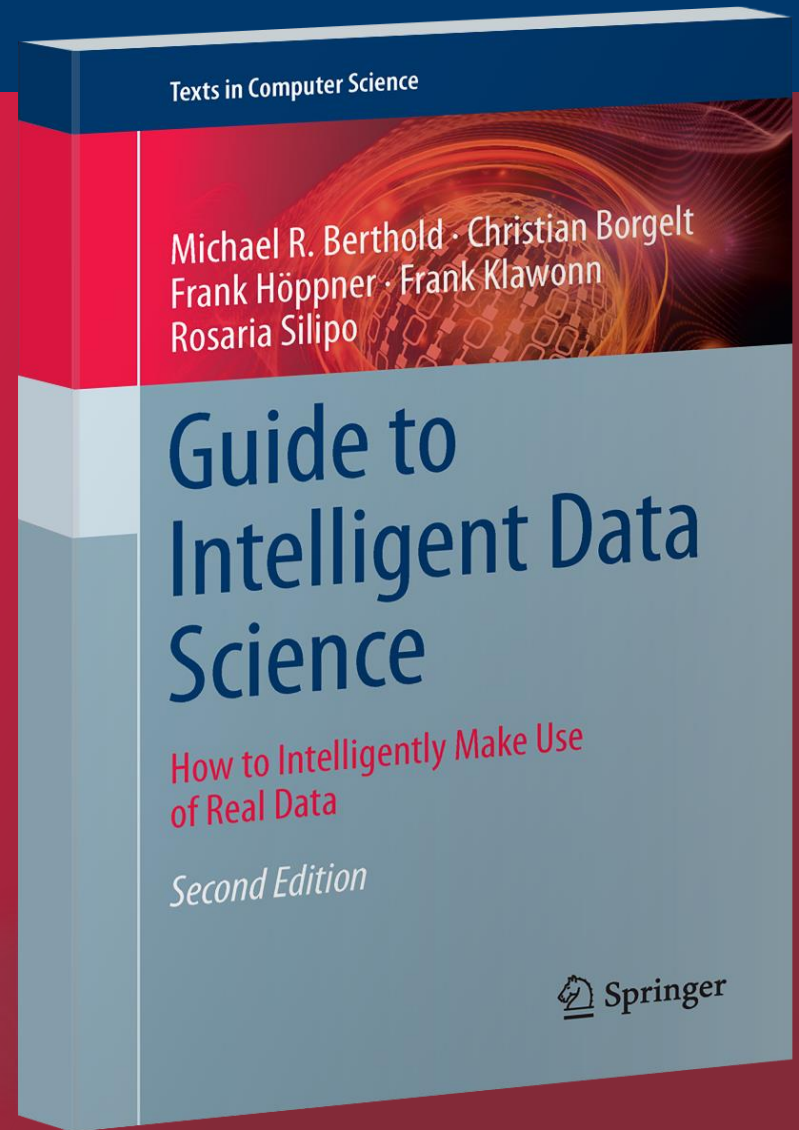


Neural Networks



*“Tell me and I forget. Teach me and I remember. Involve me and I learn.”
-Benjamin Franklin*

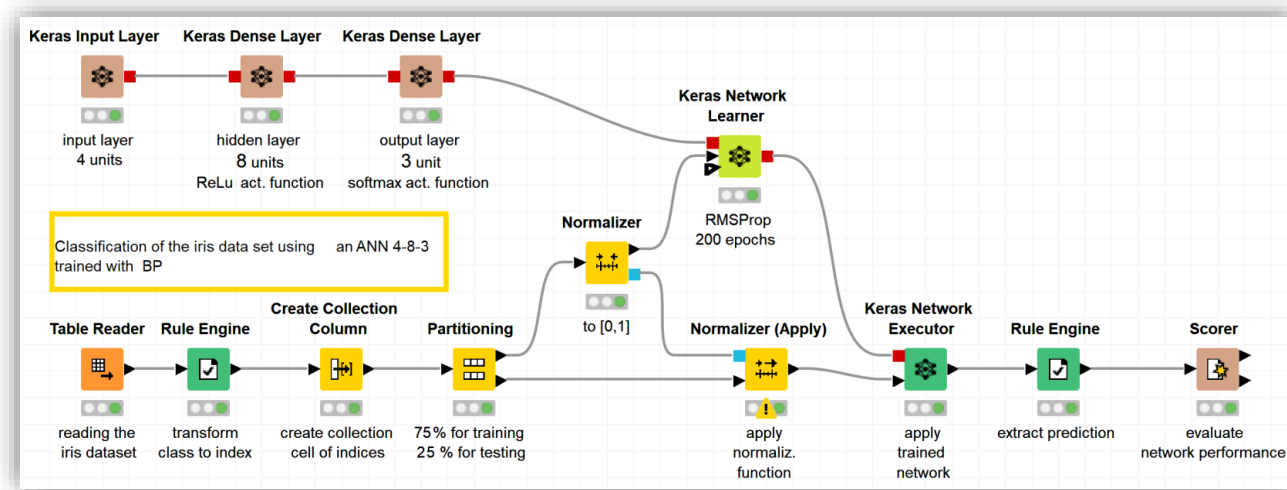
How do machines *learn*?

**This lesson refers to chapter 9 of the GIDS book*

- **Multilayer Perceptrons**
 - The Perceptron
 - Why the Perceptron is not enough
 - The MLP
- **The Back Propagation algorithm**
 - The delta rule to train the output neurons
 - Recursivity to train the hidden neurons
 - Learning rate and local minima
- **MLP and BackPropagation**
 - Pro's and Con's
 - Black-box tools
 - Overfitting
 - Techniques to avoid overfitting
 - Special architectures

Datasets

- Datasets used : iris dataset
- Example Workflows:
 - „Classifying the iris data set with ANN“ <https://kni.me/w/ei3eX9Sj5-RFEUat>
 - Keras layers
 - Multi-layer perceptron
 - Back propagation



Supervised Learning

- A target attribute is predicted based on other attributes
- Assumption: in addition to the object description \mathbf{x} , we have also the value for the target attribute \mathbf{y}

Transparent

- The decision process maps the application domain
- *How did we come to this final medical diagnosis?*

Black-box

- Abstract mathematical procedures not meaningful for the application domain
- *Recover most similar face in a million. How and why is not important.*

Biological Neuron

- Artificial Neural Networks (ANN) are among the oldest and most intensely studied Machine Learning approaches
- They took their inspiration from biological neural networks and tried to mimic the learning process of animals and humans
- However, the model of biological processes ended up to be very coarse, and several improvements to the basic approach have even abandoned the biological analogy

Advantage

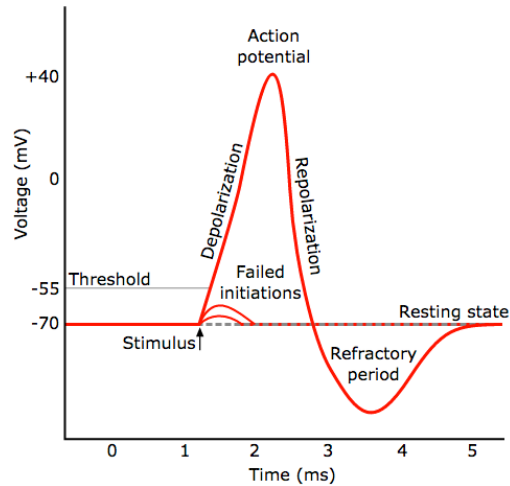
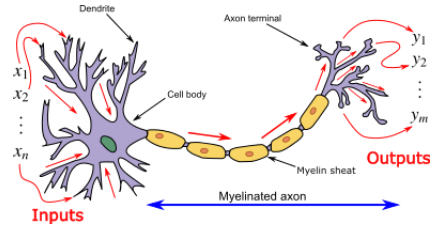
Highly flexible → good performance

Disadvantage

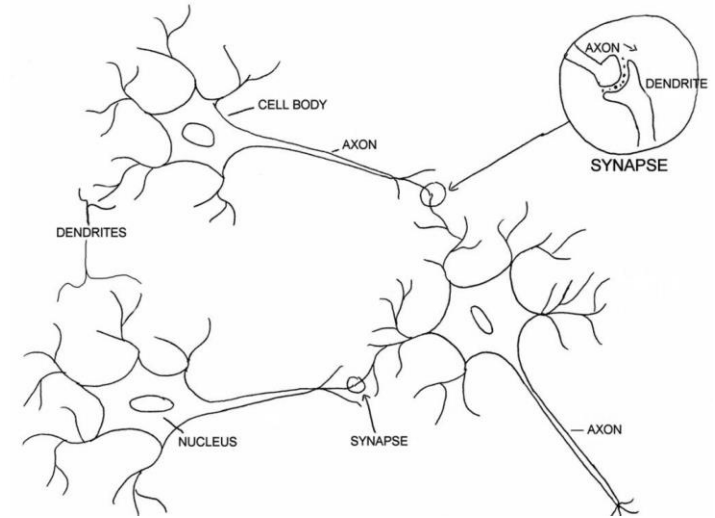
Black-box models not easy to interpret

- Human brain: ca. 10^{11} neurons.
- Each neuron connected to 10^4 other neurons on average.
- Switching time of a neuron 10^{-3} sec (computer: 10^{-10} sec ...)
- Neurons compute very basic functions
- Neuron assembly performs complex recognition tasks (faces!) in 10^{-1} sec!
- The human brain: gigantic assembly of highly connected simple processing units...

Biological Neuron



Biological Neural Networks



Perceptron

McCulloch-Pitts Model of a neuron (1943)

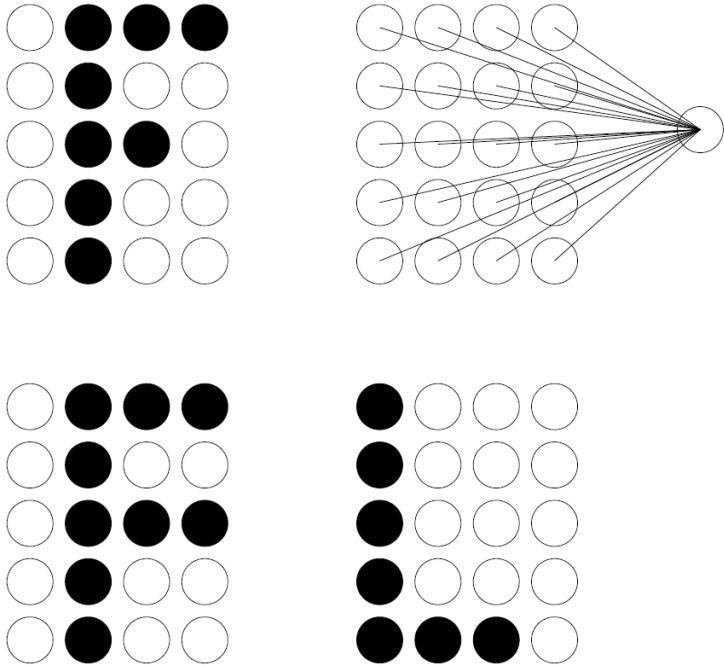
- **Aim:** neurobiological modelling and simulation to understand very elementary functions of neurons and brain.
- A neuron is a binary switch, being either active or inactive.
- Each neuron has a fixed threshold value.
- A neuron receives input signals from excitatory (positive) synapses (connections to other neuron).
- A neuron receives input signals from inhibitory (negative) synapses (connections to other neuron).
- Inputs to a neuron are accumulated (integrated) for a certain time. When the threshold value of the neuron is exceeded, the neuron becomes active and sends signals to its neighbouring neurons via its synapses.

The Perceptron (Rosenblatt, 1958)

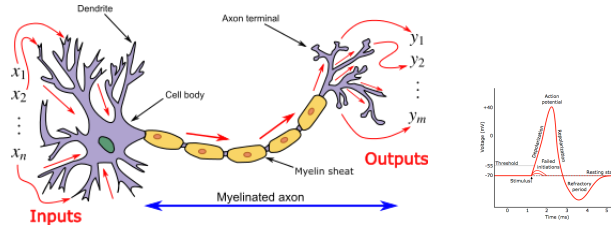
- The perceptron was introduced by Frank Rosenblatt for modelling pattern recognition abilities in 1958.
- **Aim:** Automatic learning of weights and threshold of a model of a retina to correctly classify objects.
- A simplified retina is equipped with receptors (input neurons) that are activated by an optical stimulus.
- The stimulus is passed on to an output neuron via a weighted connection (synapse).
- When the threshold of the output neuron is exceeded, the output is 1, otherwise 0.

Identifying the letter F

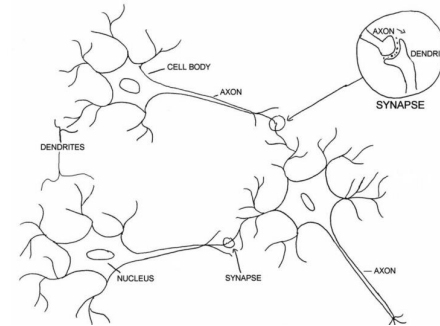
– 2 positive and 1 negative example



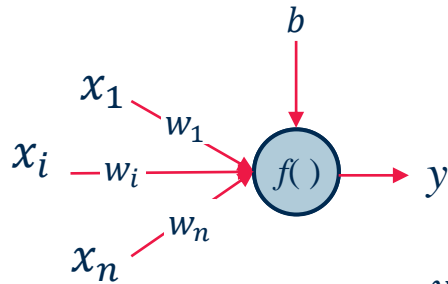
Biological Neuron



Biological Neural Networks



Artificial Neuron (Perceptron)



$$a(x) = \sum_{i=1}^n x_i w_i$$

$$y = f(x) = \begin{cases} 1 & \text{if } a(x) > b \\ 0 & \text{if } a(x) \leq b \end{cases}$$

- Numerical input attributes x_i
- Binary output class (0 or 1).
- Classifier for two-class problem
- For multiclass problems use one perceptron per class

- Initialise the weight and the threshold values randomly.
- For each data object in the training data set, check whether the perceptron predicts the correct class.
- If the perceptron predicts the wrong class, adjust the weights and threshold value to improve the prediction.
- Repeat this until no changes occur

- Whenever the perceptron makes a wrong classification
→ change weights and threshold in "**appropriate direction**".
- If the desired output is 1 and the perceptron's output is 0, the threshold is not exceeded, although it should be. Therefore, lower the threshold and adjust the weights depending on the sign and magnitude of the inputs.
- If the desired output is 0 and the perceptron's output is 1, the threshold is exceeded, although it should not be. Therefore, increase the threshold and adjust the weights depending on the sign and magnitude of the inputs.

- The **delta rule** recommends to adjust the weight and the threshold values as:

$$w_i^{new} = w_i^{old} + \Delta w_i$$

$$b^{new} = b^{old} + \Delta b$$

- w_i : A weight of the perceptron
- b : The threshold value of the perceptron
- (x_1, x_2, \dots, x_n) : An input vector
- t : the desired output for input vector (x_1, x_2, \dots, x_n)
- y : the real output of the Perceptron for input vector (x_1, x_2, \dots, x_n)
- $\eta > 0$: the Learning rate

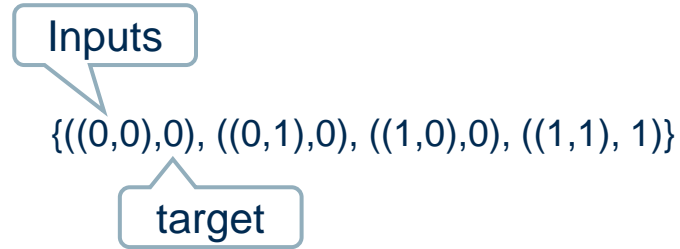
- The **delta rule** recommends to adjust the weight and the threshold values as:

$$\Delta w_i = \begin{cases} 0 & \text{if } y = t \\ +\eta x_i & \text{if } y = 0 \text{ and } t = 1 \\ -\eta x_i & \text{if } y = 1 \text{ and } t = 0 \end{cases}$$

$$\Delta b = \begin{cases} 0 & \text{if } y = t \\ -\eta & \text{if } y = 0 \text{ and } t = 1 \\ +\eta & \text{if } y = 1 \text{ and } t = 0 \end{cases}$$

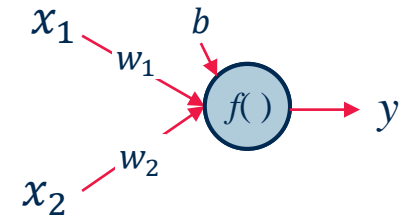
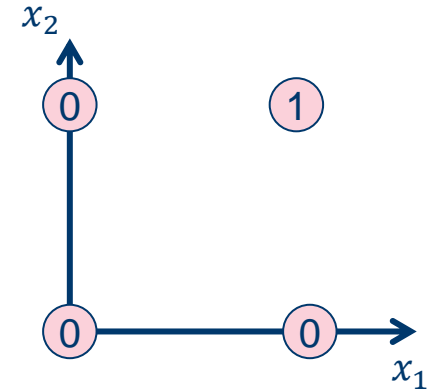
Example: Learning the logical operator AND

- Training Data:



- Learning rate $\eta = 1$
- Initialization: $w_1 = w_2 = b = 0$

	x	t	y	Δw_1	Δw_2	Δb	w_1^{new}	w_2^{new}	b^{new}
							0	0	0
Epoch 1	00	0	0	0	0	0	0	0	0
	01	0	0	0	0	0	0	0	0
	10	0	0	0	0	0	0	0	0
	11	1	0	1	1	-1	1	1	-1



Example: Learning the logical operator AND

	x	t	y	Δw_1	Δw_2	Δb	w_1^{new}	w_2^{new}	b^{new}
							1	1	-1
Epoch 2	00	0	1	0	0	1	1	1	0
	01	0	1	0	-1	1	1	0	1
	10	0	0	0	0	0	1	0	1
	11	1	0	0	1	1	2	1	0

	x	t	y	Δw_1	Δw_2	Δb	w_1^{new}	w_2^{new}	b^{new}
							2	1	0
Epoch 3	00	0	0	0	0	0	2	1	0
	01	0	1	0	-1	1	2	0	1
	10	0	1	-1	0	1	1	0	2
	11	1	0	0	1	1	2	1	1

Example: Learning the logical operator AND

	x	t	y	Δw_1	Δw_2	Δb	w_1^{new}	w_2^{new}	b^{new}
							2	1	1
Epoch 4	00	0	0	0	0	0	2	1	1
	01	0	0	0	0	0	2	1	1
	10	0	1	-1	0	1	1	1	2
	11	1	0	1	1	-1	2	2	1

	x	t	y	Δw_1	Δw_2	Δb	w_1^{new}	w_2^{new}	b^{new}
							2	2	1
Epoch 5	00	0	0	0	0	0	2	2	1
	01	0	1	0	-1	1	2	1	2
	10	0	0	0	0	0	2	1	2
	11	1	1	0	0	0	2	1	2

Example: Learning the logical operator AND

	x	t	y	Δw_1	Δw_2	Δb	w_1^{new}	w_2^{new}	b^{new}
							2	1	2
Epoch 6	00	0	0	0	0	0	2	1	2
	01	0	0	0	0	0	2	1	2
	10	0	0	0	0	0	2	1	2
	11	1	1	0	0	0	2	1	2

Perceptron Convergence

If, for a given data set with two classes, there exists a perceptron that can classify all patterns correctly, then the delta rule will adjust the weights and the threshold after a finite number of steps in such way that all patterns are classified correctly.

What classification problems can a perceptron solve?

