1.67326$	$\lambda\begin{cases} \alpha e^x & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$(-\lambda\alpha, \infty)$	C^0
Leaky rectified linear unit (Leaky ReLU)[12]		$\begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	$\begin{cases} 0.01 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$(-\infty, \infty)$	C^0
Parametric rectified linear unit (PReLU)[13]		$\begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$ with parameter α	$\begin{cases} \alpha & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$(-\infty, \infty)$	C^0
Sigmoid linear unit (SiLU,[5] Sigmoid shrinkage,[14] SiL,[15] or Swish-1[16])		$\frac{x}{1+e^{-x}}$	$\frac{1 + e^{-x} + xe^{-x}}{(1+e^{-x})^2}$	$[-0.278\ldots, \infty)$	C^∞
Gaussian		e^{-x^2}	$-2xe^{-x^2}$	$(0, 1]$	C^∞

Source: https://en.wikipedia.org/wiki/Activation_function

Neuron with ReLu activation

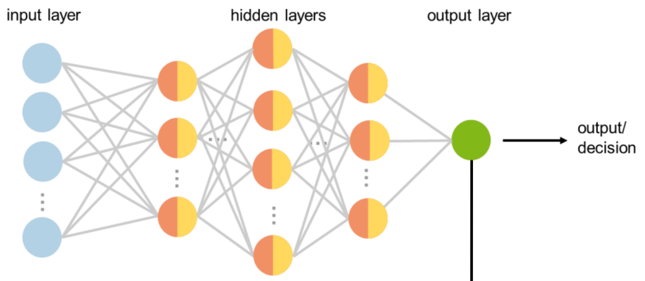
… applies an activation function to the weighted sum of its inputs



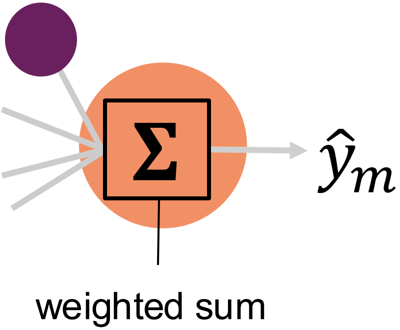
sum: $z = w_0 + w_1 x_1 + w_2 x_2 + \ \dots + w_K x_K$

output: $o = \text{act(z)} = \begin{cases} z & \text{if } z \geq 0 \\ 0 & \text{otherwise} \end{cases}$

