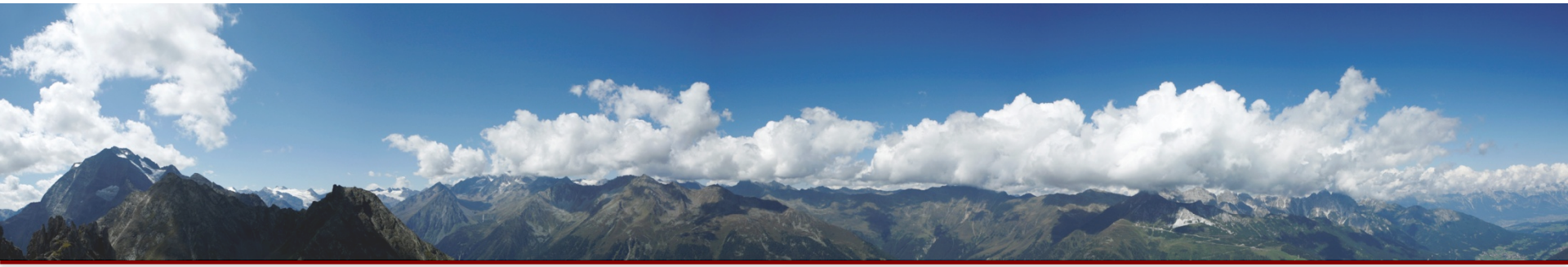
Artificial Intelligence

Neural Networks

Ioan Toma



Where are we?

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#	Title
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3	Predicate Logic
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Agenda

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

MOTIVATION

Motivation

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- 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.

Motivation

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- Neural networks are stong 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

TECHNICAL SOLUTIONS

(Artificial) Neural Networks

What are Neural Networks?

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- 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 electronical potential.
- Apart from the electrical signaling, neurotransmitter diffusion (endogenous chemicals) can effectuate the impulses.

What are Neural Networks?

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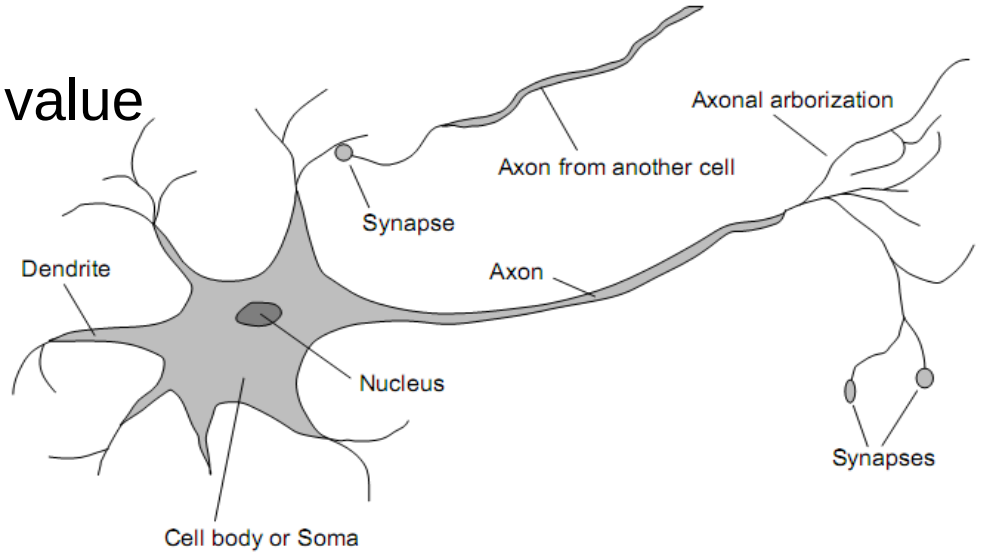
- Connections, called **synapses**, are usually formed from **axons** to **dendrites**; also other connections are possible.
- The axon is the primary conduit through which the neuron transmits impulses to neurons downstream in the signal chain
- A human has 10^{11} neurons of > 20 types, 10^{14} synapses, 1ms-10ms cycle time.
- There are 10^{11} stars 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.



What are Neural Networks?

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- 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…*

What are Neural Networks?