- Consider a perceptron with two inputs.
- Let y be the output of the perceptron for input (x_1, x_2)
- Then:

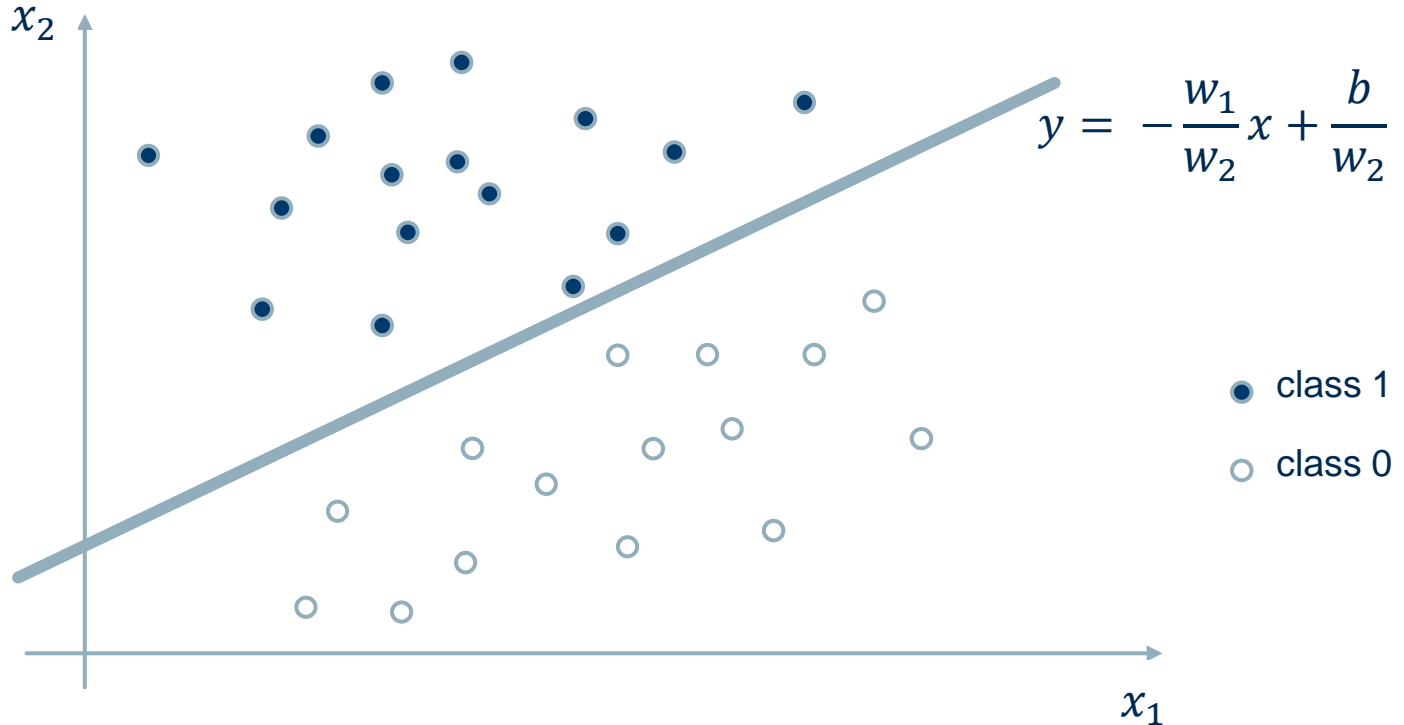
$$y = 1 \iff w_1 \cdot x_1 + w_2 \cdot x_2 > b$$

$$\iff x_2 > -\frac{w_1}{w_2}x_1 + \frac{b}{w_2}$$

- The perceptron output is 1 if and only if the input vector (x_1, x_2) is above the line:

$$y = -\frac{w_1}{w_2}x + \frac{b}{w_2}$$

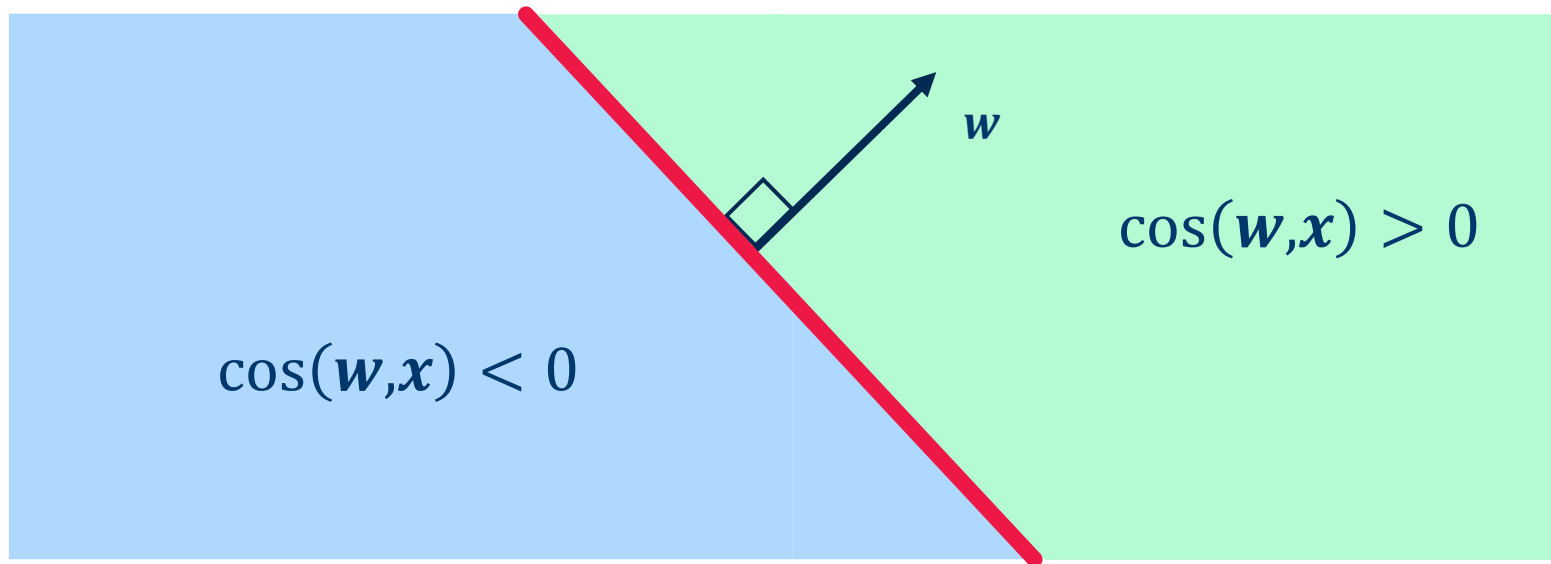
Linear Separability



The parameters w_1 , w_2 , define the line. All input patterns above this line are assigned to class 1, all input patterns below the line to class 0.

Linear Separability in hyperspaces

$$y(\mathbf{x}) = w_0 + \sum_{i=1}^n w_i x_i = w_0 + \mathbf{w}^T \cdot \mathbf{x} = w_0 + |\mathbf{x}| |\mathbf{w}| \cos(\mathbf{w}, \mathbf{x})$$

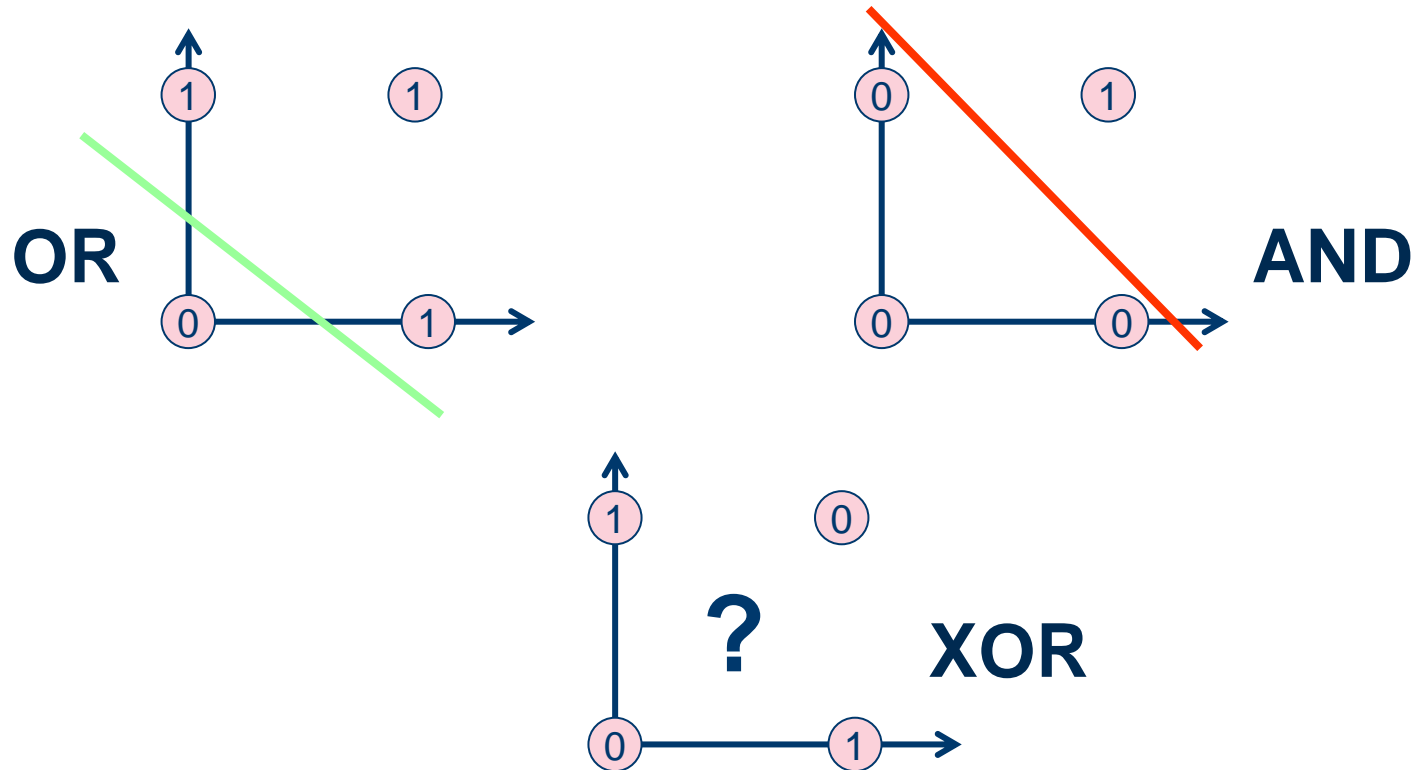


Perceptrons implements hyperplanes in the feature space

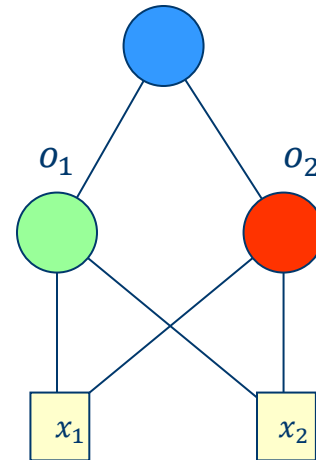
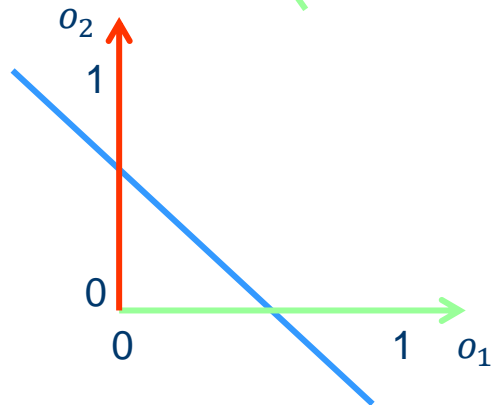
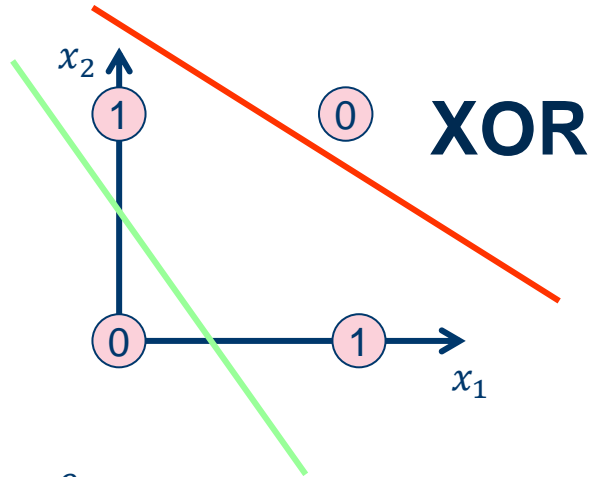
- A Perceptron with n input neurons can classify all examples from a dataset with n input variables and two classes correctly, if there exists a hyperplane separating the two classes
- Such classification problems are called **linearly separable**
- A Perceptron can only solve linearly separable problems

What can a single Perceptron do?

Example: The exclusive OR (XOR) defines a classification task which is not linearly separable.



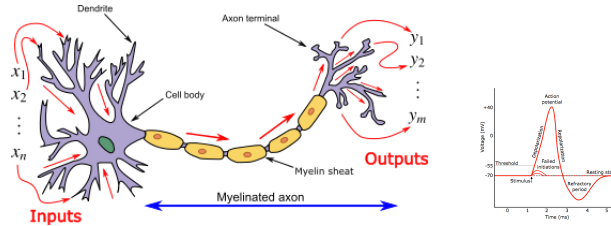
The exclusive OR (XOR) can be solved adding one more layer



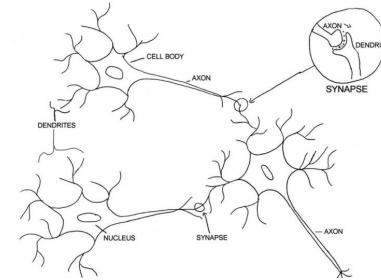
FeedForward Neural Networks

- A Perceptron with more than one layer is a **Multi-Layer Perceptron (MLP)**
- A MLP is a neural network with:
 - an *input layer*,
 - one or more *hidden layers*, and
 - an *output layer*
- Connections exist only between neurons from one layer to the next layer

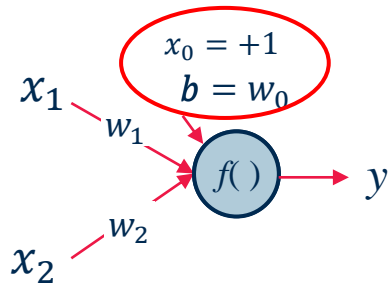
Biological Neuron



Biological Neural Networks



Artificial Neuron (Perceptron)



$$y = f(x_1w_1 + x_2w_2 + b)$$

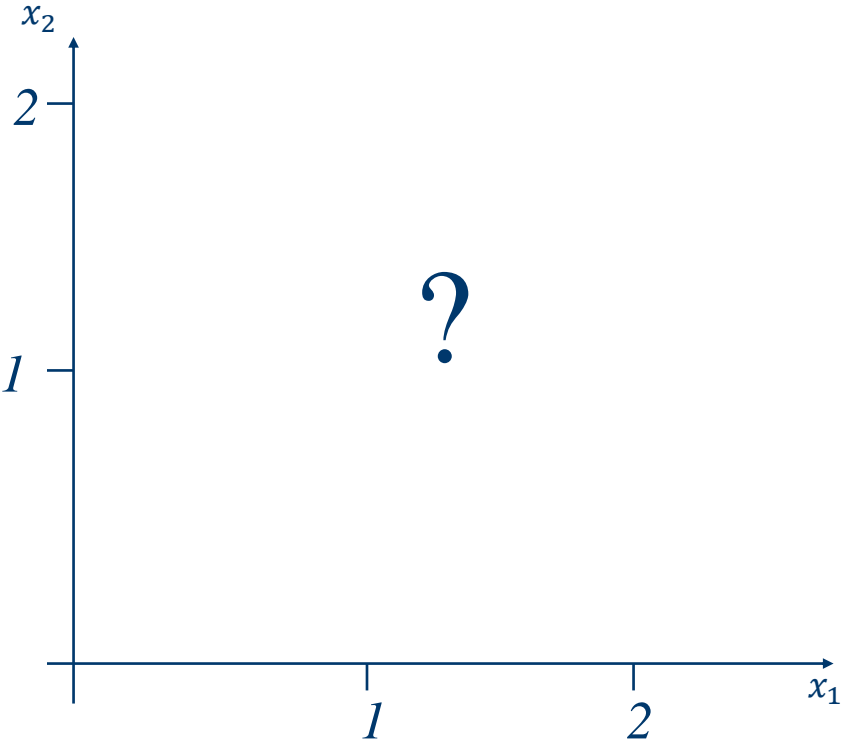
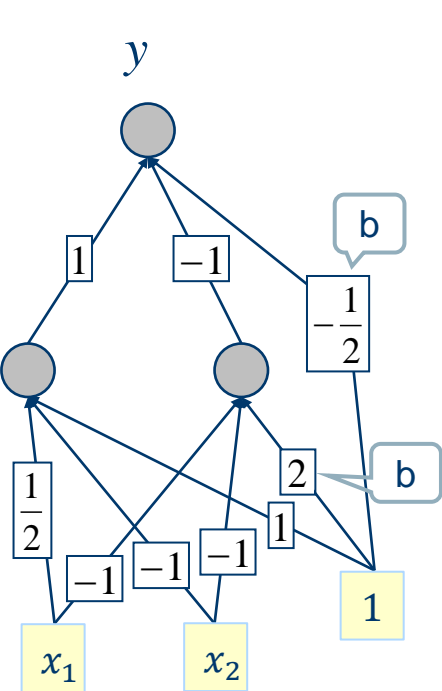
$$b = w_0$$

$$a(x) = \sum_{i=0}^n x_iw_i$$

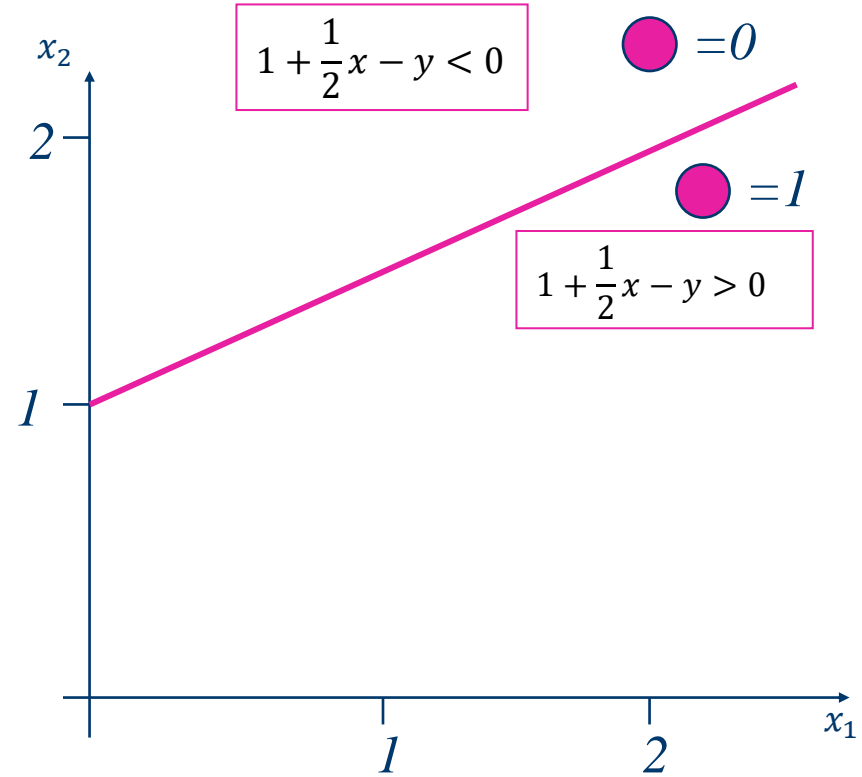
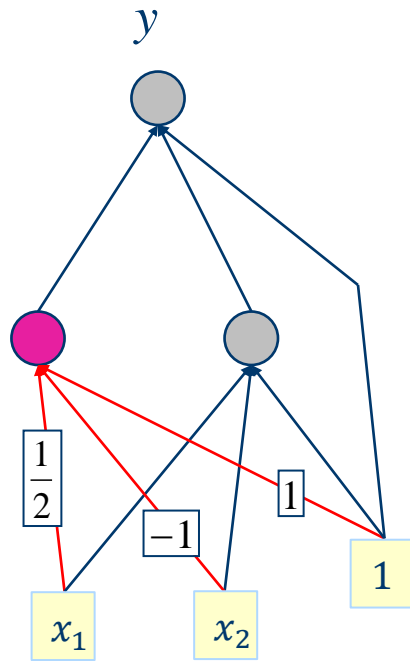
$$y(x) = f\left(\sum_{i=0}^n x_iw_i\right)$$

- Neuron bias can be considered as a weight w_0 to a constant input $x_0 = +1$

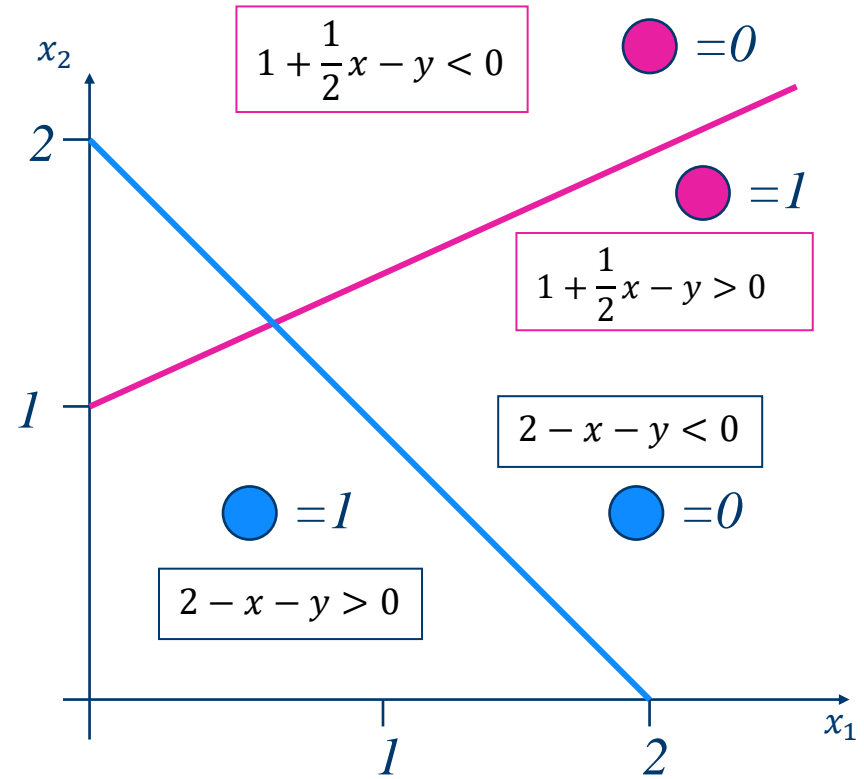
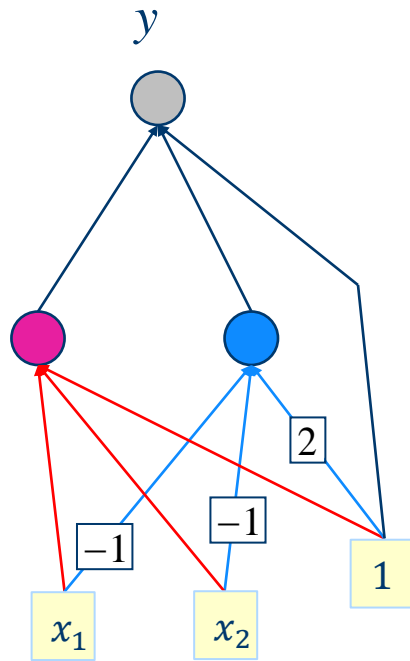
MLP: Example



