



**Artificial Intelligence**

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**Neural Networks**




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**Where are we?** 

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2	Propositional Logic
3	Predicate Logic
4	Reasoning
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**Agenda** 

- Motivation
- Technical Solution
  - (Artificial) Neural Networks
  - Perceptron
  - Artificial Neural Network Structures
  - Learning and Generalization
  - Expressiveness of Multi-Layer Perceptrons
- Illustration by Larger Examples
- Summary

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**MOTIVATION**

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**Motivation**

- A main motivation behind neural networks is the fact that symbolic rules do not reflect reasoning processes performed by humans.
- Biological neural systems can capture highly parallel computations based on representations that are distributed over many neurons.
- They learn and generalize from training data; no need for programming it all...
- They are very noise tolerant – better resistance than symbolic systems.

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**Motivation**

- Neural networks are strong in:
  - Learning from a set of examples
  - Optimizing solutions via constraints and cost functions
  - Classification: grouping elements in classes
  - Speech recognition, pattern matching
  - Non-parametric statistical analysis and regressions


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**TECHNICAL SOLUTIONS**

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**(Artificial) Neural Networks**

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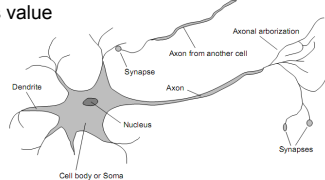
**What are Neural Networks?** 

- A biological neural network is composed of groups of chemically connected or functionally associated neurons.
- A single neuron may be connected to many other neurons and the total number of neurons and connections in a network may be extensive.
- Neurons are highly specialized cells that transmit impulses within animals to cause a change in a target cell such as a muscle effector cell or a glandular cell.
- Impulses are noisy "spike trains" of electrical potential.
- Apart from the electrical signaling, neurotransmitter diffusion (endogenous chemicals) can effectuate the impulses.


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**What are Neural Networks?** 

- Connections, called **synapses**, are usually formed from **axons to dendrites**; also other connections are possible.
- The axon is the primary conduit through which the neuron transmits impulses to neurons downstream in the signal chain
- A human has  $10^{11}$  neurons of > 20 types,  $10^{14}$  synapses, 1ms-10ms cycle time.
- There are  $10^{11}$  in a galaxy, and  $10^{11}$  galaxies in the universe.
- Not only the impulse carries value but also the frequency of oscillation, hence neural networks have an even higher complexity.




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**What are Neural Networks?** 

- Metaphorically speaking, a thought is a specific self-oscillation of a network of neurons.
- The topology of the network determines its resonance.
- However, it is the resonance in the brain's interaction with the environment and with itself that creates, reinforces or decouples interaction patterns.
- *The brain is not a static device, but a device that is created through usage...*

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**What are Neural Networks?** 

- What we refer to as Neural Networks, in this course, are mostly Artificial Neural Networks (ANN).
- ANN are approximations of biological neural networks and are built of physical devices, or simulated on computers.
- ANN are parallel computational entities that consist of multiple simple processing units that are connected in specific ways in order to perform the desired tasks.
- Remember: **ANN are computationally primitive approximations of the real biological brains.**

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# Perceptron

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## Artificial Neurons - McCulloch-Pitts „Unit“

- Output is a „squashed“ linear function of the inputs:

- A clear oversimplification of real neurons, but its purpose is to develop understanding of what networks of simple units can do.

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## Activation Functions

(a) is a step function or threshold function, signum function  
 (b) is a sigmoid function  $1/(1+e^{-x})$

- Changing the bias weight  $W_{0,i}$  moves the threshold location


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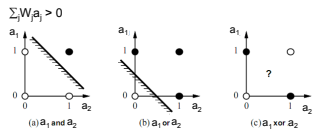
## Perceptron

- McCulloch-Pitts neurons can be connected together in any desired way to build an artificial neural network.
- A construct of one input layer of neurons that feed forward to one output layer of neurons is called **Perceptron**.


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**Expressiveness of Perceptrons** 

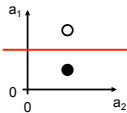
- A perceptron with  $g = \text{step function}$  can model Boolean functions and linear classification:
  - As we will see, a perceptron can represent AND, OR, NOT, but not XOR
- A perceptron represents a linear separator for the input space



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**Expressiveness of Perceptrons (2)** 

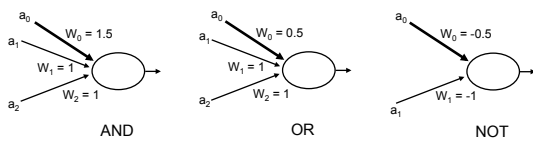
- Threshold perceptrons can represent only linearly separable functions (i.e. functions for which such a separation hyperplane exists)



- Such perceptrons have limited expressivity.
- There exists an algorithm that can fit a threshold perceptron to any linearly separable training set.