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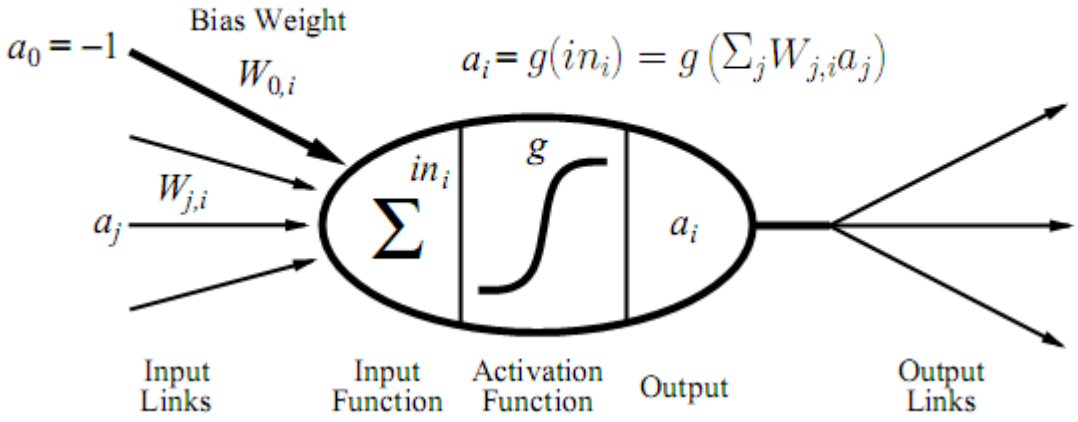
- What we refer to as Neural Networks, in this course, are mostly Artificial Neural Networks (ANN).
- ANN are approximations of biological neural networks and are built of physical devices, or simulated on computers.
- ANN are parallel computational entities that consist of multiple simple processing 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**.

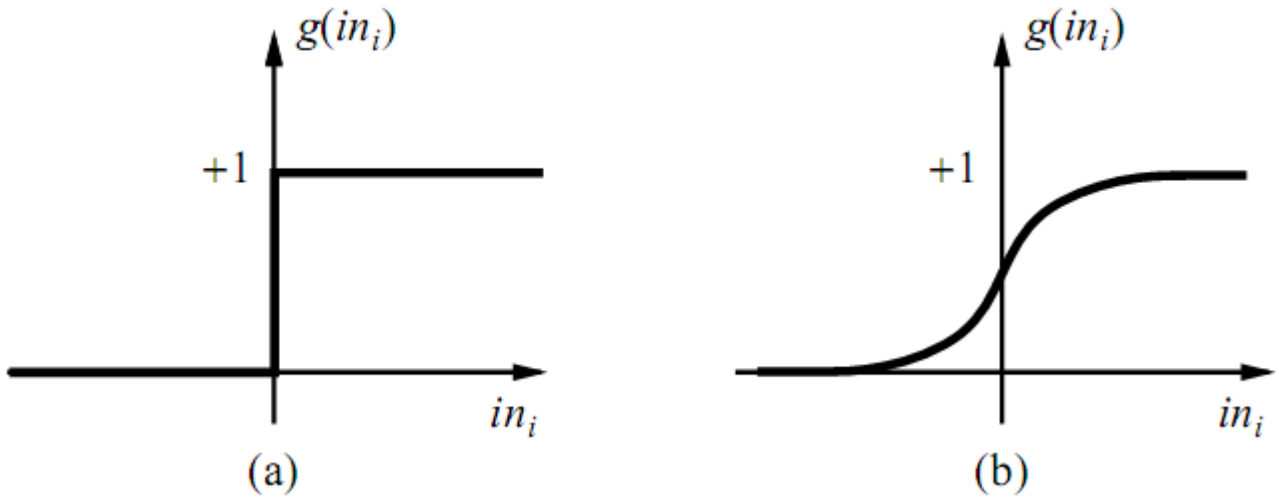
Perceptron

- 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.