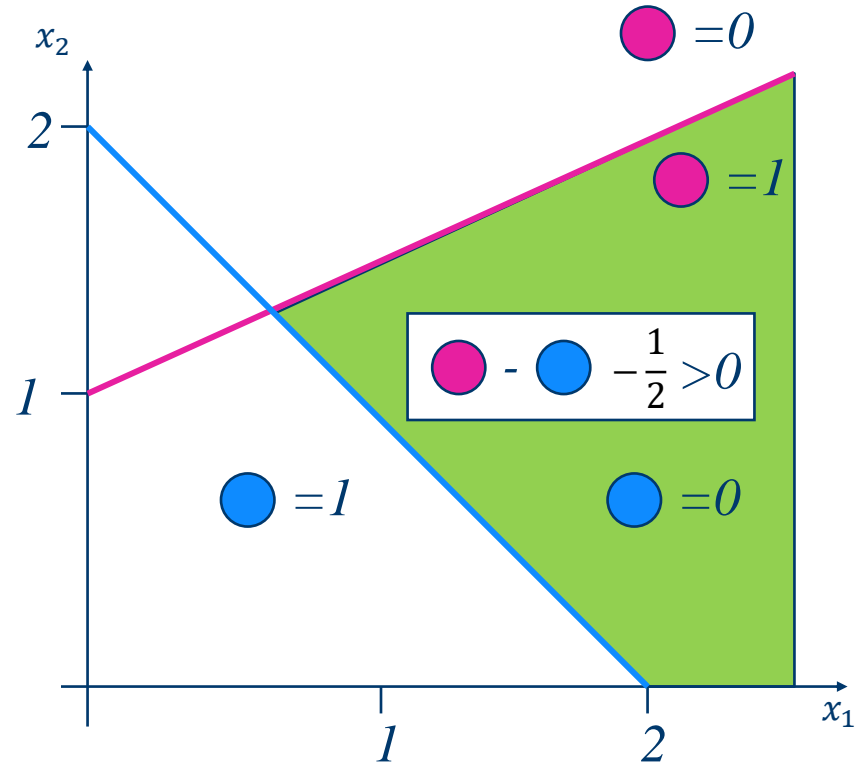
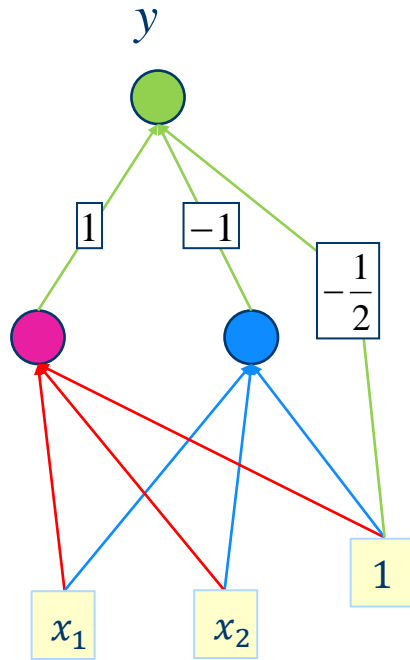
MLP: Example



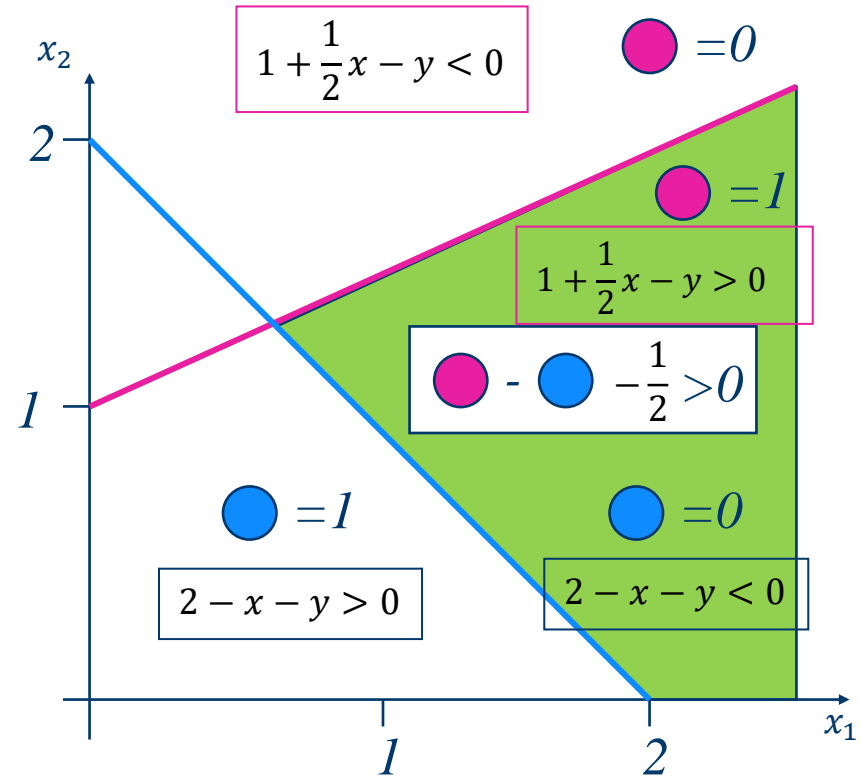
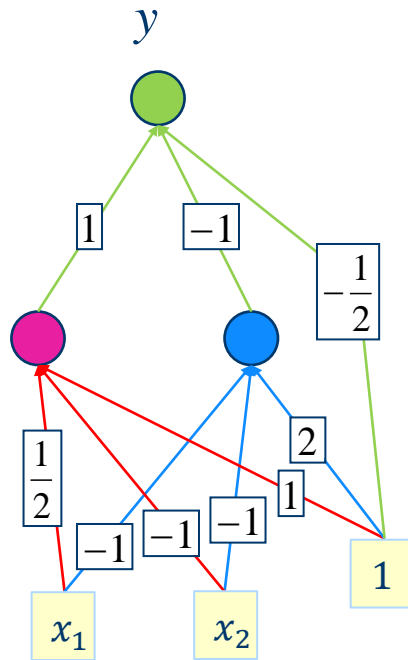
MLP: Example



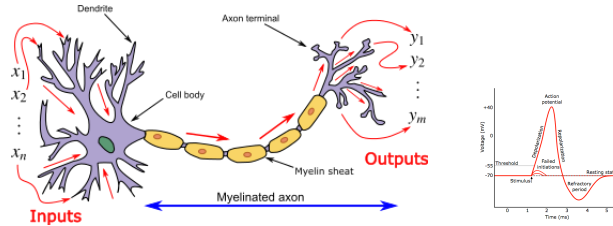
MLP: Example



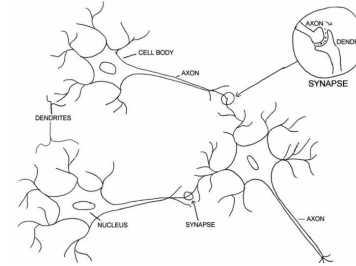
MLP: Example



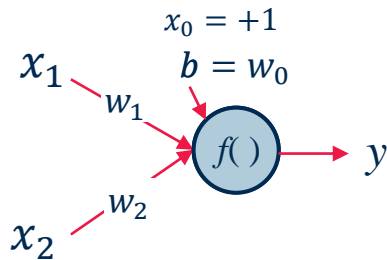
Biological Neuron



Biological Neural Networks



Artificial Neuron (Perceptron)



$$y = f(x_1w_1 + x_2w_2 + b)$$

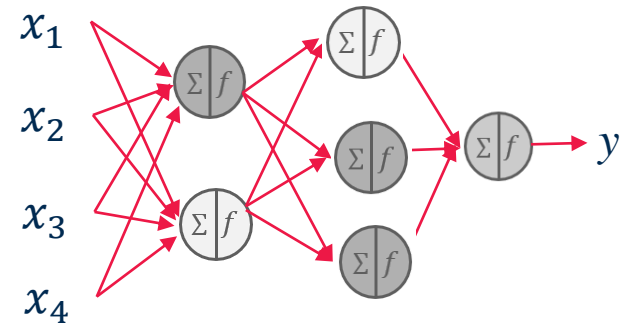
$$b = w_0$$

$$a(\mathbf{x}) = \sum_{i=0}^n x_i w_i$$

$$y(\mathbf{x}) = f\left(\sum_{i=0}^n x_i w_i\right)$$

Artificial Neural Networks

(Multilayer Perceptron, MLP)



- Let's see an example of a MLP
- 3 layers:
 - 1 input layer with $m=2$ inputs
 - 1 hidden layer with $h=3$ hidden neurons
 - 1 output layer with $n=2$ output neurons
- All **feed-forward** connections: from a neuron only to neurons in the next layer
- **Fully-connected**: that is each neuron in one layer is connected to all neurons in the next layers

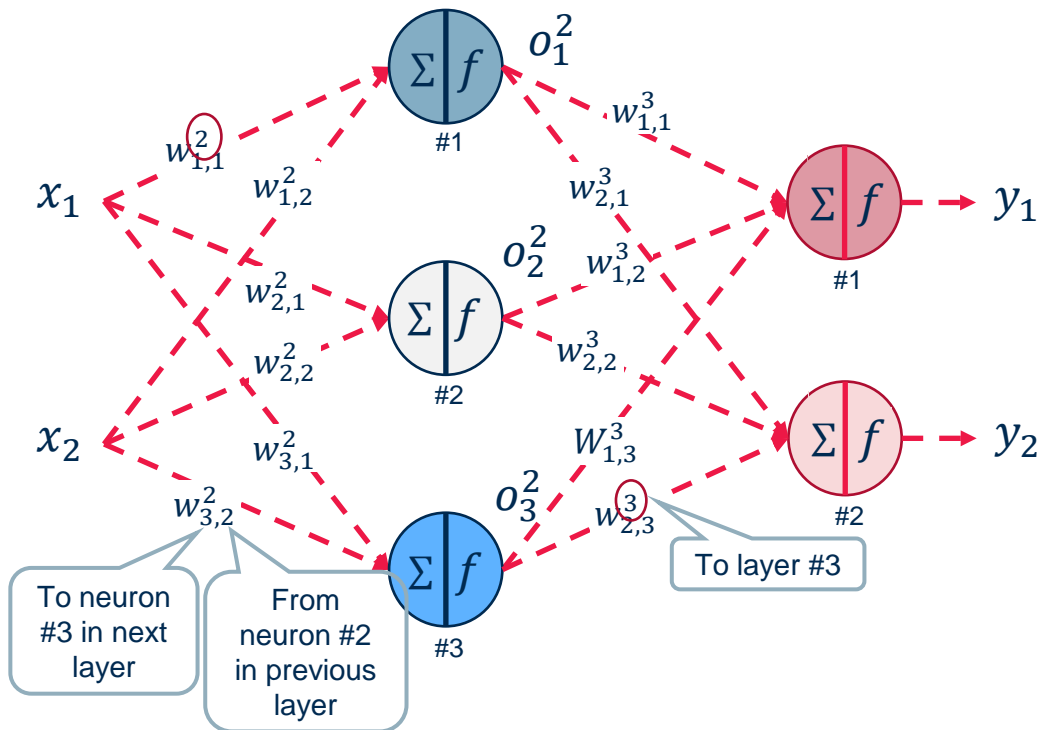
**fully connected
feed forward
neural networks**

Feed-Forward Neural Networks (FFNN)

Input
Layer #1
m=2 inputs

Hidden
Layer #2
h=3 units

Output
Layer #3
n=2 units



Forward pass:

$$o_j^2 = f\left(\sum_{i=1}^n w_{j,i}^2 x_i\right)$$

$$y_k = f\left(\sum_{j=1}^h w_{k,j}^3 o_j^2\right)$$

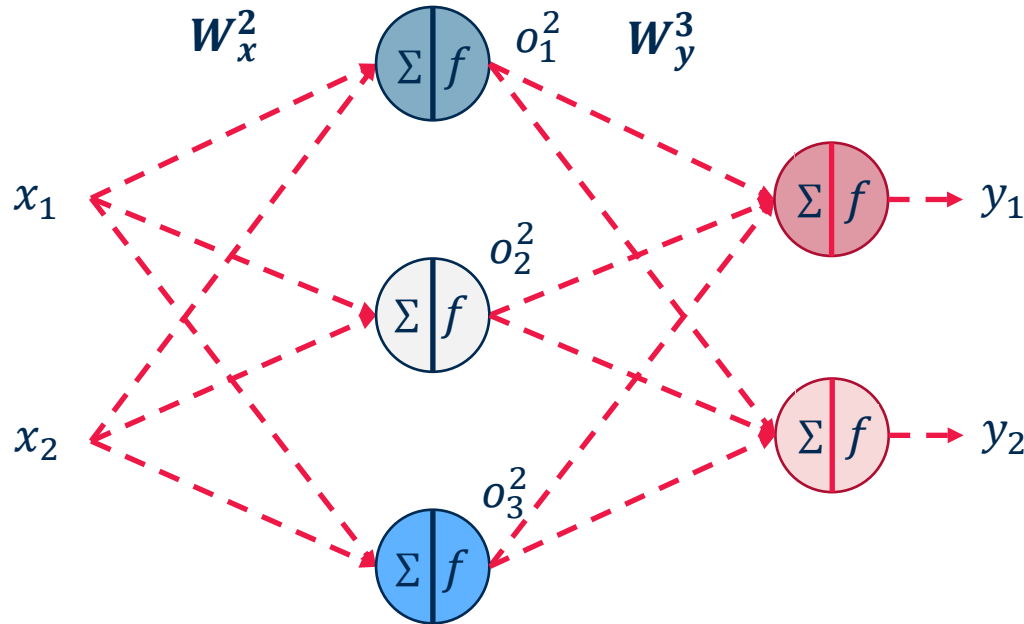
$$y_k = f\left(\sum_{j=1}^h w_{k,j}^3 f\left(\sum_{i=1}^n w_{j,i}^2 x_i\right)\right)$$

Same with Matrix Notations

Input
Layer #1
m=2 inputs

Hidden
Layer #2
h=3 units

Output
Layer #3
n=2 units



Forward pass:

$$\mathbf{o} = f(W_x^2 \mathbf{x})$$

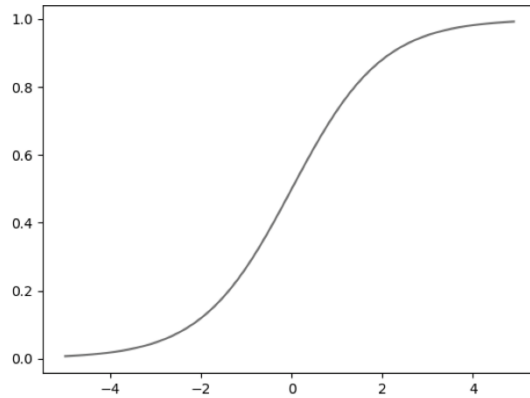
$$\mathbf{y} = f(W_y^3 \mathbf{o})$$

$$\mathbf{y} = f(W_y^3 f(W_x^2 \mathbf{x}))$$

$f()$ = activation function

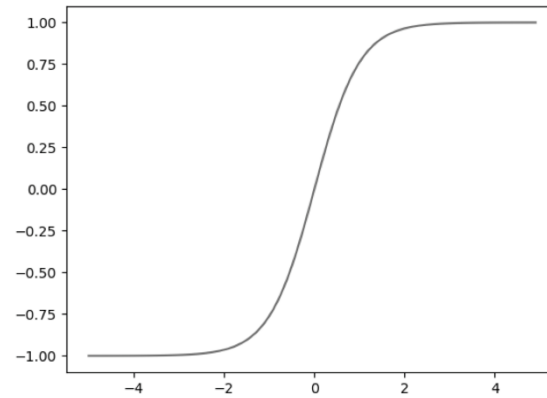
Frequently used activation functions

Sigmoid



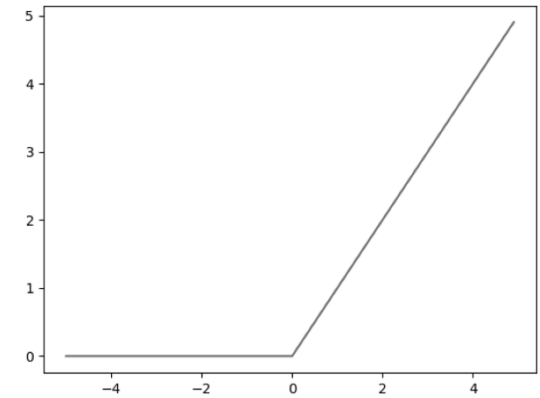
$$f(a) = \frac{1}{1 + e^{-ha}}$$

Tanh



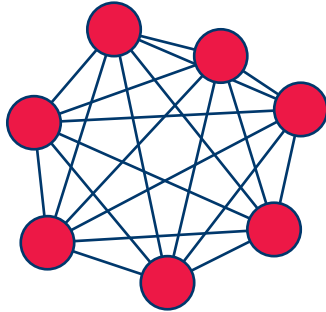
$$f(a) = \frac{e^{2ha} - 1}{e^{2ha} + 1}$$

Rectified Linear Unit (ReLU)



$$f(a) = \max\{0, ha\}$$

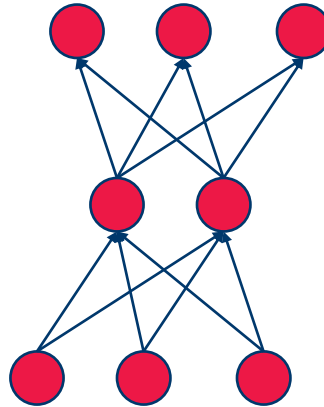
completely
connected



example:

- associative neural network
- Hopfield

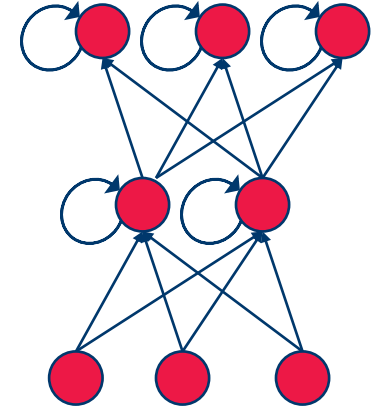
feedforward
(directed, a-cyclic)



example:

- Multi Layer Perceptron
- Auto-encoder MLP

recurrent
(feedback connections)

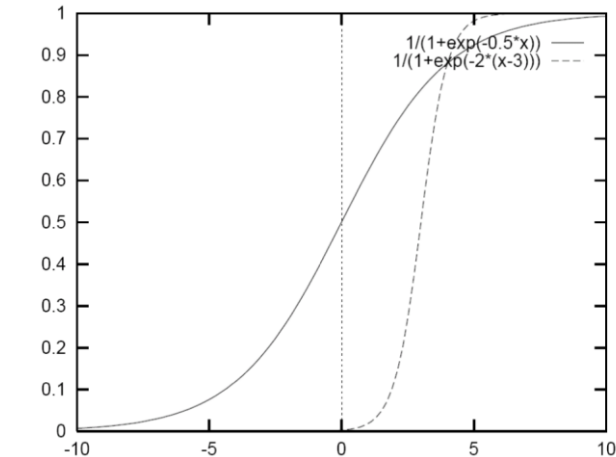


example:

- Recurrent Neural Network (for time series recognition)