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**Example: Logical Functions** 




- McCulloch and Pitts: Boolean function can be implemented with a artificial neuron (not XOR).

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**Example: Finding Weights for AND Operation** 

- There are two input weights  $W_1$  and  $W_2$  and a threshold  $W_0$ . For each training pattern the perceptron needs to satisfy the following equation:
 
$$\text{out} = g(W_1 \cdot a_1 + W_2 \cdot a_2 - W_0) = \text{sign}(W_1 \cdot a_1 + W_2 \cdot a_2 - W_0)$$
- For a binary AND there are four training data items available that lead to four inequalities:
  - $W_1 \cdot 0 + W_2 \cdot 0 - W_0 < 0 \Rightarrow W_0 > 0$
  - $W_1 \cdot 0 + W_2 \cdot 1 - W_0 < 0 \Rightarrow W_2 < W_0$
  - $W_1 \cdot 1 + W_2 \cdot 0 - W_0 < 0 \Rightarrow W_1 < W_0$
  - $W_1 \cdot 1 + W_2 \cdot 1 - W_0 \geq 0 \Rightarrow W_1 + W_2 \geq W_0$
- There is an obvious infinite number of solutions that realize a logical AND; e.g.  $W_1 = 1, W_2 = 1$  and  $W_0 = 1.5$ .


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**Limitations of Simple Perceptrons** 

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- XOR:
  - $W_1 \cdot 0 + W_2 \cdot 0 - W_0 < 0 \quad \Rightarrow W_0 > 0$
  - $W_1 \cdot 0 + W_2 \cdot 1 - W_0 \geq 0 \quad \Rightarrow W_2 \geq W_0$
  - $W_1 \cdot 1 + W_2 \cdot 0 - W_0 \geq 0 \quad \Rightarrow W_1 \geq W_0$
  - $W_1 \cdot 1 + W_2 \cdot 1 - W_0 < 0 \quad \Rightarrow W_1 + W_2 < W_0$
- The 2nd and 3rd inequalities are not compatible with inequality 4, and there is no solution to the XOR problem.
- XOR requires two separation hyperplanes!
- There is thus a need for more complex networks that combine simple perceptrons to address more sophisticated classification tasks.

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**Artificial Neural Network Structures**

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**Neural Network Structures** 

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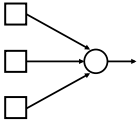
- Mathematically artificial neural networks are represented by weighted directed graphs.
- In more practical terms, a neural network has activations flowing between processing units via one-way connections.
- There are three common artificial neural network architectures known:
  - Single-Layer Feed-Forward (Perceptron)
  - Multi-Layer Feed-Forward
  - Recurrent Neural Network

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**Single-Layer Feed-Forward** 


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- A Single-Layer Feed-Forward Structure is a simple perceptron, and has thus
  - one input layer
  - one output layer
  - NO feed-back connections
- Feed-forward networks implement functions, have no internal state (of course also valid for multi-layer perceptrons).

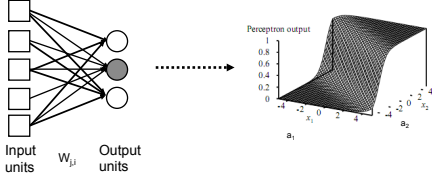


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### Single-Layer Feed-Forward: Example



- Output units all operate separately – no shared weights
- Adjusting weights moves the location, orientation, and steepness of cliff (i.e., the separation hyperplane).




Input units  $W_{ij}$  Output units

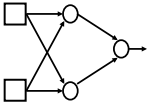
Perceptron output

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### Multi-Layer Feed-Forward




- Multi-Layer Feed-Forward Structures have:
  - one input layer
  - one output layer
  - one or many hidden layers of processing units
- The hidden layers are between the input and the output layer, and thus hidden from the outside world: no input from the world, not output to the world.

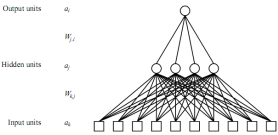


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### Multi-Layer Feed-Forward (2)



- Multi-Layer Perceptrons (MLP) have fully connected layers.
- The numbers of hidden units is typically chosen by hand; the more layers, the more complex the network (see Step 2 of Building Neural Networks)
- Hidden layers enlarge the space of hypotheses that the network can represent.
- Learning done by back-propagation algorithm → errors are back-propagated from the output layer to the hidden layers.