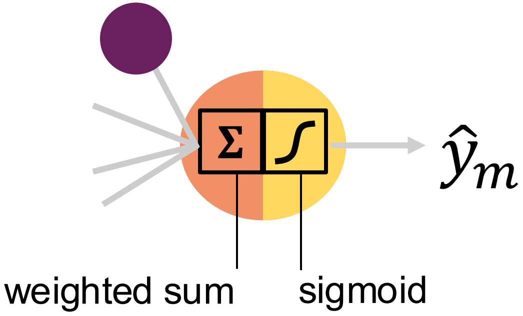
The Output Layer



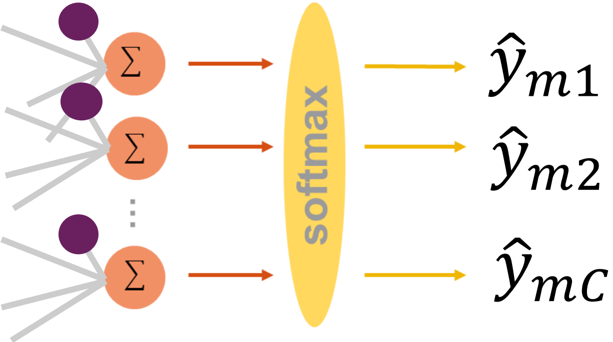
Regression: Linear Function



Binary Classification: Sigmoid



Multinomial Classification: Softmax



The output layer

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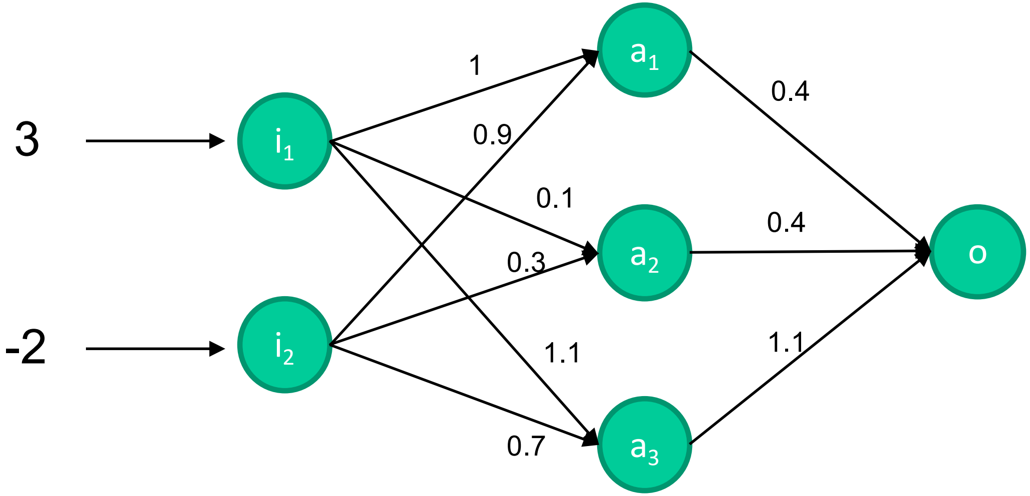
Regression tasks:
- output is a single node, the predicted value

Classification with two classes:
- output: a single value between 0..1
- decision boundary e.g. at 0.5

Classification with many classes:
- number of output values = number of classes
- sum over all output values = 1
- each output value between 0..1
- decision: largest output value is predicted class

Example



ReLU Activation function for all hidden nodes:

$$\mathrm{act}(z_{a_i}) = \mathrm{ReLu}(z_{a_i}) = \begin{cases} z_{a_i} & \text{if } z_{a_i} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

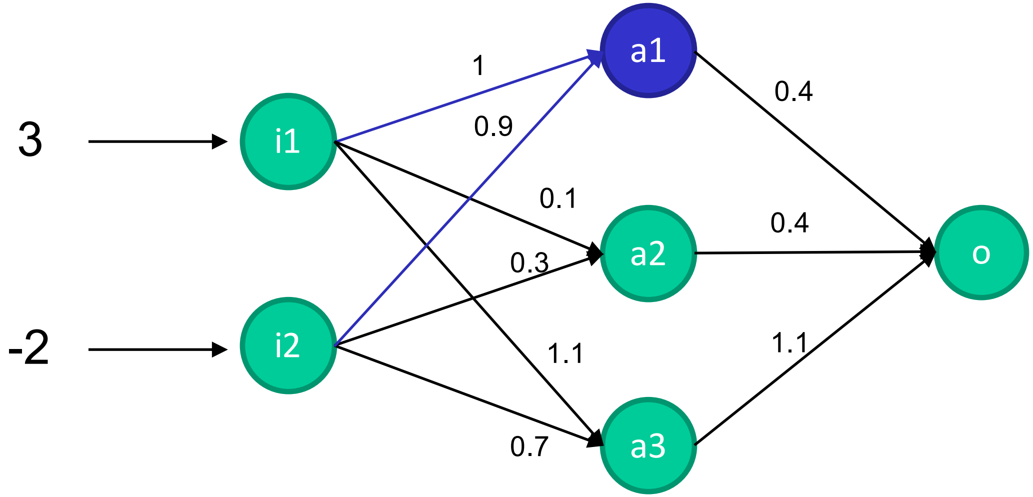
Sigmoid for output node

$$\mathrm{act}(z_o) = \sigma(z_o) = \frac{1}{1 + e^{-(z_o)}}$$

The bias (w_0) is not explicitly depicted. It is the same for all nodes:

$$\mathrm{w}_{\mathrm{a}_1,0} = \mathrm{w}_{\mathrm{a}_2,0} = \mathrm{w}_{\mathrm{a}_3,0} = w_{\mathrm{o},0} = 0.2$$