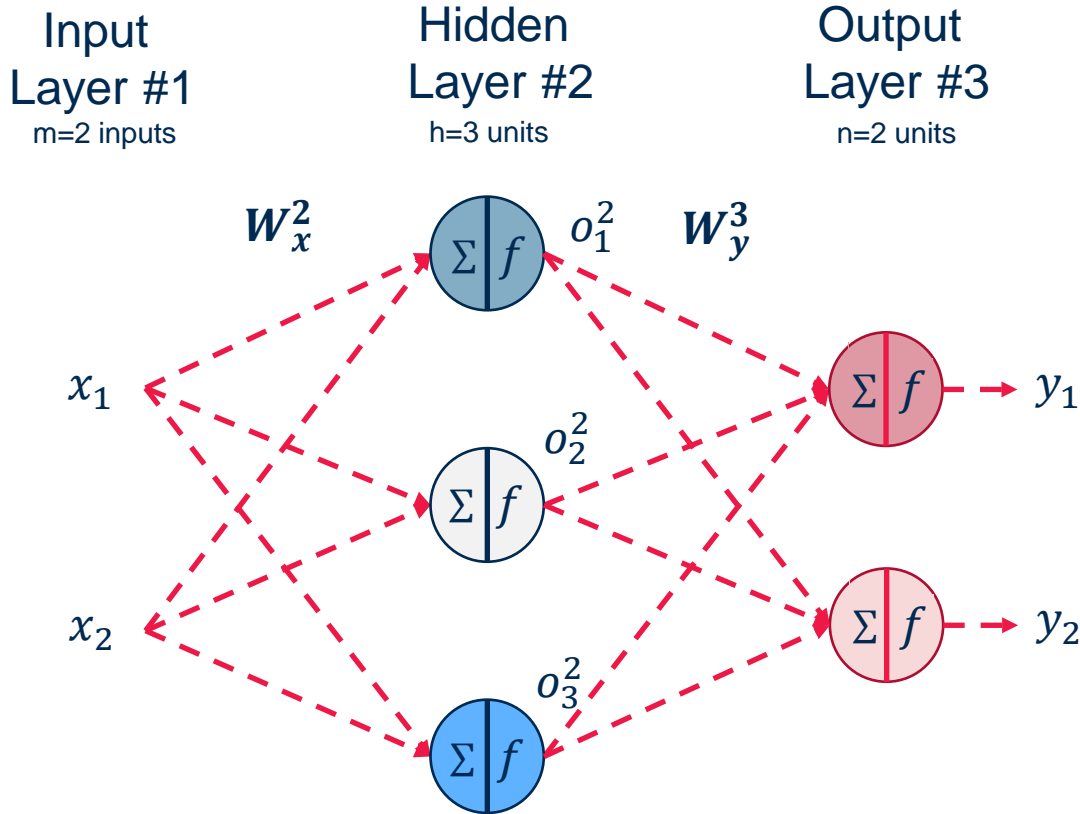
BackPropagation

- **Problem:** How do we automatically adjust the weights (and thresholds) for the neurons of the hidden layer?
- **Solution:** gradient descent
- Does not work with binary (non-differentiable) threshold function as activation function for the neurons.
- Activation function must be a **differentiable** function



- Teach (ensemble of) neuron(s) a desired input-output behavior.
- Show examples from the training set repeatedly
- Networks adjusts parameters to fit underlying function
 - topology
 - weights
 - internal functional parameters

Error Function



Number of output units

$$E = \frac{1}{2} \sum_{x \in T} \sum_{k=1}^n (y_k - t_k)^2$$

On the whole Training set

Network output value k

Target value k

Forward pass:

$$\mathbf{o} = f(W_x^2 \mathbf{x})$$

$$\mathbf{y} = f(W_y^3 \mathbf{o})$$

- Adjust the weights based on the gradient descent technique, i.e. proportionally to the gradient of the error function

$$\mathbf{w}(t + 1) = \mathbf{w}(t) + \Delta\mathbf{w}(t)$$

- with

$$\Delta\mathbf{w}(t) = -\eta \nabla(E(\mathbf{w}(t)))$$

- with $\eta > 0$ a non-zero learning rate

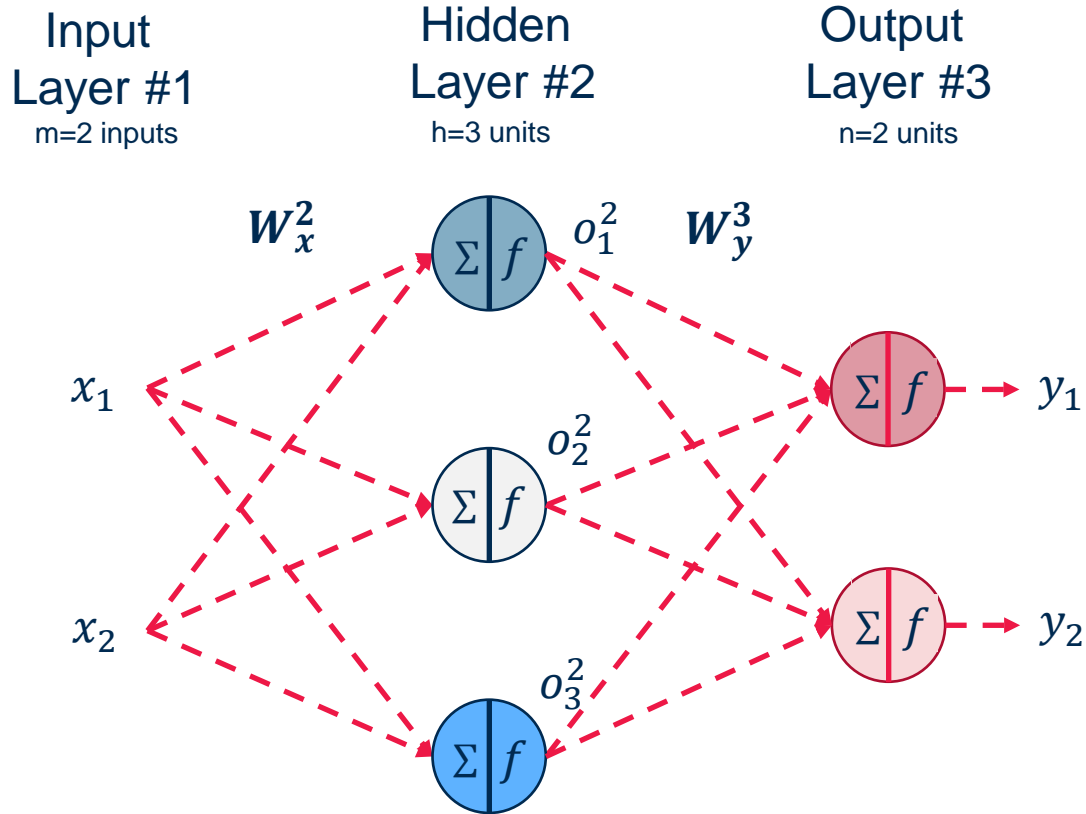
$$\Delta\mathbf{w}(t) = -\eta \nabla \left(E(\mathbf{w}(t)) \right) = -\eta \left(\frac{\partial E(\mathbf{w}(t))}{\partial w_1}, \dots, \frac{\partial E(\mathbf{w}(t))}{\partial w_m} \right)$$

- So we really need to determine only:

$$\Delta w_{u,v} = -\eta \frac{\partial E}{\partial w_{u,v}}$$

- For **each single weight** of the network.

Learning Rule from Gradient Descent



$$E = \frac{1}{2} \sum_{x \in T} \sum_{k=1}^n (y_k - t_k)^2$$

Gradient descent

$$\Delta w_{u,v} = -\eta \frac{\partial E}{\partial w_{u,v}}$$

For each weight in the output layer:

$$\Delta w_{ji}^{out} = -\eta \frac{\partial E(\mathbf{w}^{out})}{\partial w_{ji}^{out}}$$

To output neuron j
From hidden neuron i

$$\frac{\partial E}{\partial w_{ji}^{out}} = \frac{\partial \frac{1}{2} \sum_{x \in T} \sum_{k=1}^n (y_k - t_k)^2}{\partial w_{ji}^{out}} = \frac{1}{2} \sum_{x \in T} \frac{\partial (y_j - t_j)^2}{\partial w_{ji}^{out}} =$$

$$= \sum_{x \in T} (y_j - t_j) \frac{\partial y_j}{\partial w_{ji}^{out}} = \sum_{x \in T} (y_j - t_j) \frac{\partial f(\text{net}_j)}{\partial w_{ji}^{out}} =$$

Net input to output neuron j

$$= \sum_{x \in T} (y_j - t_j) \frac{\partial f(\text{net}_j)}{\partial \text{net}_j} \frac{\partial \text{net}_j}{\partial w_{ji}^{out}} = \sum_{x \in T} (y_j - t_j) f'(\text{net}_j) \frac{\partial \text{net}_j}{\partial w_{ji}^{out}} =$$

For each weight in the output layer:

$$\Delta w_{ji}^{out} = -\eta \frac{\partial E(\mathbf{w}^{out})}{\partial w_{ji}^{out}}$$

$$\frac{\partial E}{\partial w_{ji}^{out}} = \dots = \sum_{x \in T} (y_j - t_j) f'(net_j) \frac{\partial \sum_{k'=1}^h w_{j,k'}^{out} o_{k'}^{hidden}}{\partial w_{ji}^{out}} =$$

Number of neurons
in previous hidden
layer

$$= \sum_{x \in T} (y_j - t_j) f'(net_j) o_i^{hidden}$$

Output of neuron i
in previous hidden
layer

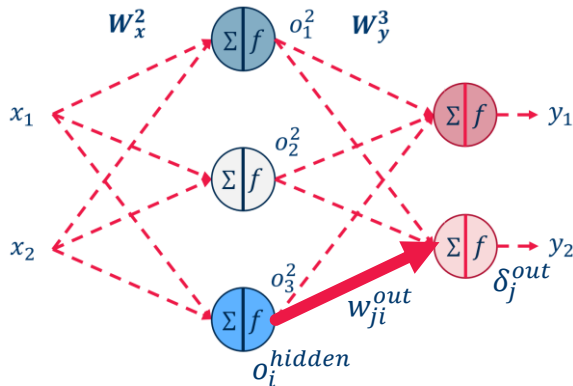
$$\Delta w_{ji}^{out} = -\eta \sum_{x \in T} \overbrace{(y_j - t_j) f'(net_j)}^{\delta_j^{out}} o_i^{hidden} = -\eta \sum_{x \in T} \delta_j^{out} o_i^{hidden}$$

Update formula for weights to the output layer after all samples in T

- Final formula to update the weight w_{ji}^{out} , after all training samples in T have passed:

$$\Delta w_{ji}^{out} = -\eta \sum_{x \in T} \delta_j^{out} o_i^{hidden}$$

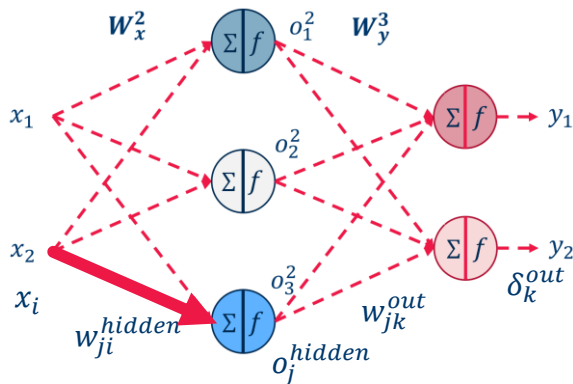
$$\delta_j^{out} = (y_j - t_j) f'(net_j)$$



In the hidden layers...

- Now, where do we get the target values for the hidden neurons?
- Let's continue with gradient descent:

$$\Delta w_{ij}^{hidden} = -\eta \frac{\partial E}{\partial w_{ij}^{hidden}}$$



... some Calculations for the Hidden Layer ...

$$\Delta w_{ji}^{hidden} = -\eta \frac{\partial \frac{1}{2} \sum_{x \in T} \sum_{k=1}^n (y_k - t_k)^2}{\partial w_{ij}^{hidden}} = -\frac{\eta}{2} \sum_{x \in T} \sum_{k=1}^n \frac{\partial (f(net_k^{out}) - t_k)^2}{\partial w_{ji}^{hidden}}$$

$$\dots = -\frac{\eta}{2} \sum_{x \in T} \sum_{k=1}^n 2(f(net_k^{out}) - t_k) \frac{\partial (f(net_k^{out}) - t_k)}{\partial w_{ji}^{hidden}}$$

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n (f(net_k^{out}) - t_k) f'(net_k^{out}) \frac{\partial net_k^{out}}{\partial w_{ji}^{hidden}}$$

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n (f(net_k^{out}) - t_k) f'(net_k^{out}) \frac{\partial \sum_{j'=1}^h w_{j'k}^{out} o_{j'}^{hidden}}{\partial w_{ji}^{hidden}}$$

If just one hidden layer

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n (f(net_k^{out}) - t_k) f'(net_k^{out}) \frac{\partial \sum_{j'=1}^h w_{j'k}^{out} f(\sum_{i'=1}^m w_{i'j'}^{hidden} \cdot x_{i'})}{\partial w_{ji}^{hidden}}$$

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n \delta_k^{out} \frac{\partial \sum_{j'=1}^h w_{j'k}^{out} f(\sum_{i'=1}^m w_{i'j'}^{hidden} \cdot x_{i'})}{\partial w_{ji}^{hidden}}$$

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n \delta_k^{out} w_{jk}^{out} \frac{\partial f(\sum_{i'=1}^m w_{i'j}^{hidden} \cdot x_{i'})}{\partial w_{ji}^{hidden}}$$

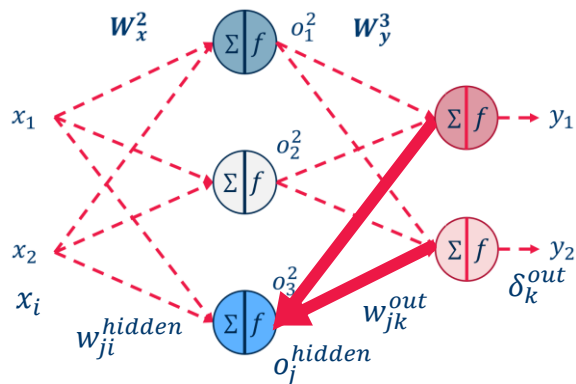
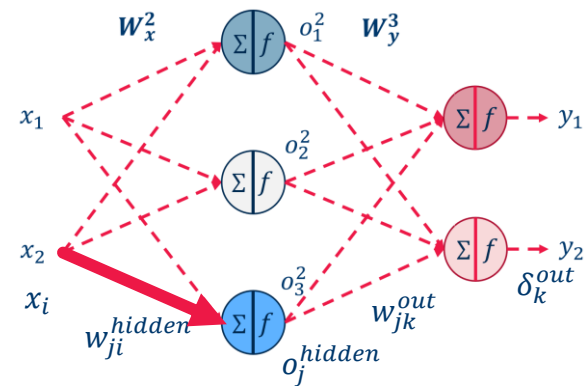
... some Calculations for the Hidden Layer ...

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n \delta_k^{out} w_{jk}^{out} \frac{\partial f(\sum_{i'=1}^m w_{i'j}^{hidden} \cdot x_{i'})}{\partial w_{ji}^{hidden}}$$

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n \delta_k^{out} w_{jk}^{out} f'(\sum_{i'=1}^m w_{i'j}^{hidden} \cdot x_{i'}) \cdot x_i$$

$$\dots = -\eta \sum_{x \in T} \sum_{k=1}^n \delta_k^{out} w_{jk}^{out} f'(net_j^{hidden}) x_i$$

$$\dots = -\eta \sum_{x \in T} \delta_j^{hidden} \cdot x_i$$



As for weights to output neurons

$$\Delta w_{ji}^{hidden} = -\eta \sum_{x \in T} \delta_j^{hidden} x_i$$

$$\delta_j^{hidden} = \sum_{k=1}^n \delta_k^{out} w_{jk}^{out} f'(net_j^{hidden})$$

δ_k^{out} is back-propagated from output to input

Error BackPropagation or Generalized Delta Rule

Update of weights to the output layer:

$$\Delta w_{ji}^{out} = -\eta \sum_{x \in T} \delta_j^{out} o_i^{hidden}$$

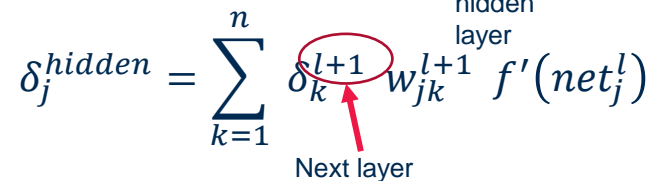
with

$$\delta_j^{out} = (y_j - t_j) f'(net_j)$$

And update of weights to hidden layers:

$$\Delta w_{ji}^l = -\eta \sum_{x \in T} \delta_j^l o_i^{l-1}$$


With

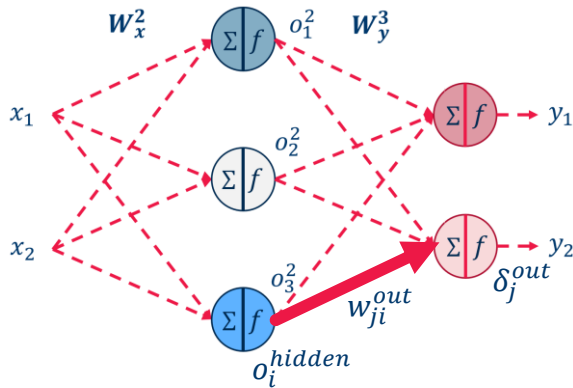
$$\delta_j^{hidden} = \sum_{k=1}^n \delta_k^{l+1} w_{jk}^{l+1} f'(net_j^l)$$


Recursive equation for updating the weights:

Update the weights to the neuron in the output layer first and then go back layer by layer and update the corresponding weights.

Update formula for weights after each sample in T

- Final formula to update the weight w_{ji}^{out} , after **one single** training sample in T :



$$E = \frac{1}{2} \sum_{k=1}^n (y_k - t_k)^2$$

← Error function after each training sample

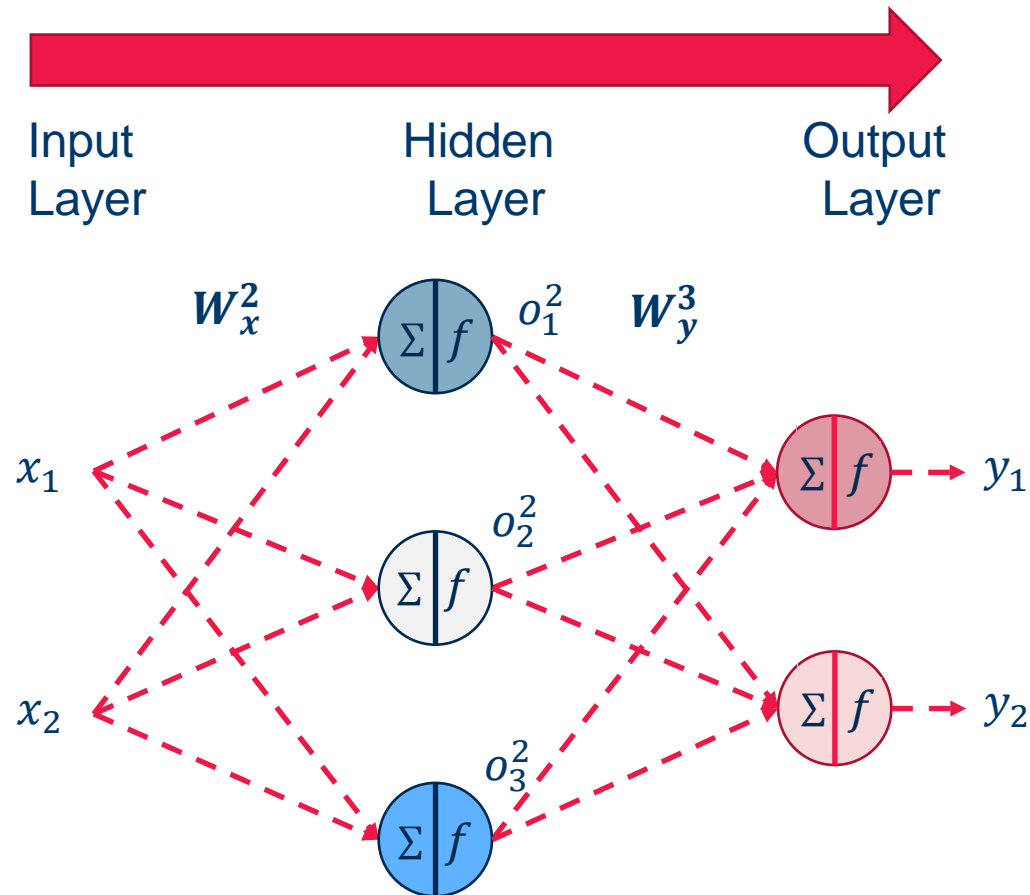
$$\Delta w_{ji}^l = -\eta \delta_j^l o_i^{l-1}$$

← No sum on training set T

$$\delta_j^l = \begin{cases} (y_j - t_j) f'(net_j^l) & l = \text{output layer} \\ \sum_{k=1}^n \delta_k^{l+1} w_{jk}^{l+1} f'(net_j^l) & l = \text{hidden layer} \end{cases}$$