Output units  $a_i$

Hidden units  $a_i$

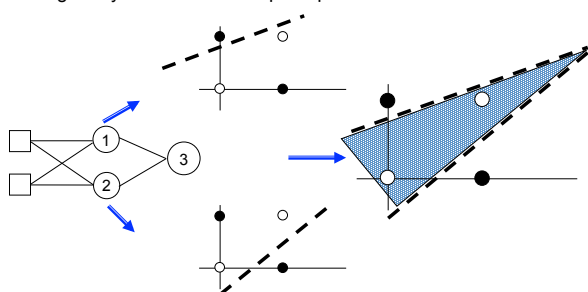
Input units  $a_i$

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### Simple MLP Example



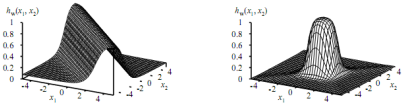
- XOR Problem: Recall that XOR cannot be modeled with a Single-Layer Feed-Forward perceptron.



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**Expressiveness of MLPs** 

- 1 hidden layer can represent all **continuous functions**
- 2 hidden layers can represent **all functions**




- Combining two opposite-facing threshold functions makes a ridge.
- Combining two perpendicular ridges makes a bump.
- Add bumps of various sizes and locations to fit any surface.
- The more hidden units, the more bumps.

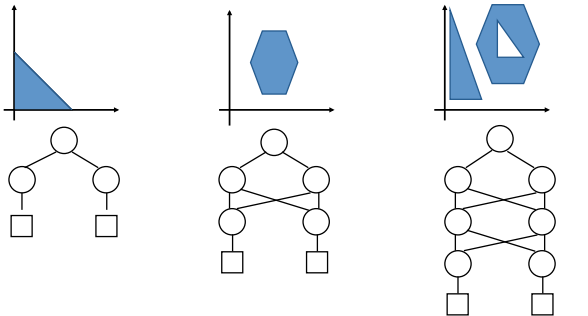
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**Number of Hidden Layers** 

- **Rule of Thumb 1**  
Even if the function to learn is slightly non-linear, the generalization may be better with a simple linear model than with a complicated non-linear model; if there is too little data or too much noise to estimate the non-linearities accurately.
- **Rule of Thumb 2**  
If there is only one input, there seems to be no advantage to using more than one hidden layer; things get much more complicated when there are two or more inputs.


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**Example: Number of Hidden Layers** 

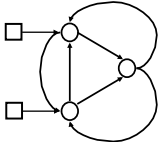


1st layer draws linear boundaries      2nd layer combines the boundaries.      3rd layer can generate arbitrarily boundaries.

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**Recurrent Network** 

- Recurrent networks have at least one feedback connection:
  - They have directed cycles with delays: they have internal states (like flip flops), can oscillate, etc.
  - The response to an input depends on the initial state which may depend on previous inputs.
  - This creates an internal state of the network which allows it to exhibit dynamic temporal behaviour; offers means to model short-time memory



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## Building Neural Networks



- Building a neural network for particular problems requires multiple steps:
  1. Determine the input and outputs of the problem;
  2. Start from the simplest imaginable network, e.g. a single feed-forward perceptron;
  3. Find the connection weights to produce the required output from the given training data input;
  4. Ensure that the training data passes successfully, and test the network with other training/testing data;
  5. Go back to Step 3 if performance is not good enough;
  6. Repeat from Step 2 if Step 5 still lacks performance; or
  7. Repeat from Step 1 if the network in Step 6 does still not perform well enough.

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## Learning and Generalization

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## Learning and Generalization



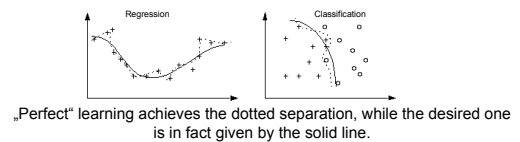
- Neural networks have two important aspects to fulfill:
  - They must learn decision surfaces from training data, so that training data (and test data) are classified correctly;
  - They must be able to generalize based on the learning process, in order to classify data sets it has never seen before.
- Note that there is an important trade-off between the learning behavior and the generalization of a neural network (called over-fitting)
- The better a network learns to successfully classify a training sequence (that might contain errors) the less flexible it is with respect to arbitrary data.