Example

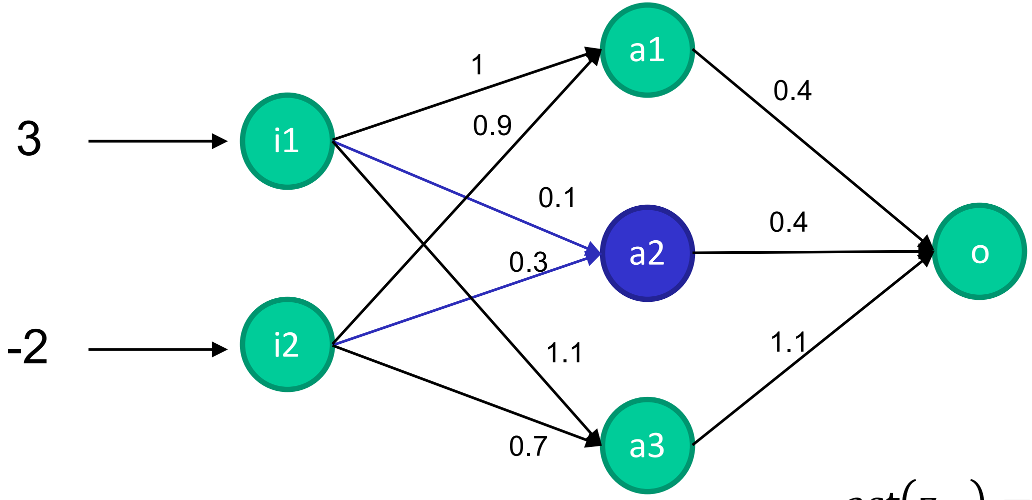


$$\mathrm{act}(z_{a_i}) = \mathrm{ReLu}(z_{a_i}) = \begin{cases} z_{a_i} & \text{if } z_{a_i} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The bias (w_0) for all nodes is the same: $\mathrm{w}_{a_1,0} = \mathrm{w}_{a_2,0} = \mathrm{w}_{a_3,0} = w_{o,0} = 0.2$

$$z_{a_1} = i_1 \cdot 1 + i_2 \cdot 0.9 + \mathrm{w}_{a1,0} = 3 \cdot 1 - 2 \cdot 0.9 + 0.2 = 1.4$$
$$a_1 = \mathrm{act}(z_{a_1}) = \mathrm{ReLu}(1.4) = 1.4$$

Example



$$\text{act}(z_{a_i}) = \text{ReLu}(z_{a_i}) \begin{cases} z_{a_i} & \text{if } z_{a_i} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The bias (w_0) for all nodes is the same: $\mathrm{w}_{a_1,0} = \mathrm{w}_{a_2,0} = \mathrm{w}_{a_3,0} = w_{o,0} = 0.2$

$$z_{a_2} = i_1 \cdot 0.1 + i_2 \cdot 0.3 + w_{a2,0} = 3 \cdot 0.1 - 2 \cdot 0.3 + 0.2 = -0.1$$

$$a_2 = \text{act}(z_{a_2}) = \text{ReLu}(-0.1) = 0$$

Example

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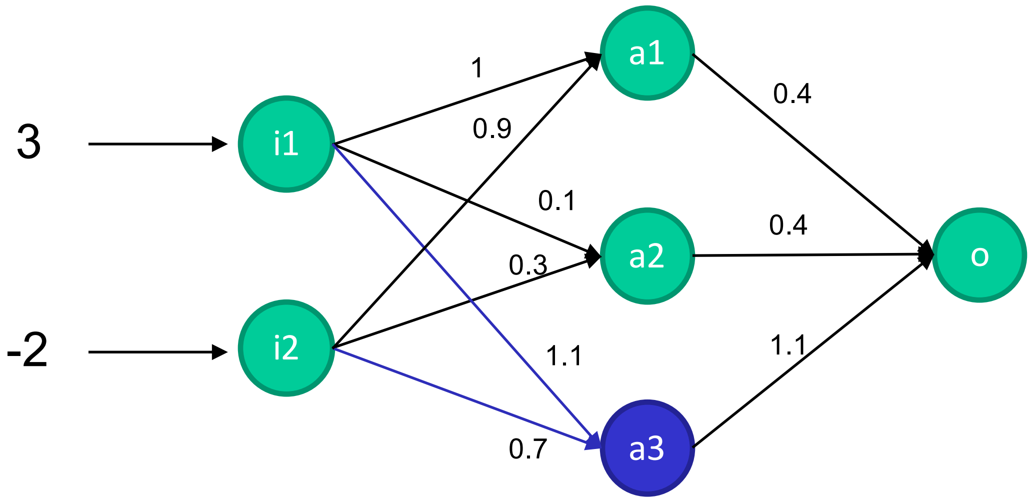