← Same as before

Step 1. Forward Pass

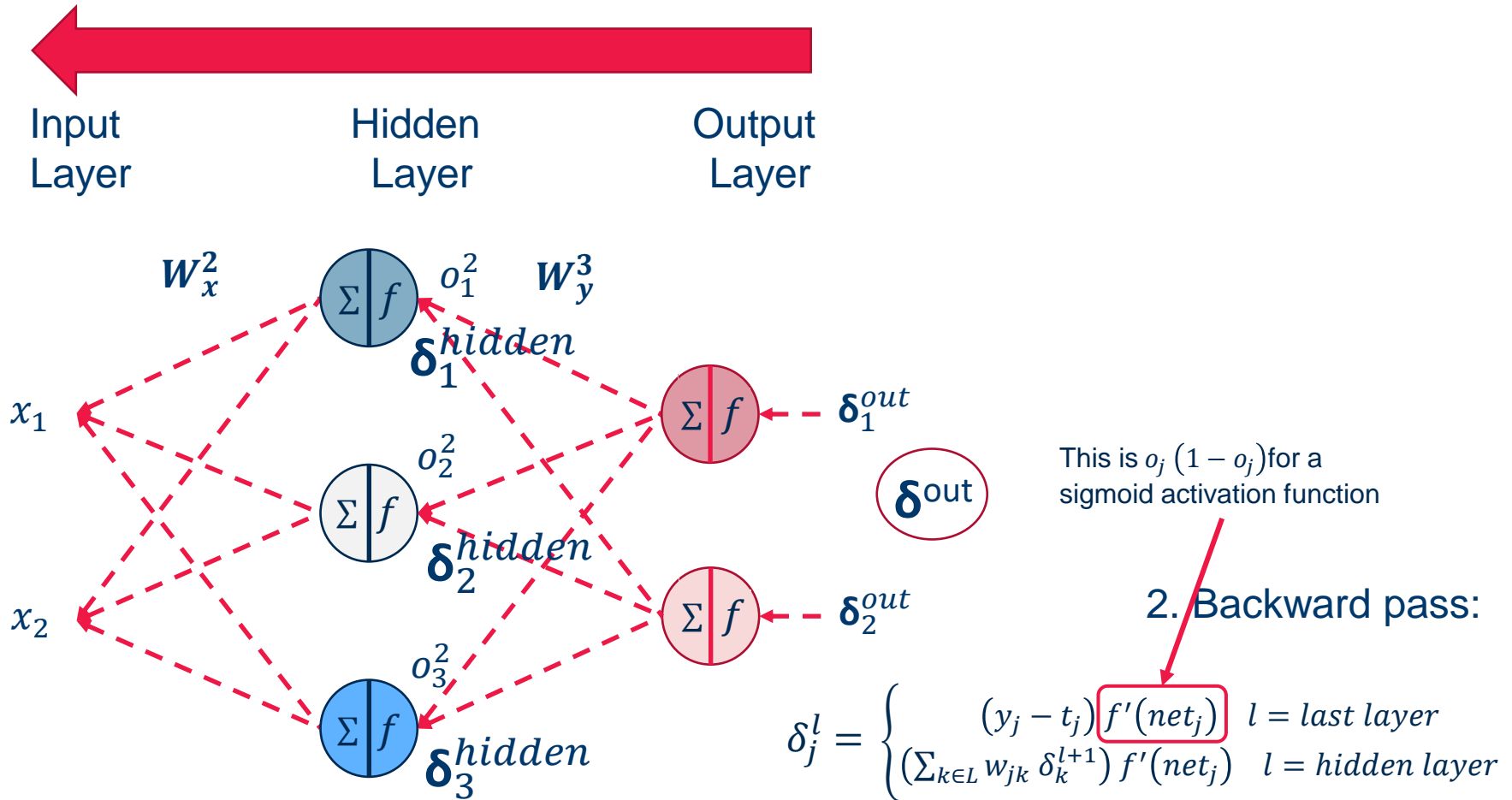


1. Forward pass:

$$o_j^2 = f\left(\sum_{i=1}^n w_{ji}^2 x_i\right)$$

$$y_k = f\left(\sum_{j=1}^h w_{kj}^3 o_j^2\right)$$

Step 2. Backward Pass - δ



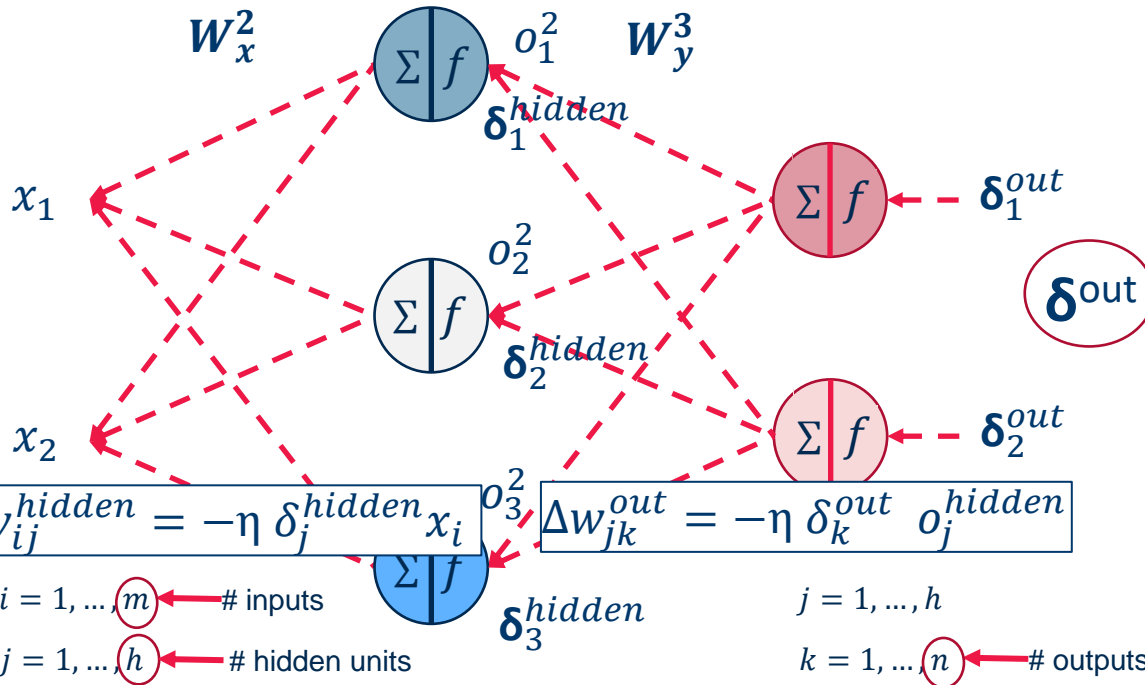
Step 3: Learning after **each** training pattern



Input Layer

Hidden Layer

Output Layer

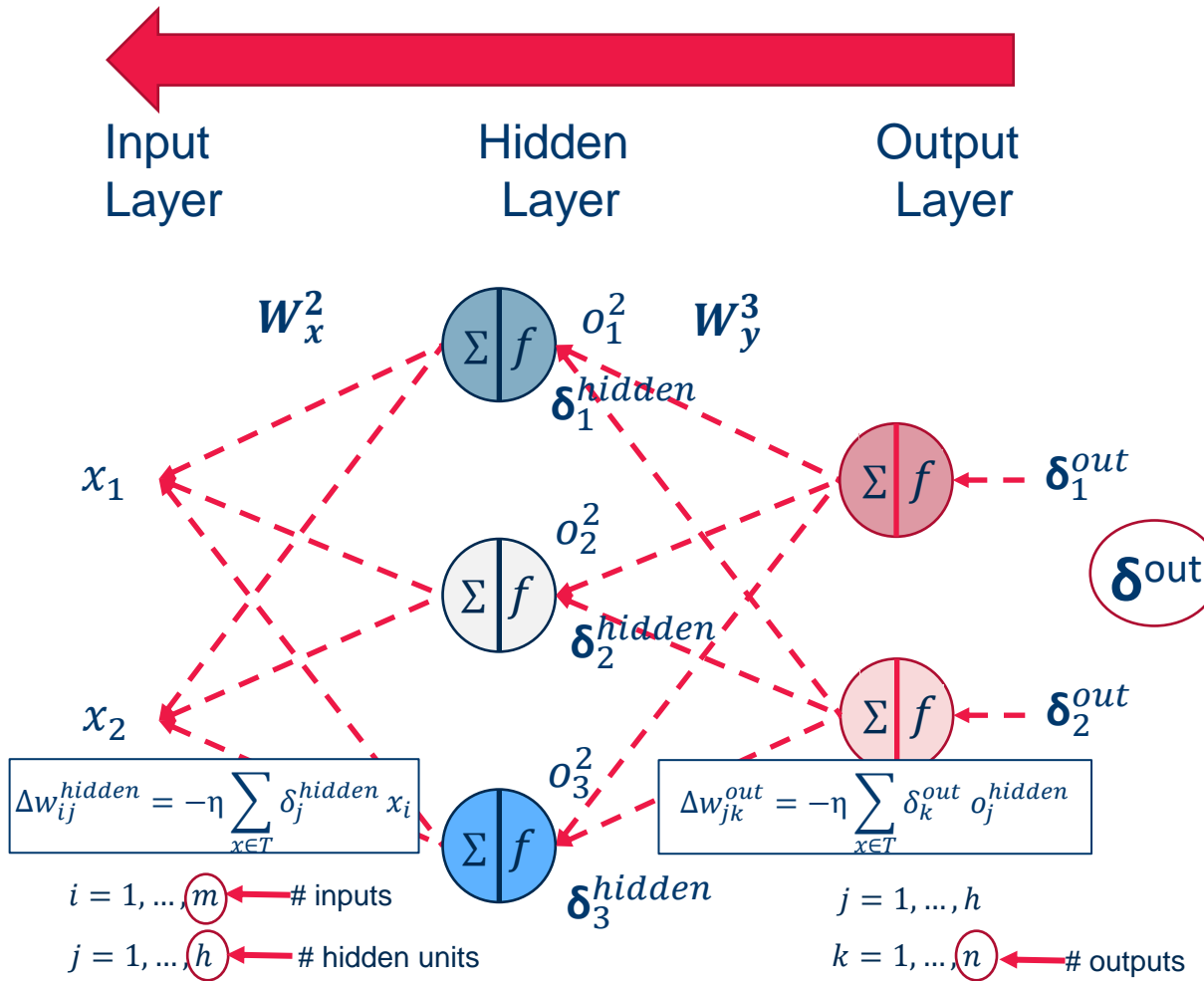


3. Weight Update after **each** training example:

$$\Delta w_{ji}^l = -\eta \delta_j^l o_i^{l-1}$$

$$w_{ji}^l(t + 1) = w_{ji}^l(t) + \Delta w_{ji}^l$$

Step 3: Learning after all training patterns



Learning rate

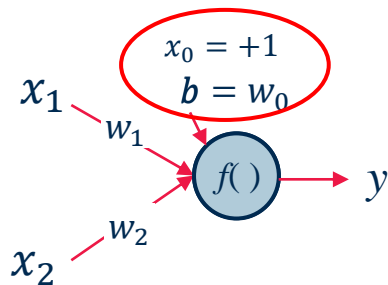
4. Weight Update after all training examples:

$$\Delta w_{ji}^l = -\eta \sum_{x \in T} \delta_j^l o_i^{l-1}$$

$$w_{ji}^l(t+1) = w_{ji}^l(t) + \Delta w_{ji}^l$$

- Remember?
- Bias values can be considered as special weights to constant inputs +1
- Therefore biases are trained together with all other weights

Artificial Neuron (**Perceptron**)



$$y = f(x_1w_1 + x_2w_2 + b)$$

$$b = w_0$$

$$a(\mathbf{x}) = \sum_{i=0}^n x_i w_i$$

$$y(\mathbf{x}) = f\left(\sum_{i=0}^n x_i w_i\right)$$

- Neuron bias can be considered as a weight w_0 to a constant input $x_0 = +1$

- **Offline Training:** Weight update after **all** training patterns
 - correct
 - computationally expensive and slow
 - works with reasonably large learning rates (fewer updates!)
- **Online (Stochastic) Training:** Weight update after **each** training pattern
 - approximation (can in theory run into oscillations)
 - faster (fewer epochs!)
 - smaller learning rates necessary
- **Batch Training:** Weight update after a batch of training patterns
 - A compromise between the two

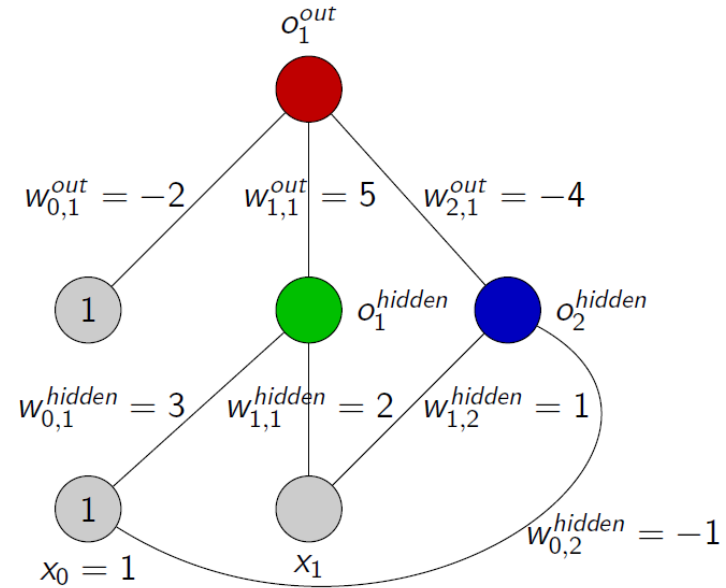
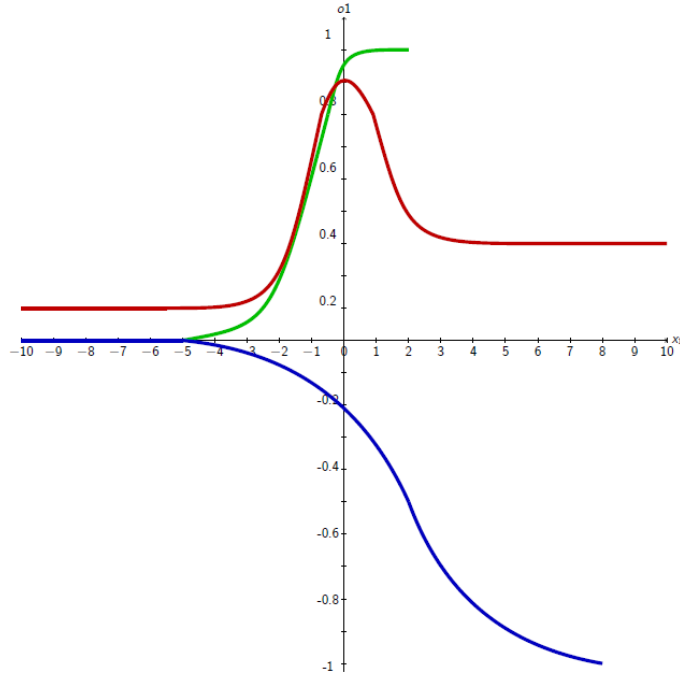
- The Sigmoid Activation Function has one really nice property (among others):

$$f'(a) = \frac{\partial}{\partial a} \left(\frac{1}{1 + e^{-ha}} \right) = - \frac{e^{-ha}}{(1 + e^{-ha})^2} = \dots = f(a)(1 - f(a))$$

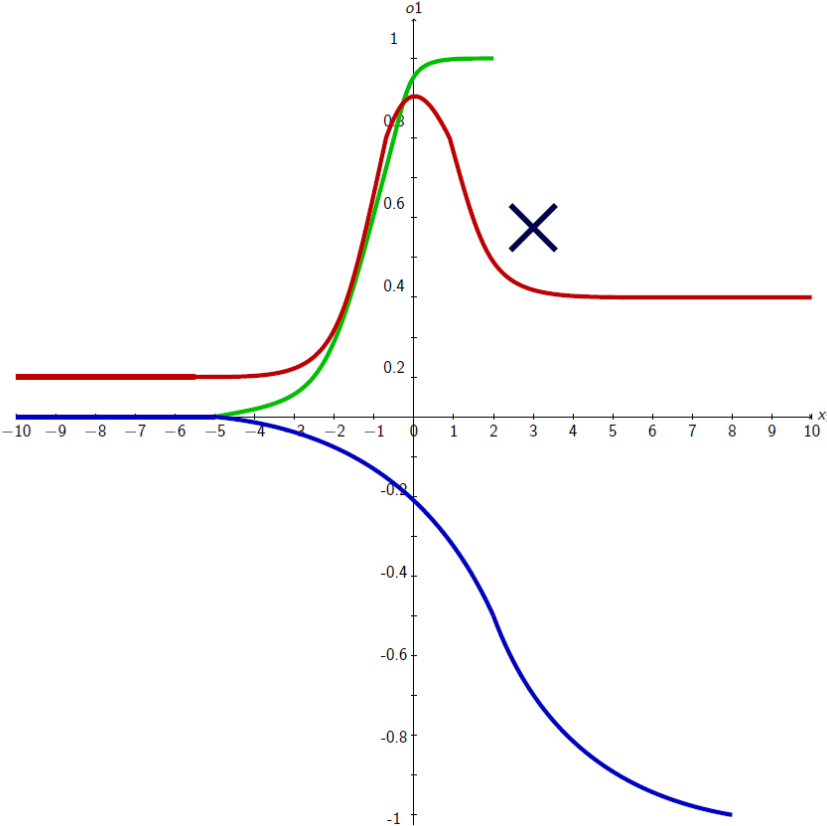
- We can compute the derivative $f'(a)$ simply from $f(a)$!

BackPropagation Example

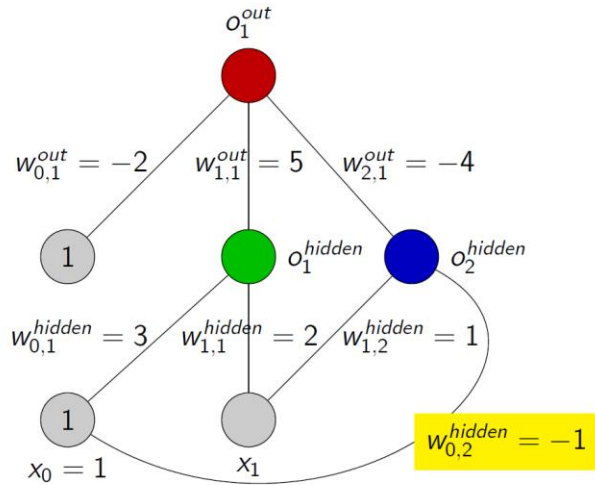
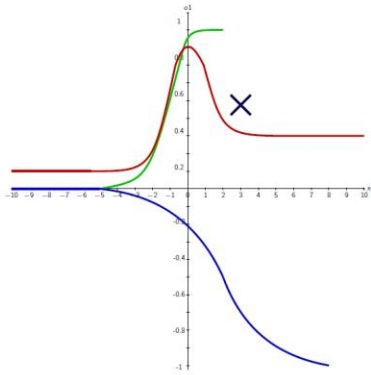
1D Example



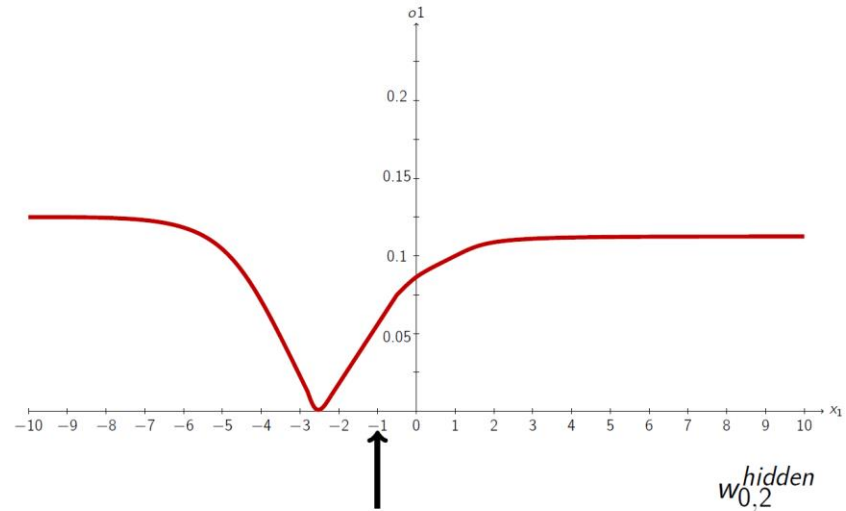
Training Pattern: $x = 3, y(x) = 0.6$



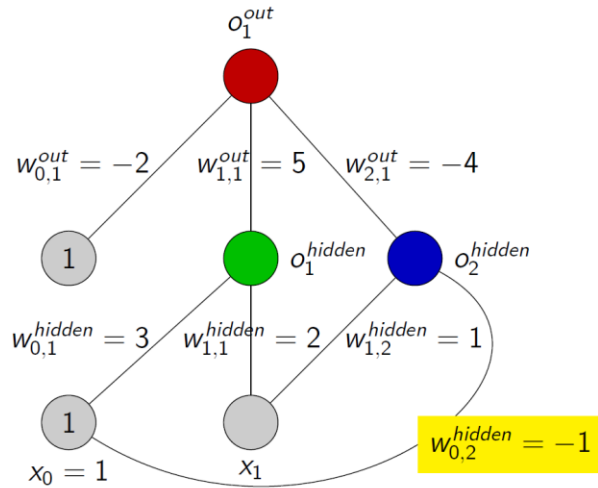
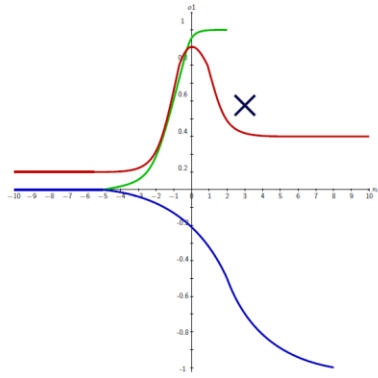
BackPropagation Example