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## Learning vs. Generalization



- Noise in the actual data is never a good thing, since it limits the accuracy of generalization that can be achieved no matter how extensive the training set is.
- Non-perfect learning is better in this case!



- However, injecting artificial noise (so-called **jitter**) into the inputs during training is one of several ways to improve generalization

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### Estimation of Generalization Error



- There are many methods for estimating generalization errors.
- Single-sample statistics
  - Statistical theory provides estimators for the generalization error in non-linear models with a "large" training set.
- Split-sample or hold-out validation.
  - The most commonly used method: reserve some data as a "test set", which must not be used during training.
  - The test set must represent the cases that the ANN should generalize to.
  - A re-run with the random test set provides an unbiased estimate of the generalization error.
  - The disadvantage of split-sample validation is that it reduces the amount of data available for both training and validation.

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### Estimation of Generalization Error



- Cross-validation (e.g., leave one out).
  - In k-fold cross-validation the data is divided into k subsets, and the network is trained k times, each time leaving one subset out for computing the error.
  - The "crossing" makes this method an improvement over split-sampling; it allows all data to be used for training.
  - The disadvantage of cross-validation is that the network must be re-trained many times (k times in k-fold crossing).
- Bootstrapping.
  - Bootstrapping works on random sub-samples (random shares) that are chosen from the full data set.
  - Any data item may be selected any number of times for validation.
  - The sub-samples are repeatedly analyzed.
- No matter which method is applied, the estimate of the generalization error of the best network will be optimistic.

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### Algorithm for ANN Learning



- Learning is based on training data, and aims at appropriate weights for the perceptrons in a network.
- Direct computation is in the general case not feasible.
- An initial random assignment of weights simplifies the learning process that becomes an iterative adjustment process.
- In the case of single perceptrons, learning becomes the process of moving hyperplanes around; parametrized over time t:  $\mathbf{W}(t+1) = \mathbf{W}(t) + \Delta\mathbf{W}(t)$

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### Perceptron Learning



- The squared error for an example with input x and desired output y is:

$$E = \frac{1}{2} \text{Err}^2 = \frac{1}{2} (y - g_w(x))^2$$


- Perform optimization search by gradient descent:

$$\frac{\partial E}{\partial W_j} = \text{Err} \times \frac{\partial \text{Err}}{\partial W_j} = \text{Err} \times \frac{\partial}{\partial W_j} (y - g(\sum_{j=0}^n W_j x_j)) = -\text{Err} \times g'(in) \times x_j$$

- Simple weight update rule:  $W_j \leftarrow W_j + \alpha \times \text{Err} \times g'(in) \times x_j$
- Positive error  $\Rightarrow$  increase network output
  - increase weights on positive inputs,
  - decrease on negative inputs

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### Perceptron Learning (2)



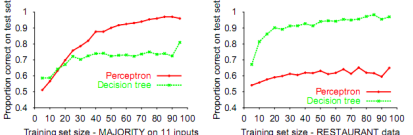
- The weight updates need to be applied repeatedly for each weight  $W_j$  in the network, and for each training suite in the training set.
- One such cycle through all weights is called an **epoch** of training.
- Eventually, mostly after many epochs, the weight changes converge towards zero and the training process terminates.
- The perceptron learning process always finds a set of weights for a perceptron that solves a problem correctly with a finite number of epochs, if such a set of weights exists.
- If a problem can be solved with a separation hyperplane, then the set of weights is found in finite iterations and solves the problem correctly.

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### Perceptron Learning (3)




- Perceptron learning rule converges to a consistent function for any linearly separable data set



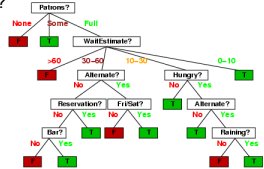
- Perceptron learns majority function easily, Decision-Tree is hopeless
- Decision-Tree learns restaurant function easily, perceptron cannot represent it.

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### Example Functions




- Majority Function: the output is false when  $n/2$  or more inputs are false, and true otherwise.
- Restaurant Function: decide whether to wait for a table or not:
  - How many guests (**patron**) are in the restaurant?
  - What is the **estimated waiting** time?
  - Any **alternative** restaurant nearby?
  - Are we **hungry**?
  - Do we have a **reservation**?
  - Is it **Friday or Saturday**?
  - Is there a comfortable **bar** area to wait in?
  - Is it **raining** outside?