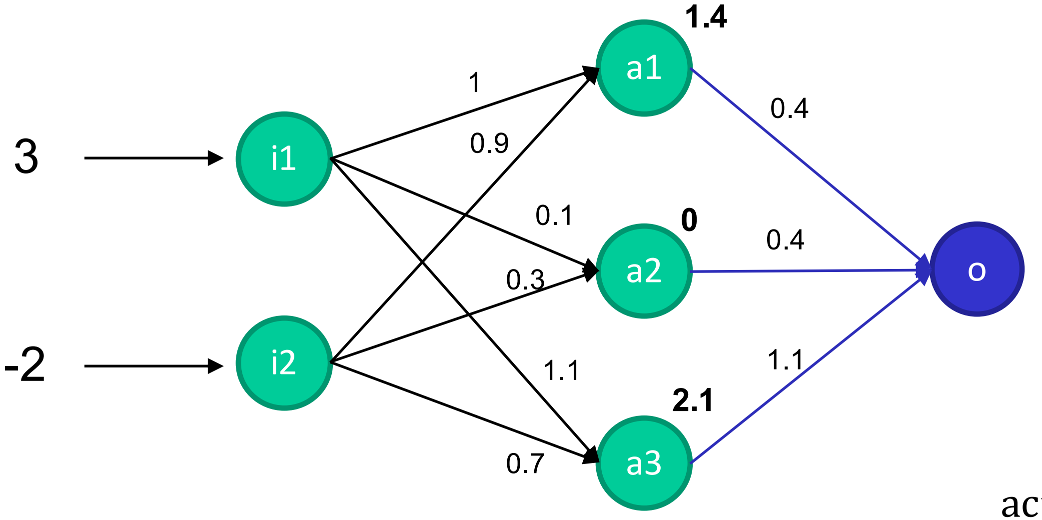
$$\mathrm{act}(z_{a_i}) = \mathrm{ReLu}(z_{a_i}) = \begin{cases} z_{a_i} & \text{if } z_{a_i} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The bias (w_0) for all nodes is the same: $\mathrm{w}_{\mathrm{a}_1,0} = \mathrm{w}_{\mathrm{a}_2,0} = \mathrm{w}_{\mathrm{a}_3,0} = w_{\mathrm{o},0} = 0.2$

$$z_{a_3} = i_1 \cdot 1.1 + i_2 \cdot 0.7 + w_{\mathrm{a}3,0} = 3 \cdot 1.1 - 2 \cdot 0.7 + 0.2 = 2.1$$

$$a_3 = \mathrm{act}(z_{a_3}) = \mathrm{ReLu}(2.1) = 2.1$$

Example



$$\mathrm{act}(z_o) = \sigma(z_o) = \frac{1}{1 + e^{-(z_o)}}$$

The bias (w_0) for all nodes is the same: $\mathrm{w}_{\mathrm{a}_1,0} = \mathrm{w}_{\mathrm{a}_2,0} = \mathrm{w}_{\mathrm{a}_3,0} = w_{\mathrm{o},0} = 0.2$

$$z_o = a_1 \cdot 0.4 + a_2 \cdot 0.4 + a_3 \cdot 2.1 + w_{\mathrm{o},0} = 1.4 \cdot 0.4 + 0 \cdot 0.4 + 2.1 \cdot 1.1 + 0.2 = 3.07$$

$$\hat{y} = \mathrm{act}(z_o) = \frac{1}{1 + e^{-(z_o)}} = 0.96$$

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Training Neural Networks

The cost function for neural networs

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Regression: Average sum of squared residuals

$$J(\boldsymbol{W}) = \frac{1}{2M}\sum_{m=1}^{M}(y_m - \hat{y}_m)^2$$

Classification: Average Cross Entropy

- Binary (logistic):

$$\mathrm{J}(\boldsymbol{W}) = -\frac{1}{M}\sum_{m=1}^{M} y_m \log \hat{y}_m + (1 - y_m)\log(1 - \hat{y}_m)$$

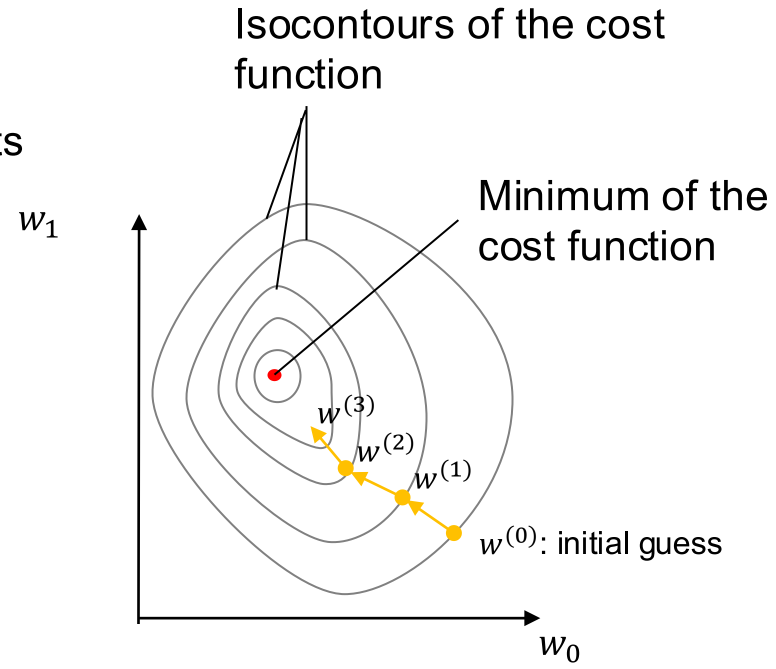
- Multinomial, i.e. multiclass (softmax):

$$\mathrm{J}(\boldsymbol{W}) = -\frac{1}{M}\sum_{m=1}^{M} y_{mk} \log \hat{y}_{mk} \text{ (where } k \text{ is the correct class index for sample } m\text{)}$$