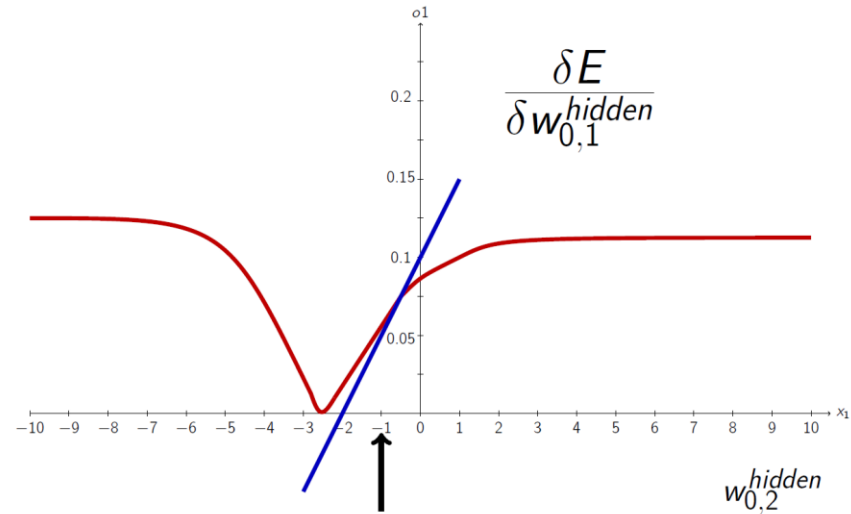
$$E(w_{0,2}^{hidden})$$



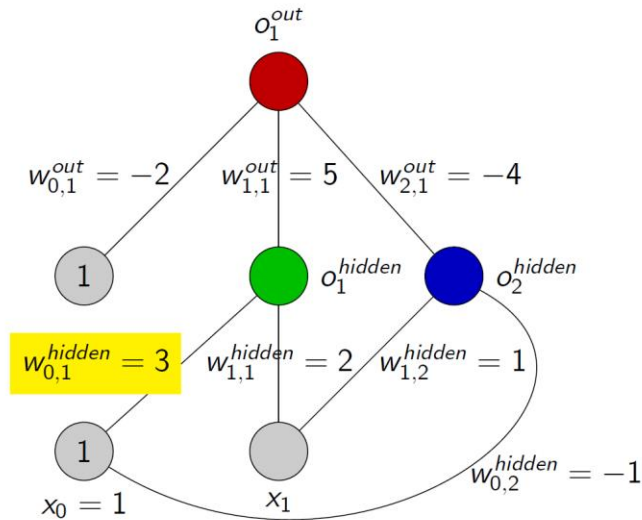
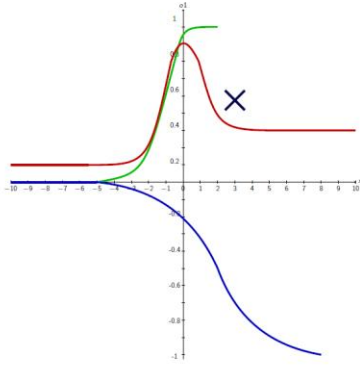
BackPropagation Example



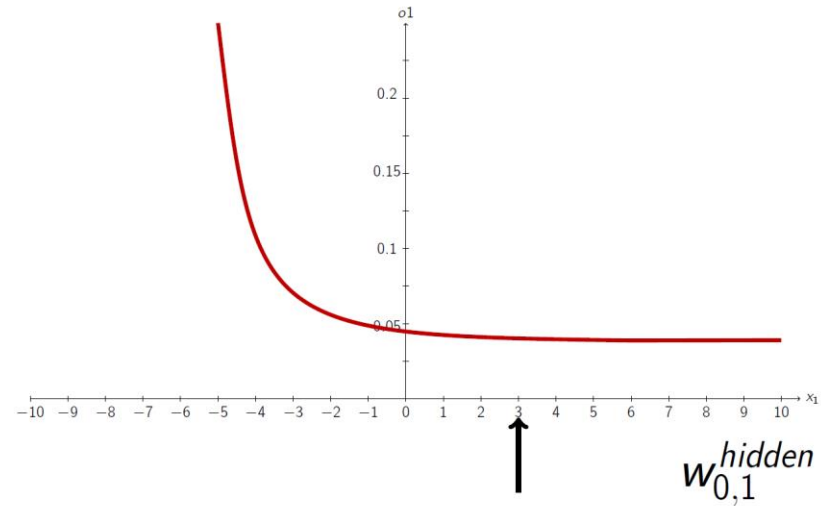
$$E(w_{0,2}^{hidden})$$



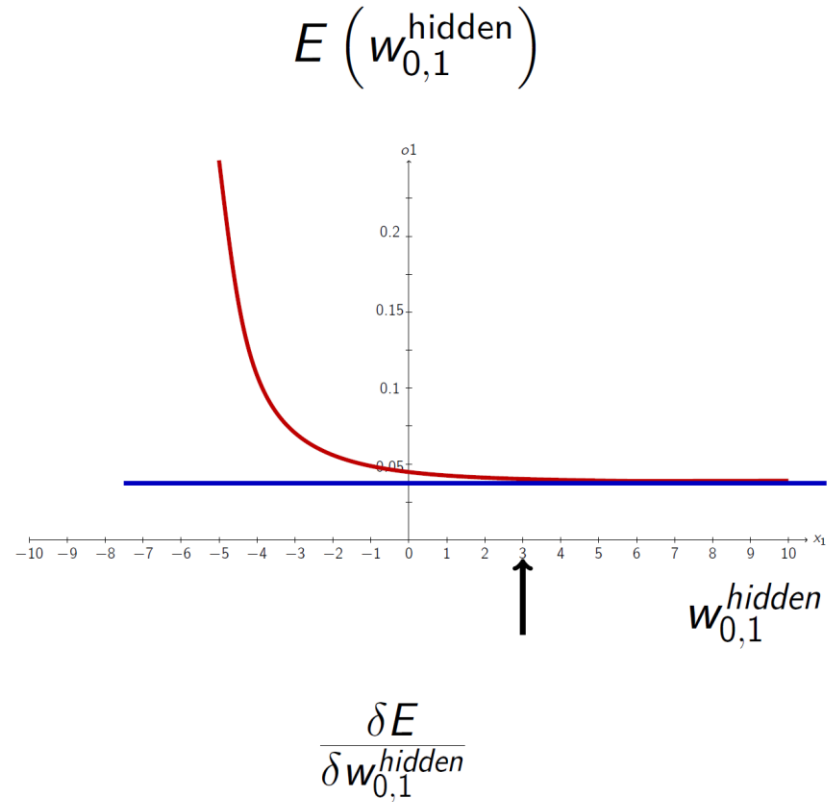
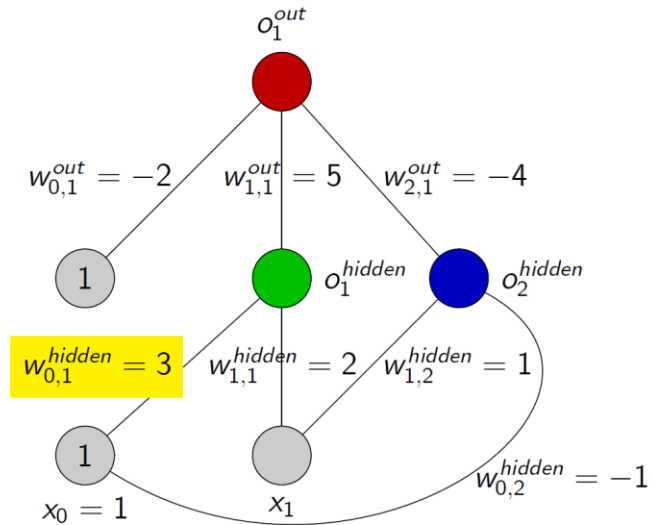
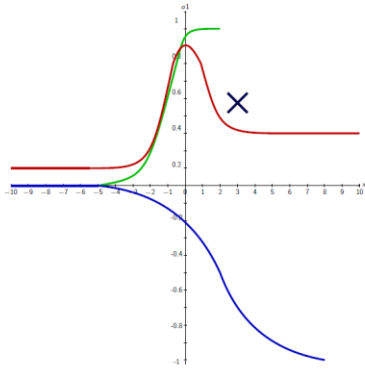
BackPropagation Example



$$E(w_{0,1}^{hidden})$$



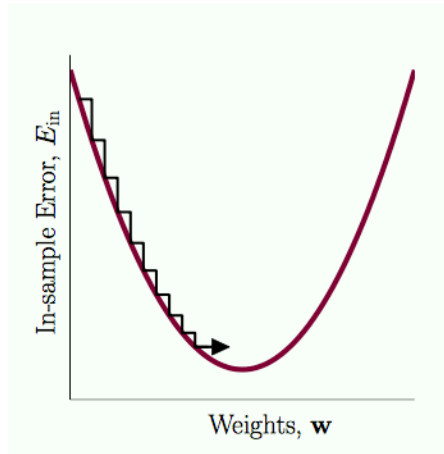
BackPropagation Example



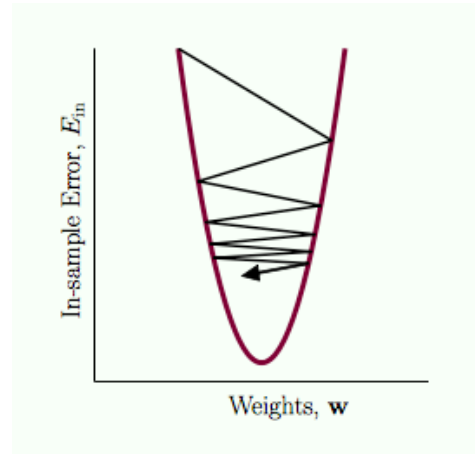
Variations of BackPropagation

- Backpropagation as a gradient descent technique can only find a local minimum.
- Training the networks with different random initialisations can lead to a different weight configuration on a different local minimum.
- The learning rate η defines the step width of the gradient descent technique.
 - A very large η leads to skipping minima or oscillations.
 - A very small η leads to starving, i.e. slow convergence or even convergence before the (local) minimum is reached.

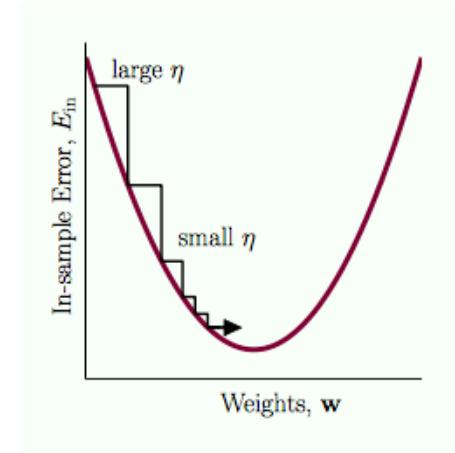
η too small



η too large



η just right



- Feed-Forward Neural Networks can potentially describe very complex relationships
- FFNNs are very simple but very flexible neural architectures
- It is easy to:
 - Expand the architecture by adding more units/layers
 - Experiment with new activation functions
- Too many parameters!
- Danger of fitting training data too well: Overfitting
 - Modeling of particularities in training data instead of underlying concept
 - ⇒ Modeling of artifacts or outliers

- Overfitting can be prevented by keeping the weights small
- **Weight Decay:**
 - push all weights to zero
 - only those weights that are really needed will “survive”
- **Momentum Term:**
 - increase weight updates as long as they have the same sign
- **Resilient Backpropagation (or RPROP):**
 - estimate optimum for weights based on assumption that the error surface is a polynomial.
- **Regularization:**
 - a regularization term is added to the Error function as to force the weights to stay small or few.

- Introduce a **momentum term**:
- For the weight update, the previous weight update is taken into account:

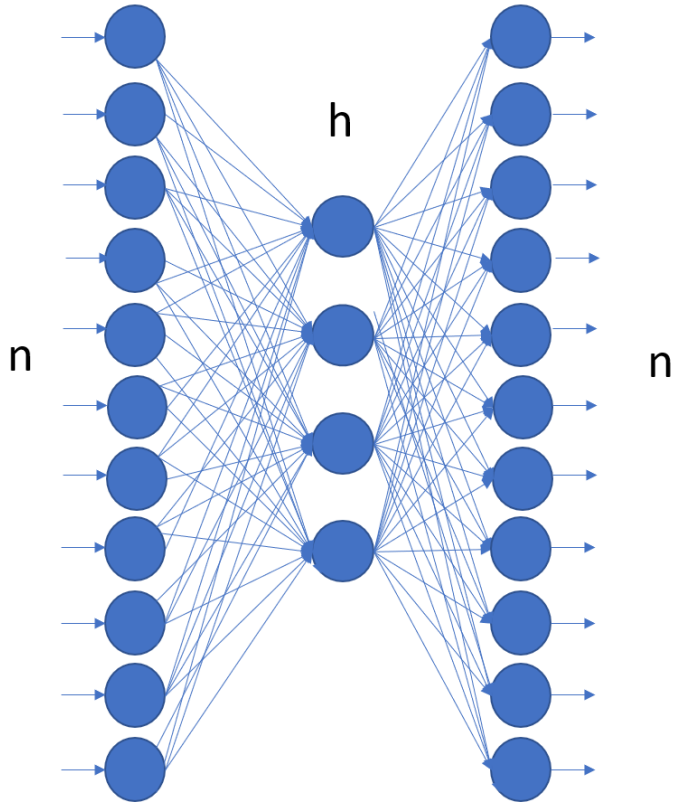
$$\Delta_p W(u, v) = \eta \delta_v^p o_u^p + \beta \Delta_q W(u, v)$$

- $\Delta_q W(u, v)$ is the weight update at the previous step q of the gradient descent algorithm.
- If weight is updated continuously in the same direction, the weight update increases, otherwise it decreases.
- Typical choices: $\eta = 0.2$, $\beta = 0.8$

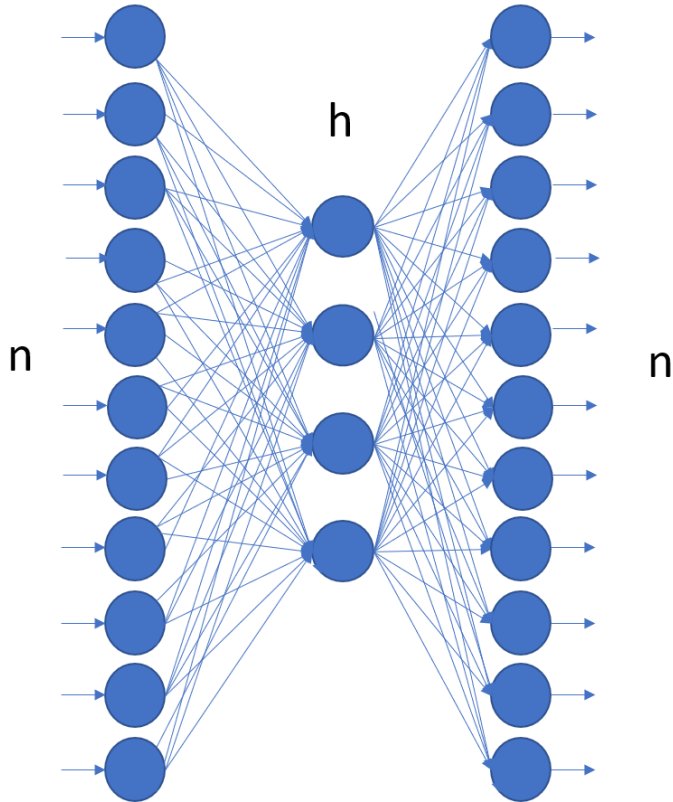
- MLPs are powerful but black boxes
- Rule extraction only possible in some cases
 - VI-Analysis (interval propagation)
 - extraction of decision trees
- Problems:
 - Global influence of each neuron
 - Interpretation of hidden layer(s) complicated
- Possible Solution:
 - Local activity of neurons in hidden layer: Local Basis Function Networks

- Usually, weights are not updated after a whole epoch, i.e. after all patterns have been presented once (offline training), or after the presentation of each input pattern (online training, but after a batch of input patterns (batch training)).
- There is no general rule on how to choose the number of hidden layers and the size of the hidden layers.
 - Small neural networks might not be flexible enough to fit the data.
 - Large neural networks tend to overfit the data (note: Deep Learning...).
- The steepness of the activation function is usually fixed and is not adjusted.
- A perceptron learns only in those regions where the activation function is not close to zero or one, otherwise the derivative is almost zero (the problem of the vanishing gradient).

The autoencoder architecture



- **Dimensionality reduction**
- Input and output are identical, i.e. the neural network should learn the identity function. (Auto-associative network)
- Introduce a hidden layer with only $h < n$ neurons: the bottleneck.
- Train the neural network with the data.
- After training, input the data into the network and use the outputs of the bottleneck neurons as a representation of the input data in a lower dimension
- If $h = 2$ then the outputs of the bottleneck neurons represent the two dimensions for the graphical representation of the data

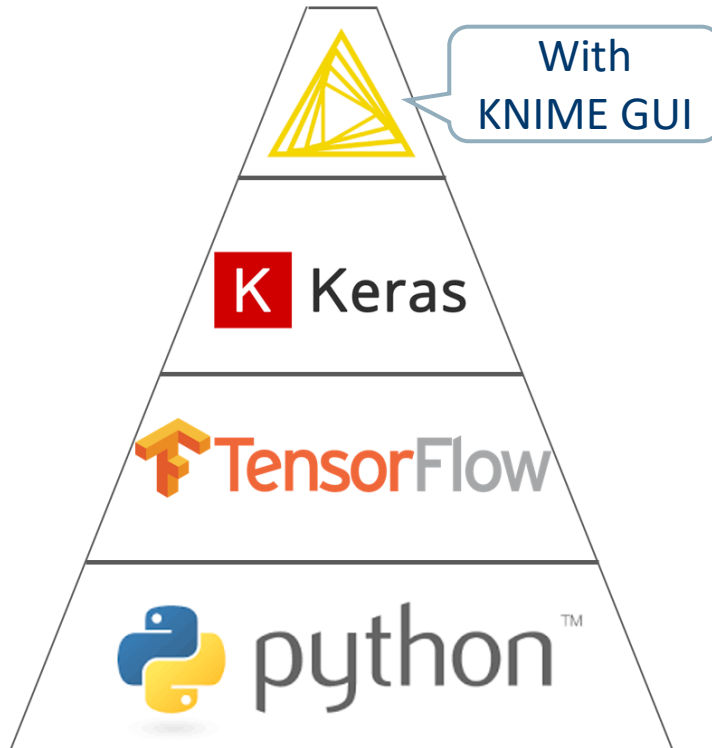


- **Anomaly Detection**
- Input and output are identical, i.e. the neural network should learn the identity function. (Auto-associative network)
- Train the neural network with the data.
- After training, input the data into the network and calculate the distance between input and output layer.
- If input data is similar to training data, then distance is small.
- If input data is an anomaly not present in the training data, then distance is large

- (Hard/Soft) Competitive Learning
- Learning Vector Quantization
- Self Organizing Maps
- Radial (and other) Basis Function Networks
- Many connections to Kernel Methods and Support Vector Machines...

- What is a Perceptron?
- Why do we need MLPs?
- The BackPropagation algorithm to train the hidden layers
- Issues with MLPs and BackPropagation
- The autoencoder architecture

KNIME Deep Learning Keras Extension



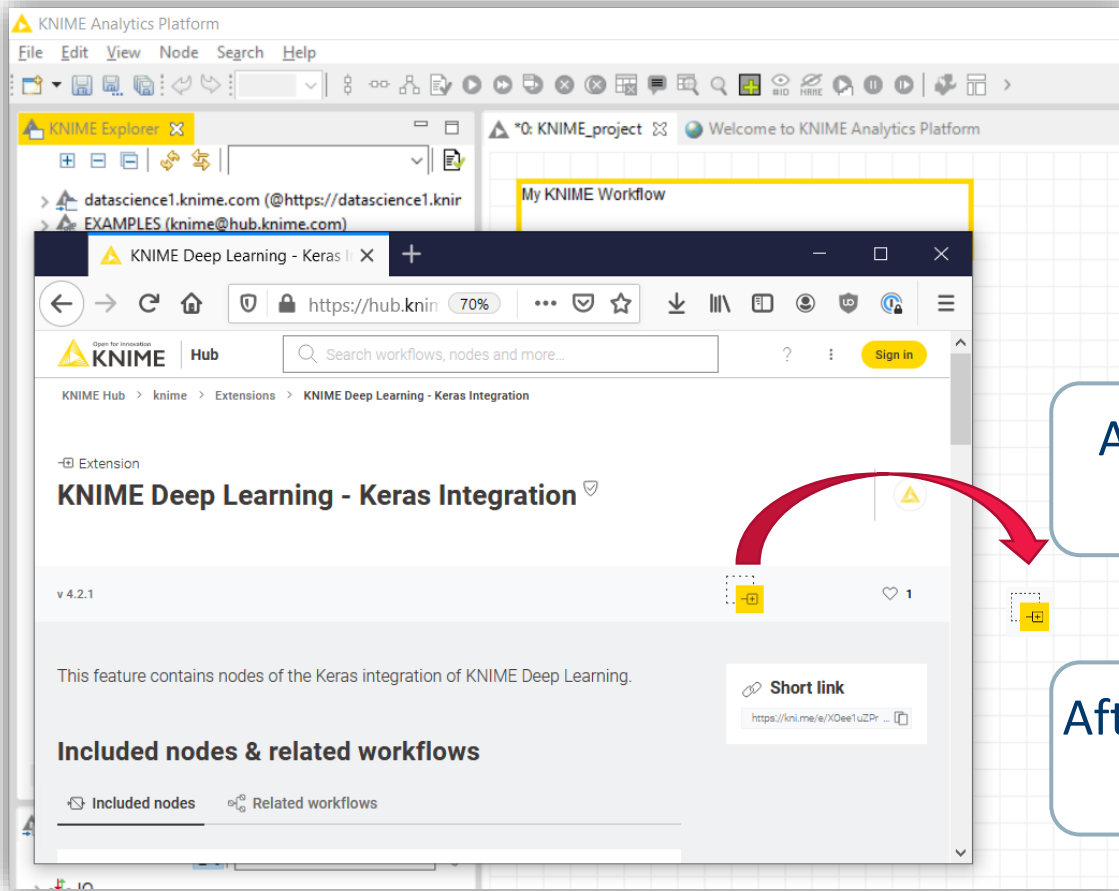
- KNIME Deep Learning Extension builds on top of the Keras Libraries
- The Keras libraries build on top of TensorFlow
- Deep Learning libraries from TensorFlow and Keras are accessible via Python ...
- ... And KNIME with the Deep Learning Keras Integration.