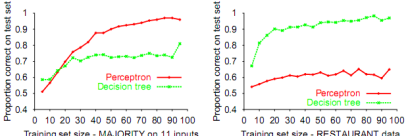


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### Perceptron Learning (3)




- Perceptron learning rule converges to a consistent function for any linearly separable data set




- Perceptron learns majority function easily, Decision-Tree is hopeless
- Decision-Tree learns restaurant function easily, perceptron cannot represent it.

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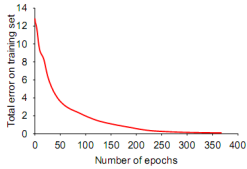
**Back-Propagation Learning** 

- The errors (and therefore the learning) propagate backwards from the output layer to the hidden layers.
- Learning at the output layer is the same as for single-layer perceptron:  $W_j \leftarrow W_j + \alpha \times Err \times g'(in) \times x_j$
- Hidden layer neurons get a "blame" assigned for the error (back-propagation of error), giving greater responsibility to neurons connected by stronger weight.
- Back-propagation of error updates the weights of the hidden layer; the principle thus stays the same.

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**Back-Propagation Learning (2)** 

- Training curve for 100 restaurant examples converges to a perfect fit to the training data




- MLPs are quite good for complex pattern recognition tasks, but resulting hypotheses cannot be understood easily
- Typical problems: slow convergence, local minima

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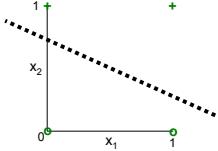


**ILLUSTRATION BY AN EXAMPLE**


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**Perceptron Learning Example** 

- The applied algorithm is as follows
  - Initialize the weights and threshold to small random numbers.
  - Present a vector  $\mathbf{x}$  to the neuron inputs and calculate the output.
  - Update the weights according to the error.
- Applied learning function:  $W_j(t+1) = W_j(t) + \alpha \times (y - g_w(x)) \times x_j$
- Example with two inputs  $x_1, x_2$




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**Perceptron Learning Example** 


- Data: (0,0)→0, (1,0)→0, (0,1)→1, (1,1)→1
- Initialization:  $W_1(0) = 0.9286$ ,  $W_2(0) = 0.62$ ,  $W_0(0) = 0.2236$ ,  $\alpha = 0.1$
- Training – epoch 1:
  - $out1 = \text{sign}(0.92 \cdot 0 + 0.62 \cdot 0 - 0.22) = \text{sign}(-0.22) = 0$  ✓
  - $out2 = \text{sign}(0.92 \cdot 1 + 0.62 \cdot 0 - 0.22) = \text{sign}(0.7) = 1$  ✗
  - $W_1(1) = 0.92 + 0.1 \cdot (0 - 1) \cdot 1 = 0.82$  ✓
  - $W_2(1) = 0.62 + 0.1 \cdot (0 - 1) \cdot 0 = 0.62$  ✓
  - $W_0(1) = 0.22 + 0.1 \cdot (0 - 1) \cdot (-1) = 0.32$  ✓
  - $out3 = \text{sign}(0.82 \cdot 0 + 0.62 \cdot 1 - 0.32) = \text{sign}(0.5) = 1$  ✓
  - $out4 = \text{sign}(0.82 \cdot 1 + 0.62 \cdot 1 - 0.32) = 1$  ✓

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**Perceptron Learning Example** 


- Training – epoch 2:
  - $out1 = \text{sign}(0.82 \cdot 0 + 0.62 \cdot 0 - 0.32) = \text{sign}(0.32) = 0$  ✓
  - $out2 = \text{sign}(0.82 \cdot 1 + 0.62 \cdot 0 - 0.32) = \text{sign}(0.5) = 1$  ✗
  - $W_1(2) = 0.82 + 0.1 \cdot (0 - 1) \cdot 1 = 0.72$  ✓
  - $W_2(2) = 0.62 + 0.1 \cdot (0 - 1) \cdot 0 = 0.62$  ✓
  - $W_0(2) = 0.32 + 0.1 \cdot (0 - 1) \cdot (-1) = 0.42$  ✓
  - $out3 = \text{sign}(0.72 \cdot 0 + 0.62 \cdot 1 - 0.42) = \text{sign}(0.3) = 1$  ✓
  - $out4 = \text{sign}(0.72 \cdot 1 + 0.62 \cdot 1 - 0.42) = 1$  ✓
- Training – epoch 3:
  - $out1 = \text{sign}(0.72 \cdot 0 + 0.62 \cdot 0 - 0.42) = 0$  ✓
  - $out2 = \text{sign}(0.72 \cdot 1 + 0.62 \cdot 0 - 0.42) = 1$  ✗
  - $W_1(3) = 0.72 + 0.1 \cdot (0 - 1) \cdot 1 = 0.62$  ✓
  - $W_2(3) = 0.62 + 0.1 \cdot (0 - 1) \cdot 0 = 0.62$  ✓
  - $W_0(3) = 0.42 + 0.1 \cdot (0 - 1) \cdot (-1) = 0.52$  ✓