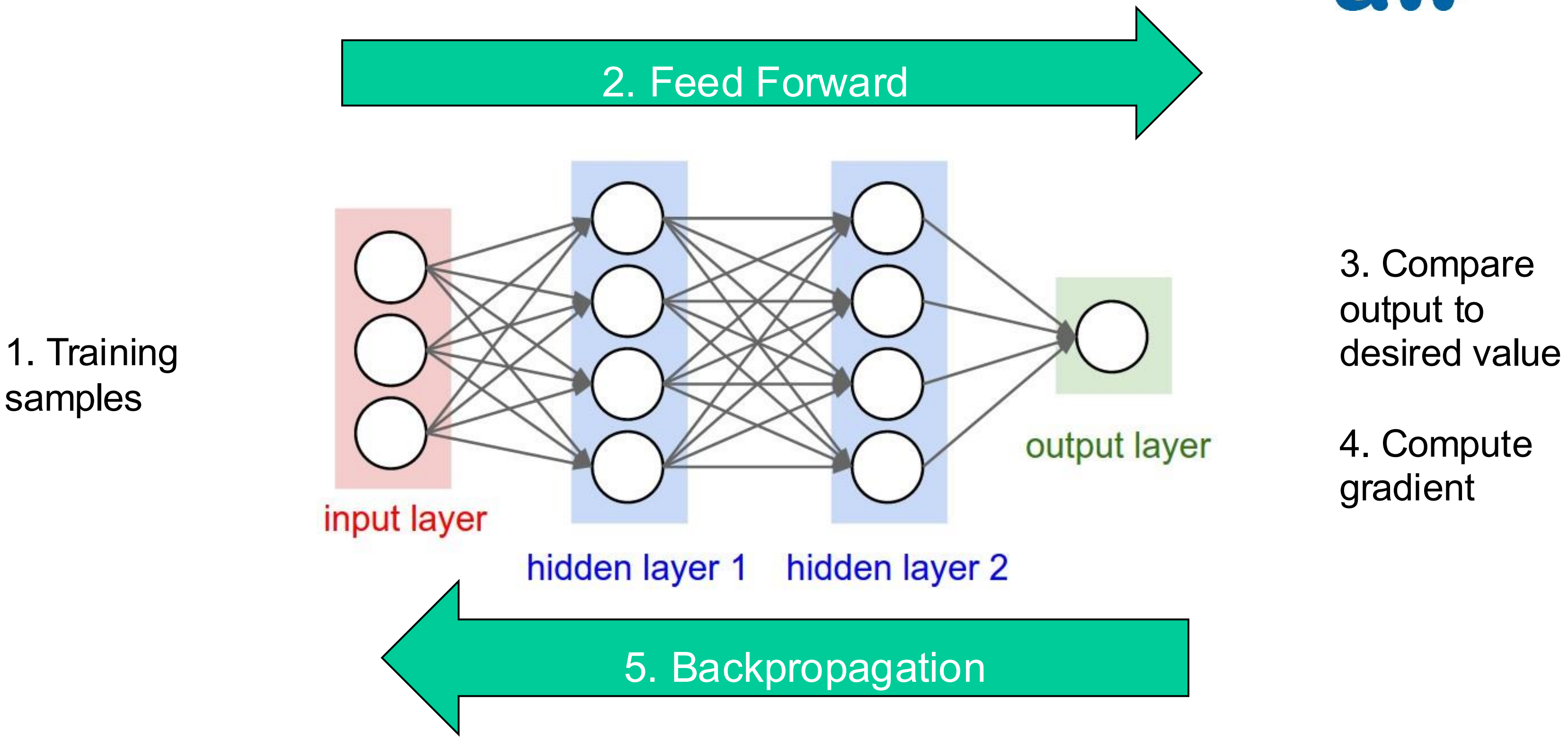
Minimisation by gradient descent

- Initial guess for the model parameters: the weights
- Repeat until stopping criterium is reached:
    1. compute **gradient** of the cost function with respect to parameters
    2. **adjust the parameters** in the opposite direction of the gradient by a small step, i.e. the **learning rate** α

$$w_{kl} \leftarrow w_{kl} - \alpha \frac{\partial J(\boldsymbol{W})}{\partial w_{kl}}$$