Installation

- Deep Learning in KNIME Analytics Platform comes with a specific integration. Few simple steps are necessary to get it up and running.
- On your machine:
 - **Anaconda** with Python3 correctly installed
- Extensions installed on KNIME Analytics Platform
 - **KNIME Deep Learning - Keras Integration**
 - **KNIME TensorFlow Integration**

NOTE: This is a just quick start guide to start using Deep Learning with your KNIME Analytics Platform. If you are experiencing issues or want to customize your installation, please refer to [KNIME Deep Learning Integration Installation Guide](#)

Installation of KNIME Extensions

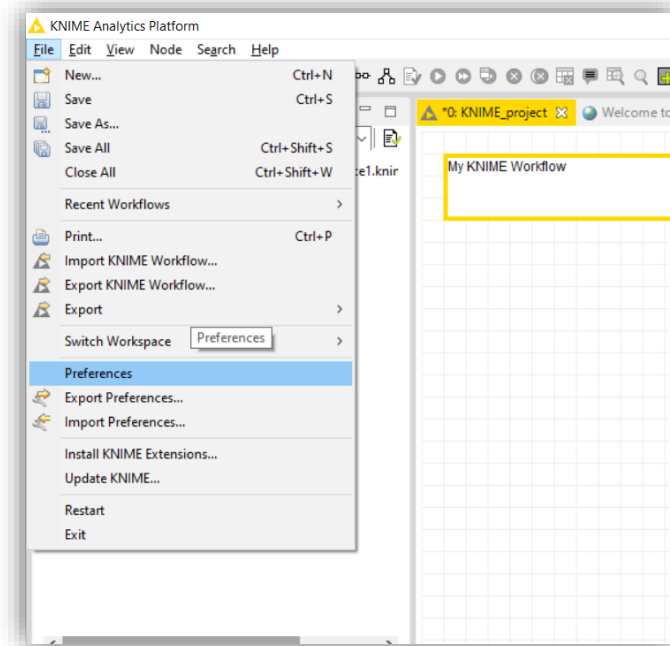


Drag and drop the icon into the KNIME Workbench

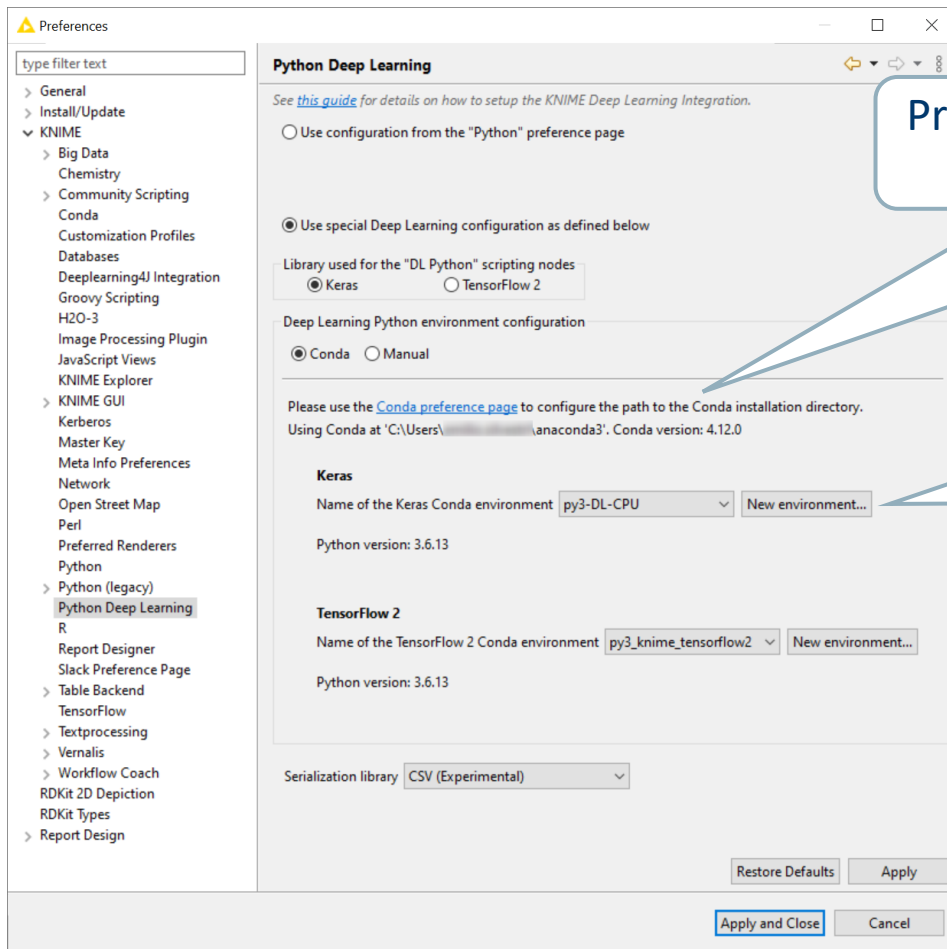
A window will pop up asking to install the Extension

After installation you will be asked to restart KNIME

- Go to the Python Deep Learning Preference page located at *File > Preferences*



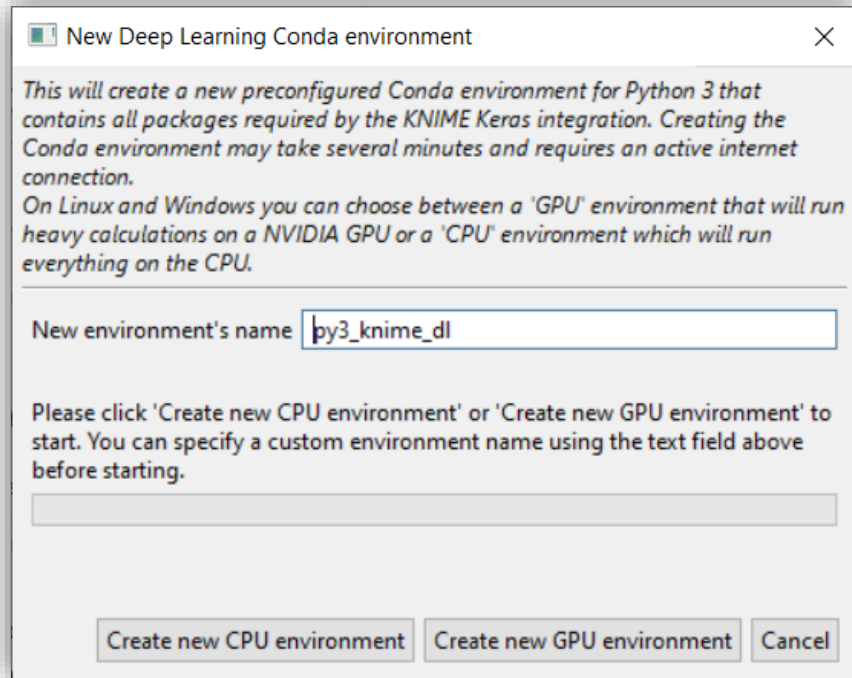
- From the window that pops up, select *KNIME > Python Deep Learning* from the list on the left.



Provide the path to the folder containing your Anaconda installation

Click on **New Environment** to set up a new ready-to-go environment containing all the required dependencies

NOTE: You can also select an existing Python Deep Learning environment from the drop down menu, if you have already set up one



- Provide a name for the new environment
- Choose if you want to create a new CPU or GPU environment
- This creates a new *conda* environment containing all required Python Deep Learning dependencies

Only choose GPU if you have a TensorFlow compatible GPU available. More information about Python Deep Learning GPU support can be found [here](#)

Deep Learning Nodes

Layer Overview (optional)

▼ Deep Learning

▼ Keras

▼ Layers

▶ Advanced Activations

▶ Convolution

▶ Core

▶ Embedding

▶ Locally Connected

▶ Merge

▶ Noise

▶ Normalization

▶ Pooling

▶ Recurrent

⊗ Keras Collect Layer

⊗ Keras Freeze Layers

▼ Advanced Activations

- ⊗ Keras ELU Layer
- ⊗ Keras Leaky ReLU Layer
- ⊗ Keras PReLU Layer
- ⊗ Keras Softmax Layer
- ⊗ Keras Thresholded ReLU Layer

▼ Convolution

- ⊗ Keras Convolution 1D Layer
- ⊗ Keras Convolution 2D Layer
- ⊗ Keras Convolution 3D Layer
- ⊗ Keras Cropping 1D Layer
- ⊗ Keras Cropping 2D Layer
- ⊗ Keras Cropping 3D Layer
- ⊗ Keras Separable Convolution 1D Layer
- ⊗ Keras Separable Convolution 2D Layer
- ⊗ Keras Transposed Convolution 2D Layer
- ⊗ Keras Upsampling 1D Layer
- ⊗ Keras Upsampling 2D Layer
- ⊗ Keras Upsampling 3D Layer
- ⊗ Keras Zero-Padding 1D Layer
- ⊗ Keras Zero-Padding 2D Layer
- ⊗ Keras Zero-Padding 3D Layer

▼ Core

- ⊗ Keras Activation Layer
- ⊗ Keras Activity Regularization Layer
- ⊗ Keras Dense Layer
- ⊗ Keras Dropout Layer
- ⊗ Keras Flatten Layer
- ⊗ Keras Input Layer
- ⊗ Keras Masking Layer
- ⊗ Keras Permute Layer
- ⊗ Keras Repeat Layer
- ⊗ Keras Reshape Layer

▼ Embedding

- ⊗ Keras Embedding Layer

▼ Locally Connected

- ⊗ Keras Locally Connected 1D Layer
- ⊗ Keras Locally Connected 2D Layer

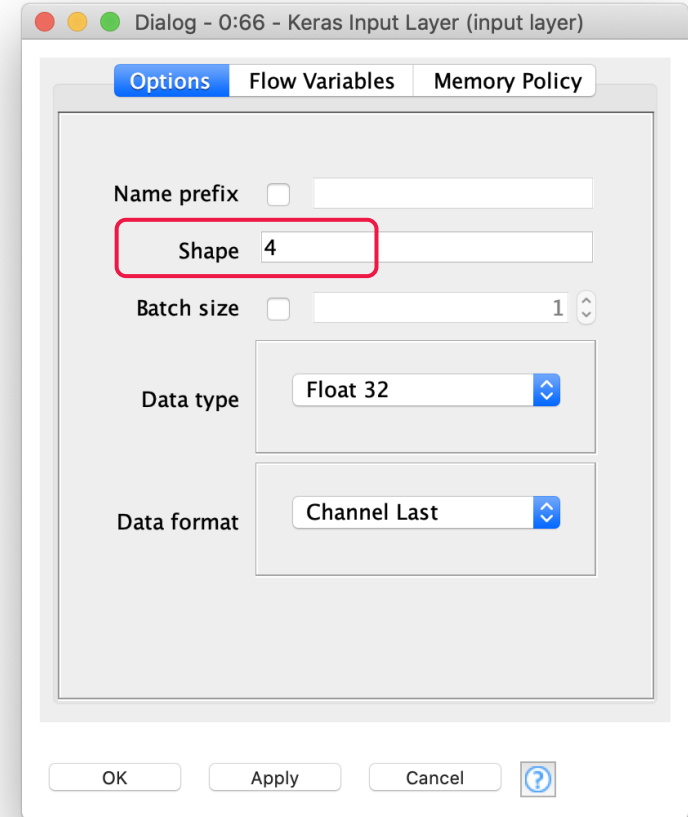
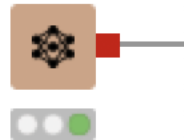
▼ Merge

- ⊗ Keras Add Layer
- ⊗ Keras Average Layer
- ⊗ Keras Concatenate Layer
- ⊗ Keras Dot Layer
- ⊗ Keras Maximum Layer
- ⊗ Keras Multiply Layer
- ⊗ Keras Subtract Layer

Keras Input Layer

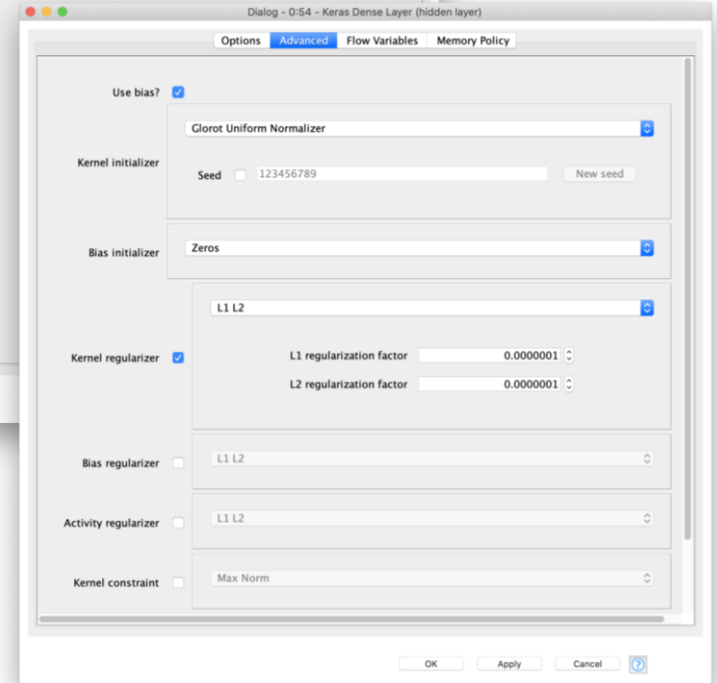
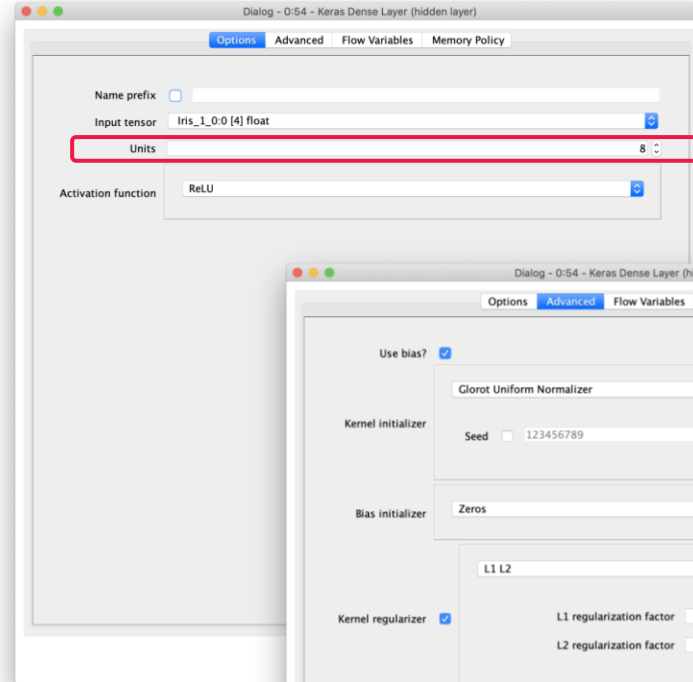
- Allows to define the input shape
- Use $[x,y]$ for sequential data
 - x = sequence length
 - y = dimension of one element in the sequence

Keras Input Layer

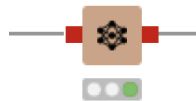


Keras Dense Layer

- Important settings
 - Number of Units
 - Selection of the activation function
- Regularization support
- Can be used as hidden layer and as output layer
- Tip: Add Name prefix if used as output layer

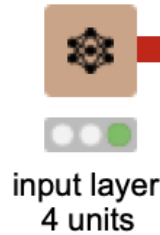


Keras Dense Layer

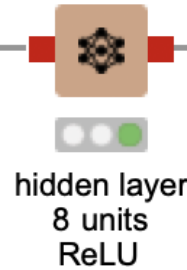


Simple Network Example

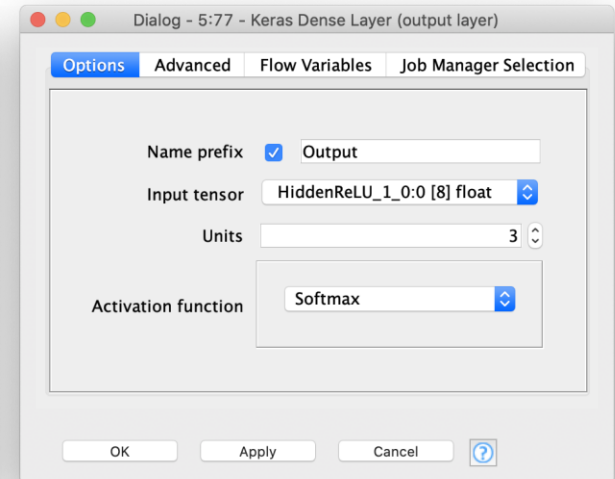
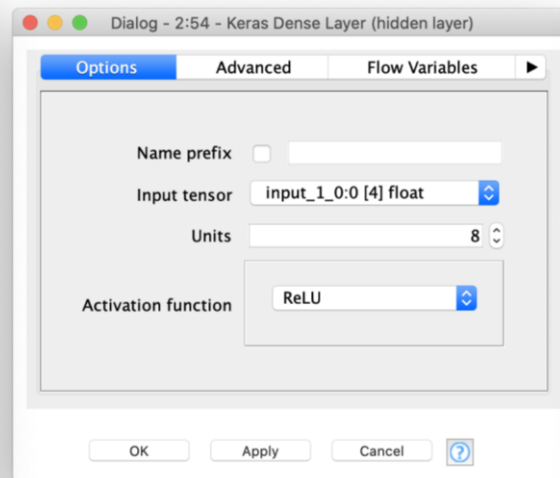
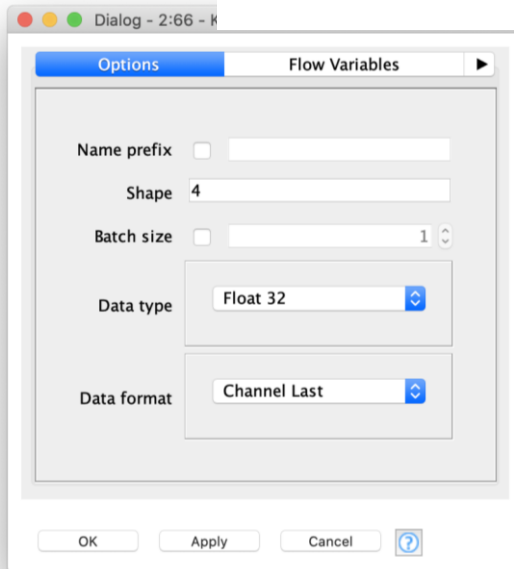
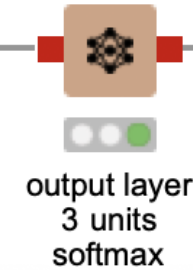
Keras Input Layer



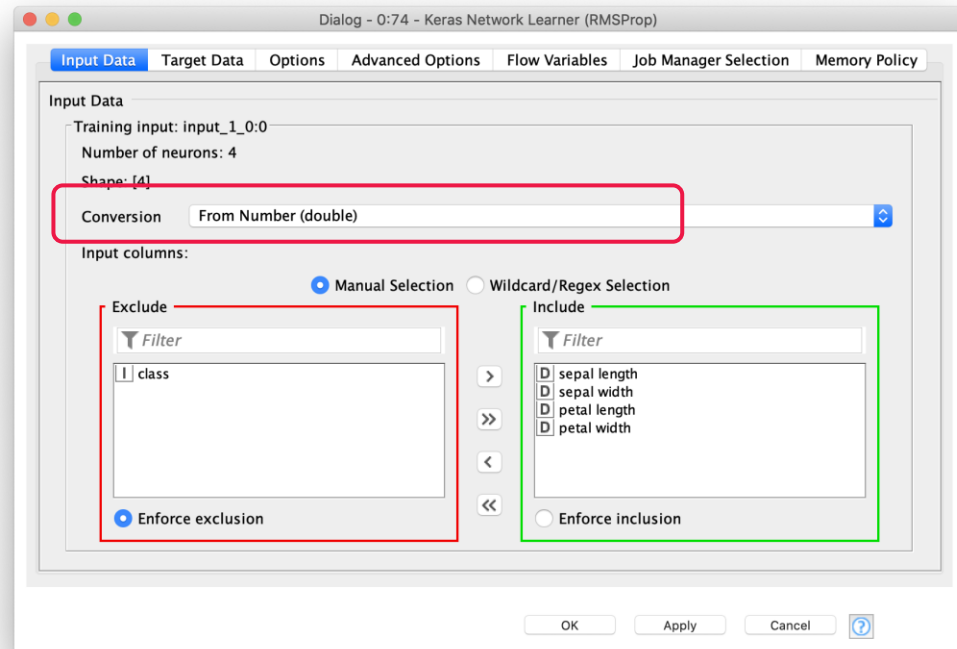
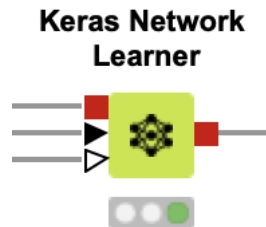
Keras Dense Layer