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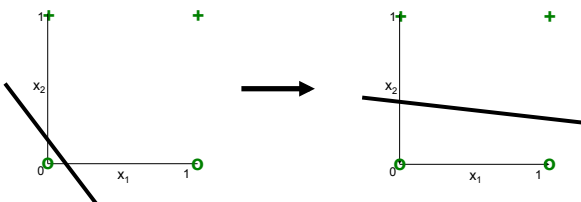
**Perceptron Learning Example** 

- $out3 = \text{sign}(0.62 \cdot 0 + 0.62 \cdot 1 - 0.52) = 1$  ✓
  - $out4 = \text{sign}(0.62 \cdot 1 + 0.62 \cdot 1 - 0.52) = 1$  ✓
- Training – epoch 4:
  - $out1 = \text{sign}(0.62 \cdot 0 + 0.62 \cdot 0 - 0.52) = 0$  ✓
  - $out2 = \text{sign}(0.62 \cdot 1 + 0.62 \cdot 0 - 0.52) = 1$  ✗
  - $W_1(4) = 0.62 + 0.1 \cdot (0 - 1) \cdot 1 = 0.52$  ✓
  - $W_2(4) = 0.62 + 0.1 \cdot (0 - 1) \cdot 0 = 0.62$  ✓
  - $W_0(4) = 0.52 + 0.1 \cdot (0 - 1) \cdot (-1) = 0.62$  ✓
  - $out3 = \text{sign}(0.52 \cdot 0 + 0.62 \cdot 1 - 0.62) = 0$  ✗
  - $W_1(4) = 0.52 + 0.1 \cdot (1 - 0) \cdot 0 = 0.52$  ✓
  - $W_2(4) = 0.62 + 0.1 \cdot (1 - 0) \cdot 1 = 0.72$  ✓
  - $W_0(4) = 0.62 + 0.1 \cdot (1 - 0) \cdot (-1) = 0.52$  ✓
  - $out4 = \text{sign}(0.52 \cdot 1 + 0.72 \cdot 1 - 0.52) = 1$  ✓


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**Perceptron Learning Example** 

- Finally:
  - $out1 = \text{sign}(0.12 \cdot 0 + 0.82 \cdot 0 - 0.42) = 0$  ✓
  - $out2 = \text{sign}(0.12 \cdot 1 + 0.82 \cdot 0 - 0.42) = 0$  ✓
  - $out3 = \text{sign}(0.12 \cdot 0 + 0.82 \cdot 1 - 0.42) = 1$  ✓
  - $out4 = \text{sign}(0.12 \cdot 1 + 0.82 \cdot 1 - 0.42) = 1$  ✓



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**Further Application Examples** 

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- There are endless further examples: :
  - Handwriting Recognition
  - Time Series Prediction
  - Kernel Machines (Support Vectore Machines)
  - Data Compression
  - Financial Predication
  - Speech Recognition
  - Computer Vision
  - Protein Structures
  - ...

0	1	2	3	4	5	6	7	8	9
0	1	0	7	4	5	6	7	8	9


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**SUMMARY**

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**Summary** 

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- Most brains have lots of neurons, each neuron approximates a linear-threshold unit.
- Perceptrons (one-layer networks) approximate neurons, but are as such insufficiently expressive.
- Multi-layer networks are sufficiently expressive; can be trained to deal with generalized data sets, i.e. via error back-propagation.
- Multi-layer networks allow for the modeling of arbitrary separation boundaries, while single-layer perceptrons only provide linear boundaries.
- Endless number of applications: Handwriting Recognition, Time Series Prediction, Bioinformatics, Kernel Machines (Support Vectore Machines), Data Compression, Financial Predication, Speech Recognition, Computer Vision, Protein Structures...


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**REFERENCES**

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**References** 

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**Mandatory Readings:**

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- Supervised learning demo (perceptron learning rule) at <http://lcn.epfl.ch/tutorial/english/perceptron/html>

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**References** 

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**Next lecture** 


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**Questions?** 

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