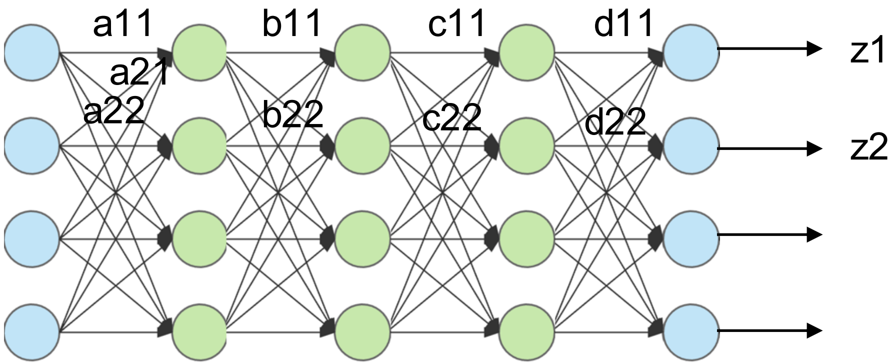


Backpropagation: efficient computation of the partial derivatives in gradient descent



https://www.pyimagesearch.com/wp-content/uploads/2016/08/simple_neural_network_header.jpg

Re-use of Partial Derivative Chains



$$\frac{\partial z1}{\partial a11} = \frac{\partial z1}{\partial d11} \frac{\partial d11}{\partial c11} \frac{\partial c11}{\partial b11} \frac{\partial b11}{\partial a11} + \dots$$

$$\frac{\partial z1}{\partial a21} = \dots + \frac{\partial z1}{\partial d11} \frac{\partial d11}{\partial c11} \frac{\partial c11}{\partial b11} \frac{\partial b11}{\partial a21} \dots$$

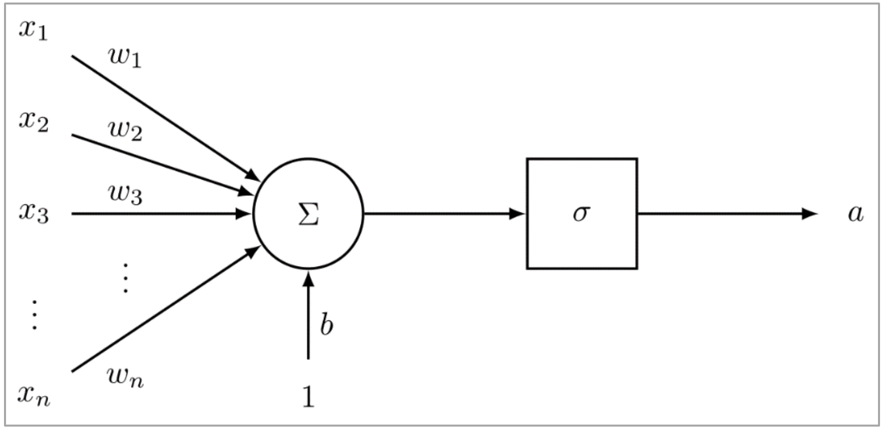
$$\frac{\partial z2}{\partial a11} = \dots + \frac{\partial z22}{\partial d12} \frac{\partial d12}{\partial c11} \frac{\partial c11}{\partial b11} \frac{\partial b11}{\partial a11} \dots$$

In each path for the partial derivatives, we can re-use sub-paths from previous calculations. This makes backpropagation efficient.

History:

- First described by Werbos 1974
- Re-discovered by Parker 1982 and **Rumelhart et al. 1986**

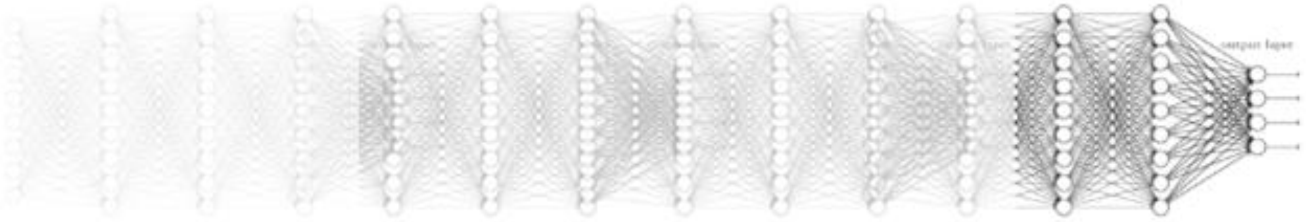
Key factor: Differentiability



If all components in a neural network are differentiable, we can efficiently compute the gradient of the cost function with respect to the weights and optimise using gradient descent