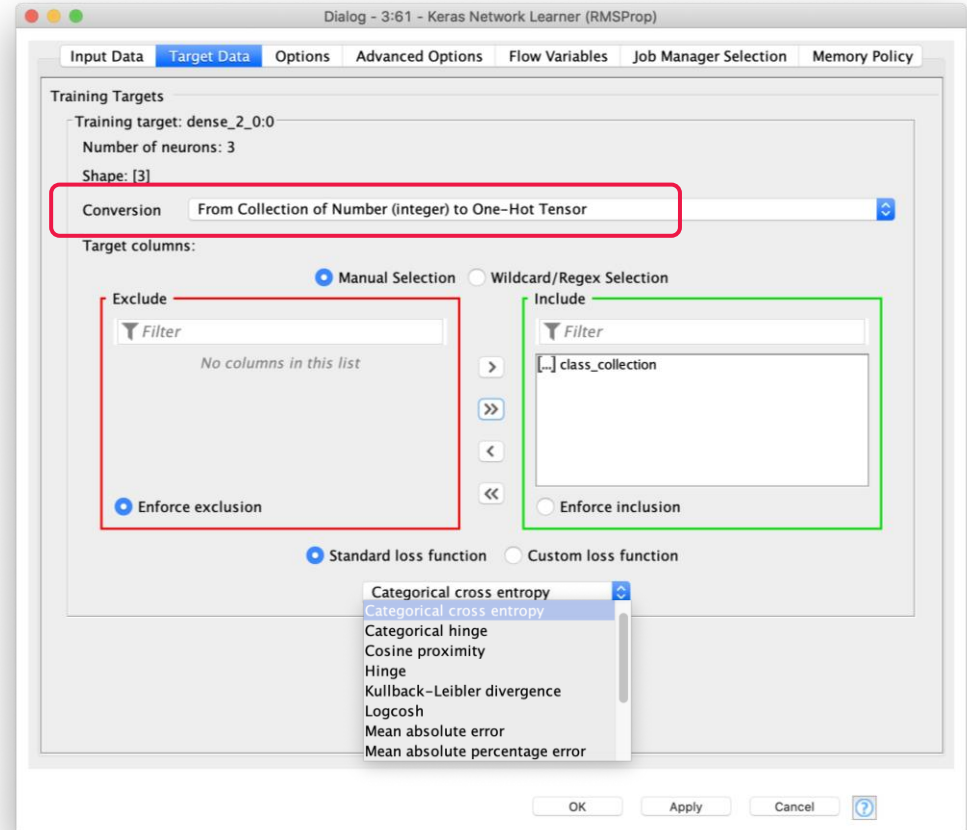
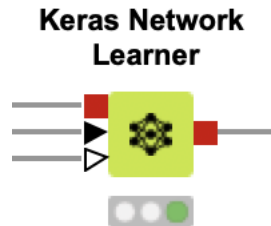
Keras Dense Layer



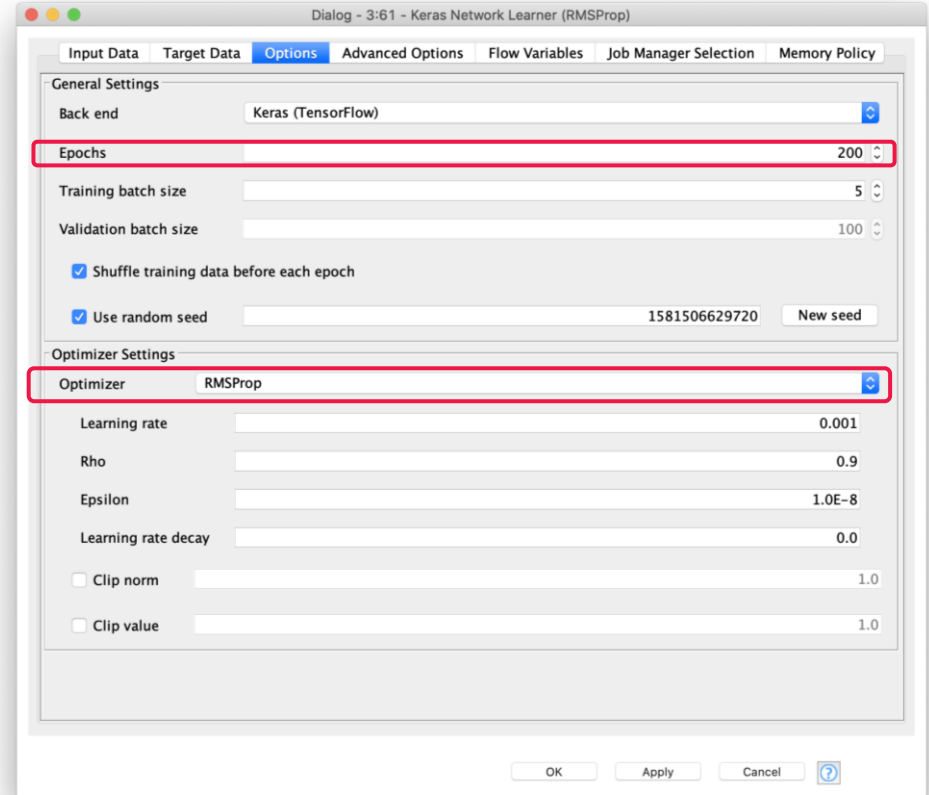
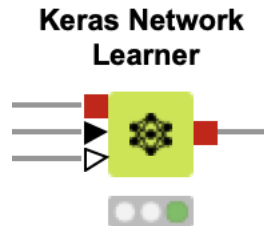
- Select input columns for the network and correct conversion
- Conversion "From Collection of Number (integer) to One-Hot Vector" can be used to transform index encoding to one-hot encoding



- Select target column and correct conversion
- Select a standard loss function or define your custom loss function

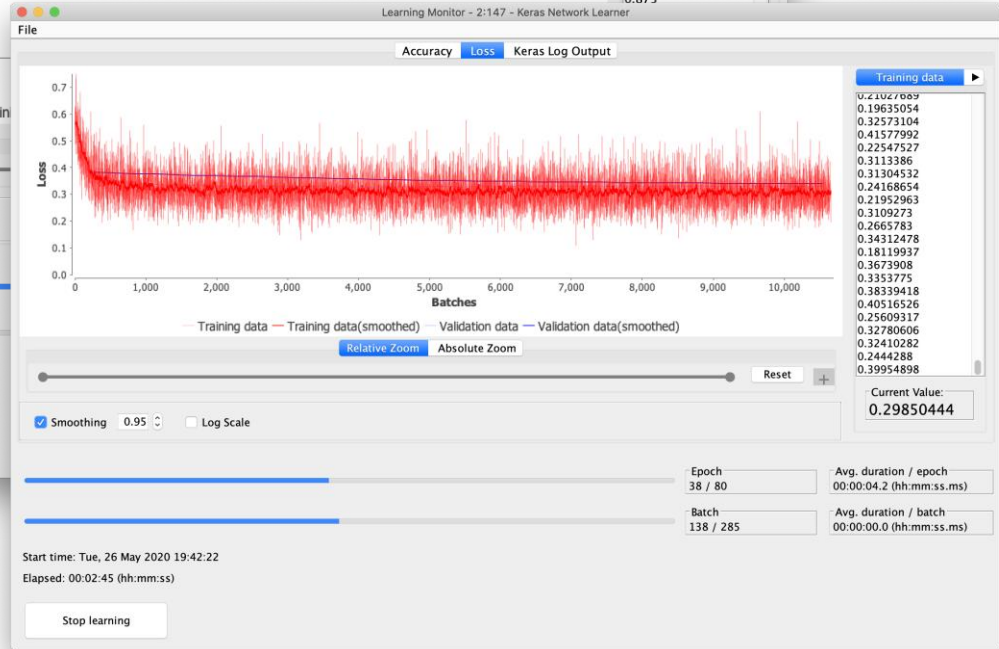
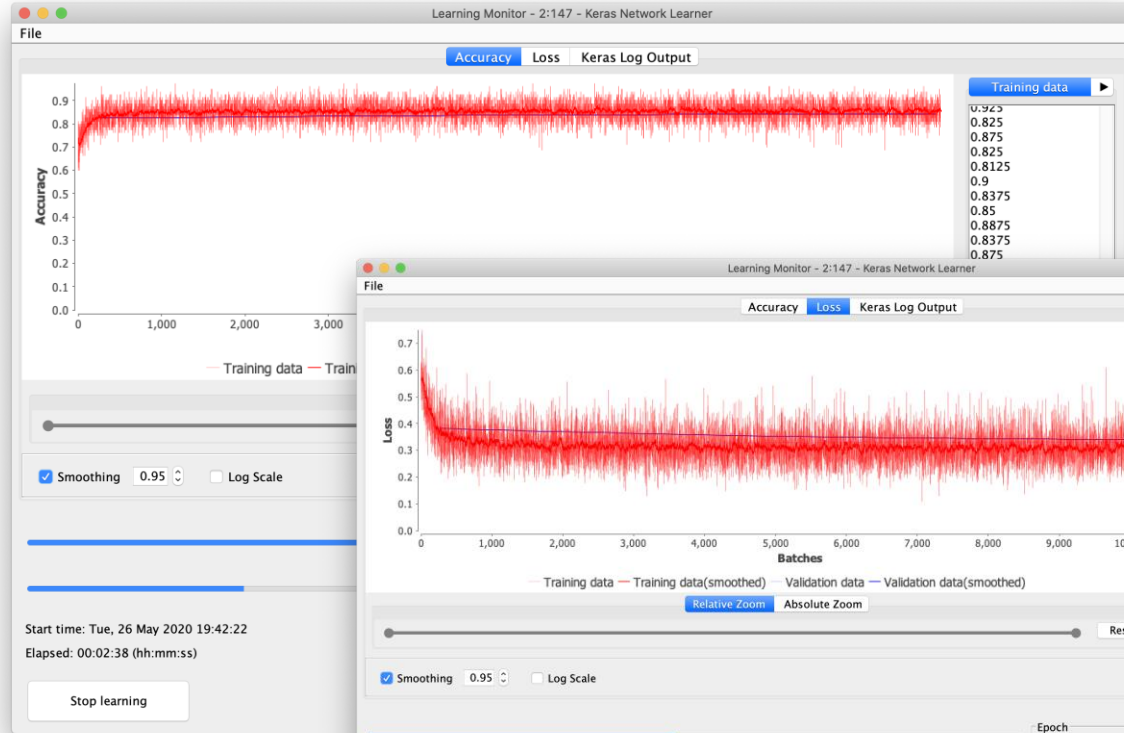


- Allows to define the training settings
- Important settings
 - Epochs
 - Training batch size
 - Shuffle training data...
 - Optimizer

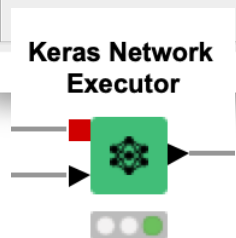
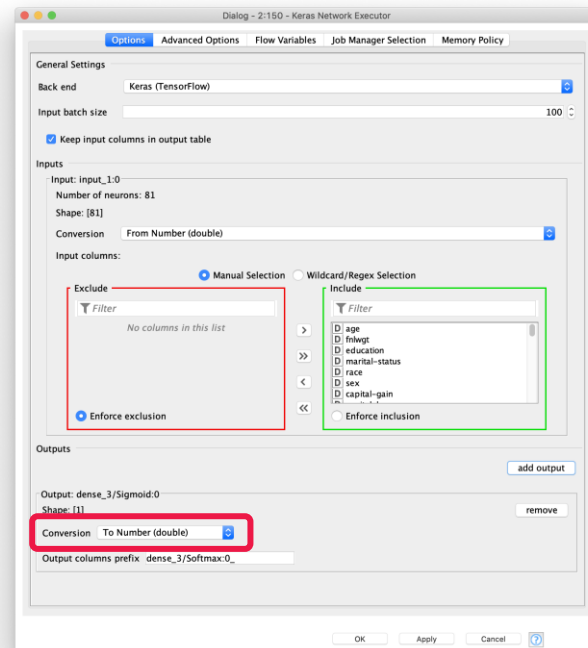
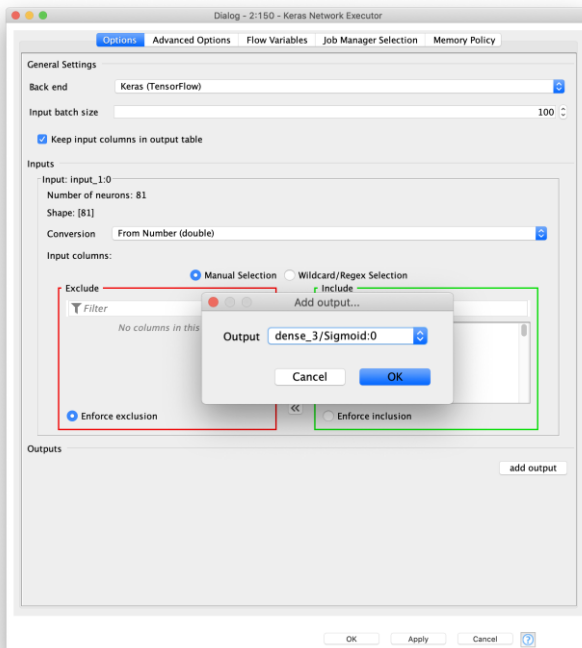
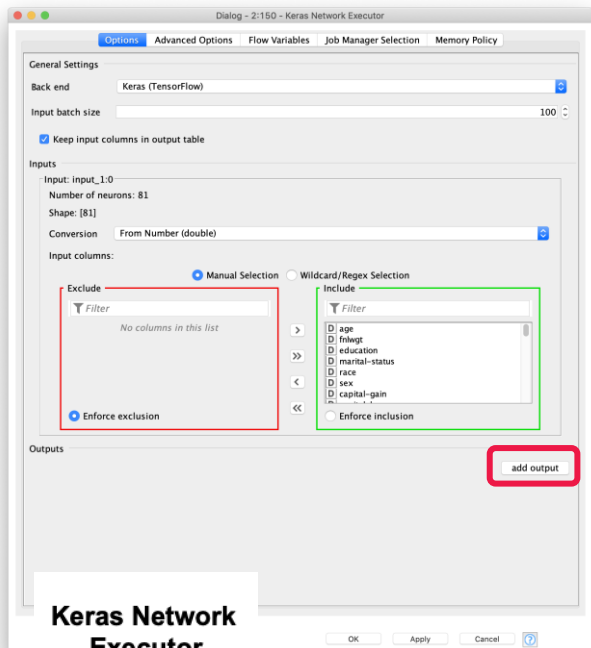


Learning Monitor View of the Keras Network Learner

A screenshot of the context menu for the 'Keras Network Learner' node in a workflow editor. The menu items include: Configure... (F6), Execute (F7), Execute and Open Views (⇧F10), Cancel (F9), Reset (F8), Edit Node Description... (⌘F2), New Workflow Annotation, Connect selected nodes (⌘L), Disconnect selected nodes (⇧⌘L), Create Metanode..., Create Component..., View: Learning Monitor (highlighted in blue), and Compare Nodes. Below the menu, there are sections for 'Show Flow Variable Ports' and standard editing actions: Cut, Copy, Paste, Undo, Redo, and Delete. The 'Keras Network' icon is visible at the bottom of the menu.



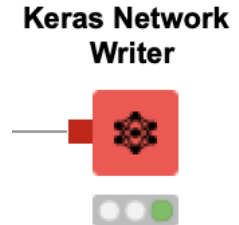
Keras Network Executor



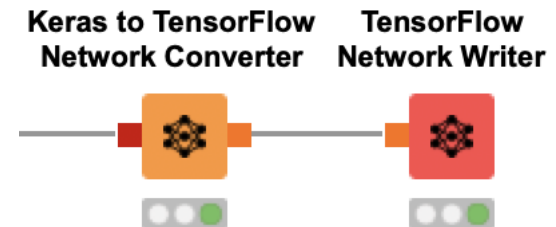
Different Option to Save a Trained Model

- The Keras Network Writer node saves the trained model as .h5 file

knime://knime.workflow/<filename>



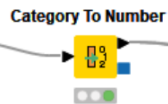
- Convert your model to a TensorFlow Network for faster execution during deployment and save it as .zip file using the TensorFlow Writer node



Index-based encoding and One-hot Encoding

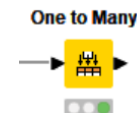
Index-based

Education	Index
10th	0
11th	1
12th	2
Assoc-acdm	3
Assoc-voc	4
Bachelors	5
Doctorate	6
HS-grad	7
Masters	8
Prof-school	9
Some-college	10



One-hot Encoding

	10th	11th	12th	Assoc-admin	Assoc-voc	Bach.	Doc.	HS-grad	Masters	Prof-school	Some-college
Masters	0	0	0	0	0	0	0	0	1	0	0
11th	0	1	0	0	0	0	0	0	0	0	0
Some-college	0	0	0	0	0	0	0	0	0	0	1
Bach.	0	0	0	0	0	1	0	0	0	0	0
10th	1	0	0	0	0	0	0	0	0	0	0
Doc.	0	0	0	0	0	0	1	0	0	0	0
Prof-school	0	0	0	0	0	0	0	0	0	1	0
HS-grad	0	0	0	0	0	0	0	1	0	0	0



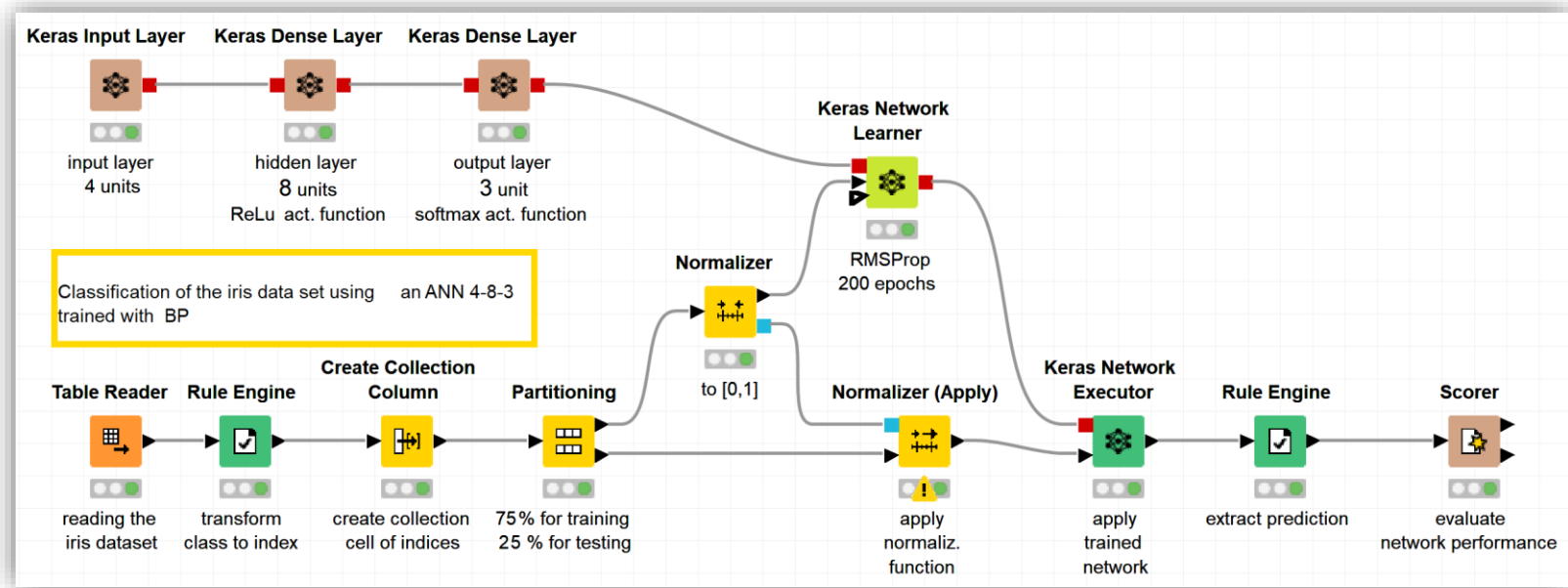
Normalization

- Input to NN must be in $[0,1]$
- Normalization is needed



Practical Examples with KNIME Analytics Platform

- A multilayer perceptron with layers (4–8–3) is trained to classify the iris data set using the backpropagation algorithm, as set in the Keras Network Learner node



Thank you

Guide to Intelligent Data Science Second Edition, 2020