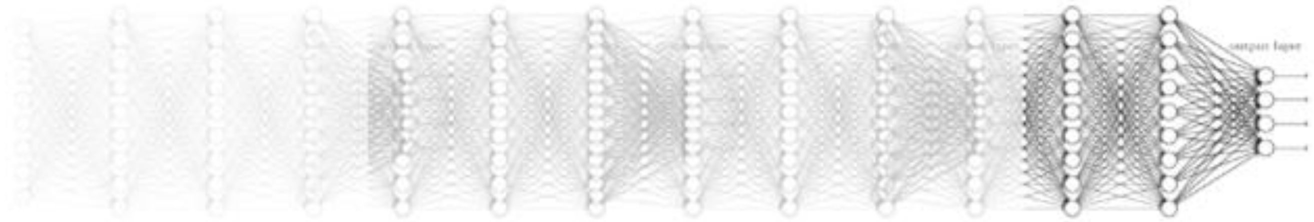
Disadvantages of Backpropagation

- Requires large amount of labelled training data
- Learning time is slow for multiple hidden layers
- Can get stuck in local optima (although not a big problem in high dimensions)
- **Vanishing Gradient Problem**



Vanishing Gradient Problem
Sepp Hochreiter 1991

- **Observation:** if we have many hidden layers, and if all partial derivatives are between -1 and 1 (sigmoid function), then multiplying them makes them exponentially small
- Thus, changes in the first layers will diminish since the gradient becomes extremely small
- Depths of a network can be easily up to 150 layers
- In practice, this results in very slowly changing weights, thus, very long training times
- Less of problem with ReLu (question: why?)
- Advanced network architectures avoid this problem



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Neural networks for non-linear problems

Non-linear decision boundaries with neural networks

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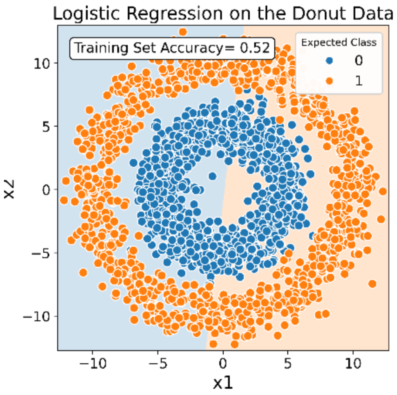
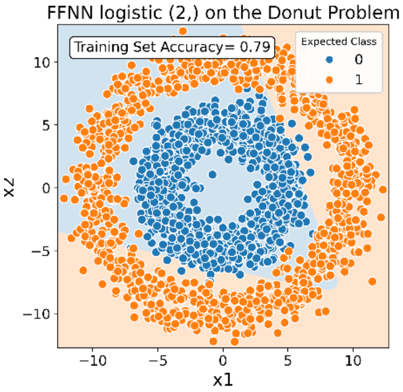
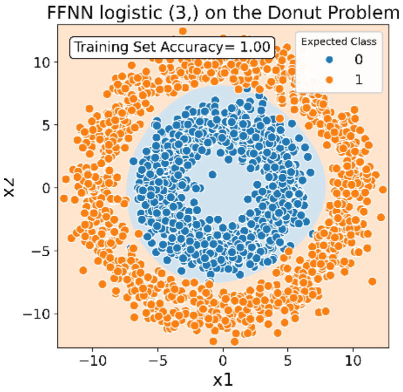
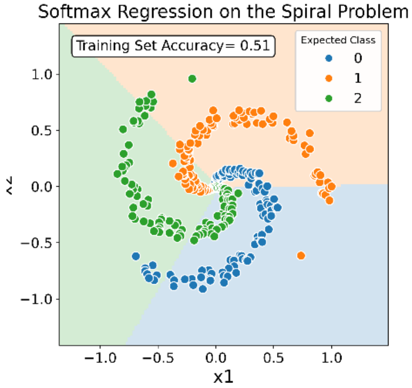
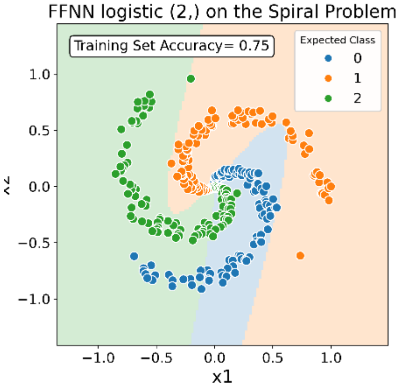
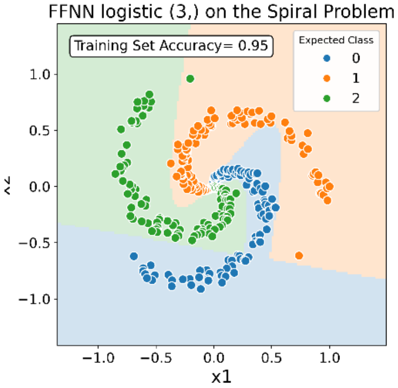






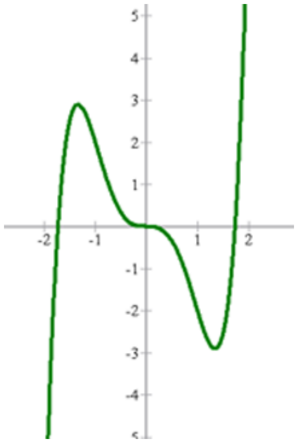


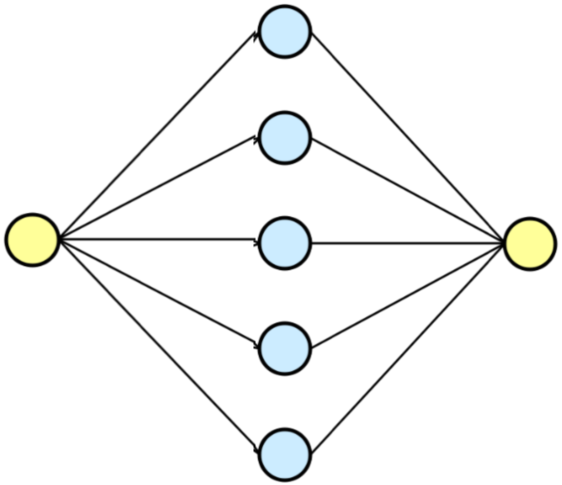




Universality Theorem
Hornik 1991

A neural net with one hidden layer and arbitrary number of neurons can approximate any given continuous function.





Proof Idea of Universality Theorem

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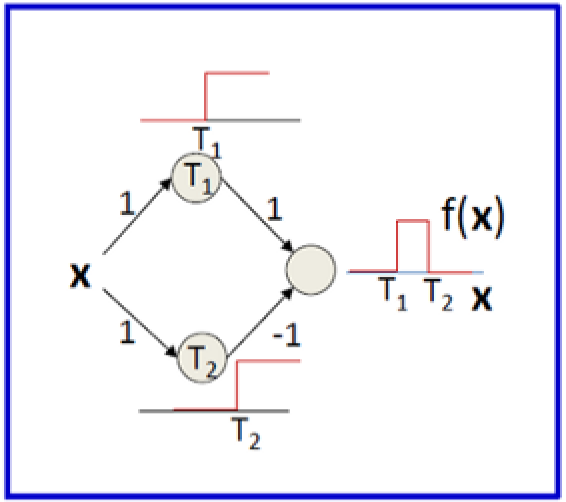
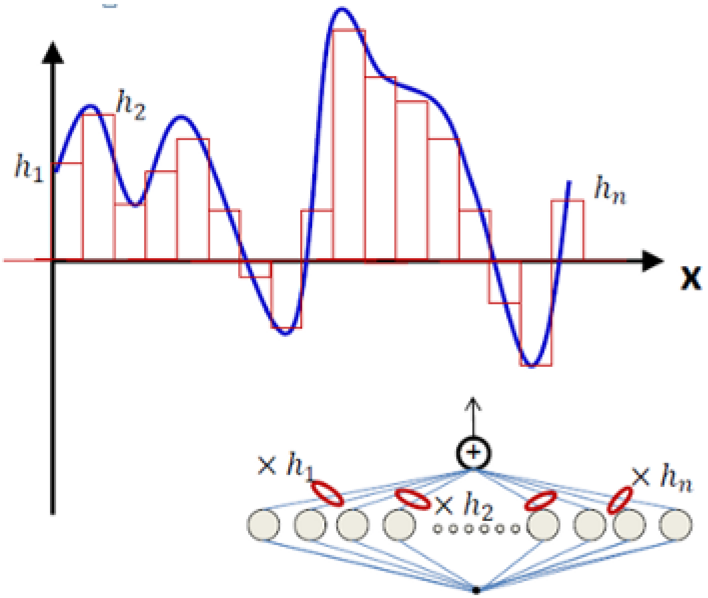
Idea: Cut a given function *f* in sufficient amount of small pieces, then use 2 neurons that model a partial linear function to approximate each of these pieces





https://medium.com/analytics-vidhya/neural-networks-and-the-universal-approximation-theorem