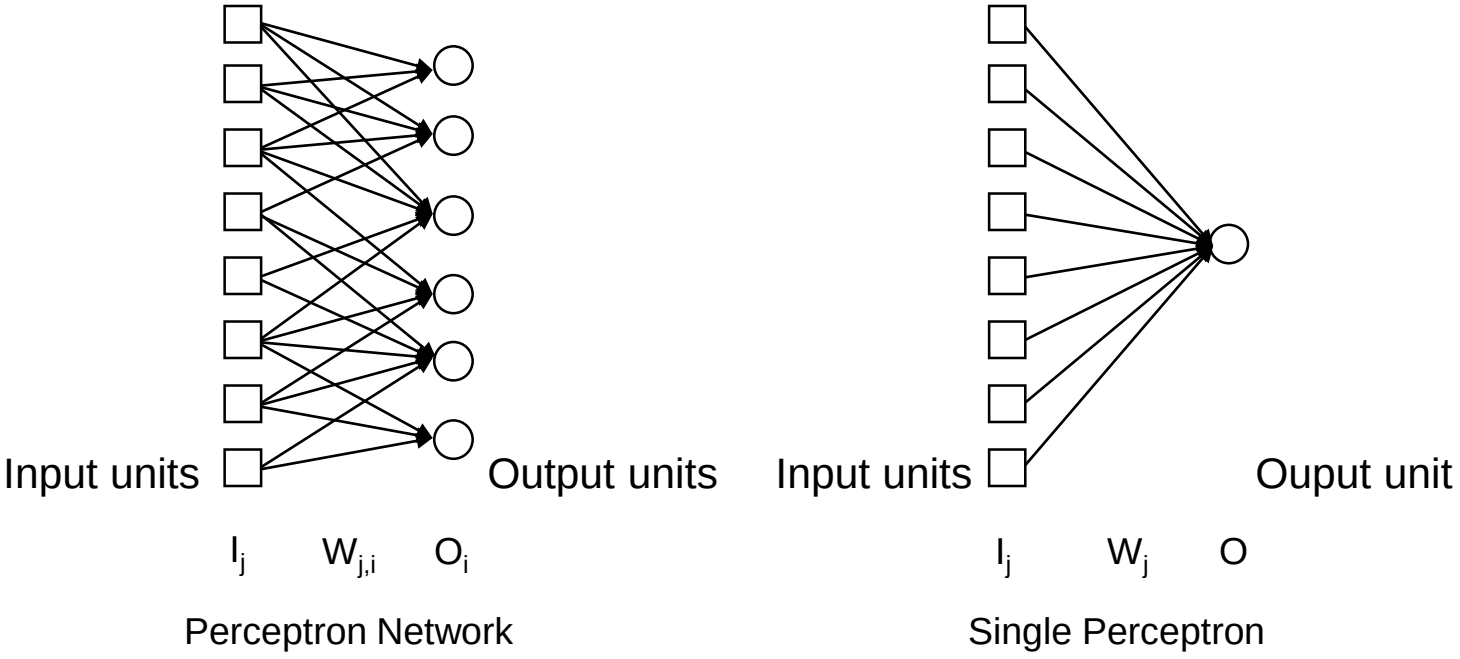
Activation Functions



(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

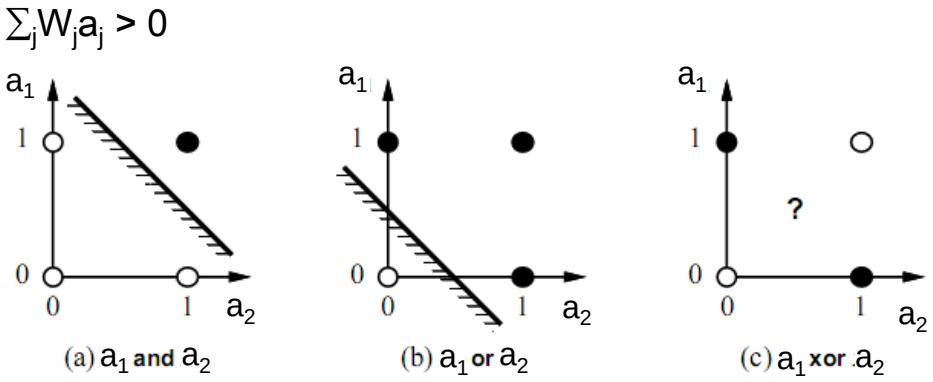
- McCulloch-Pitts neurons can be connected together in any desired way to build an artificial neural network.
- A construct of one input layer of neurons that feed forward to one output layer of neurons is called **Perceptron**.



Expressiveness of Perceptrons

- A perceptron with g = 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



Expressiveness of Perceptrons (2)

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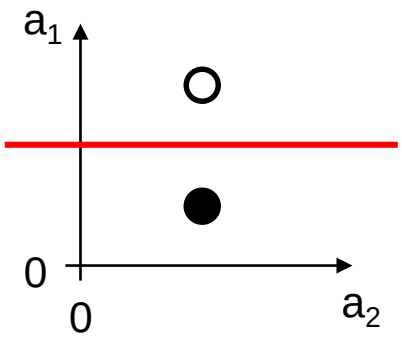
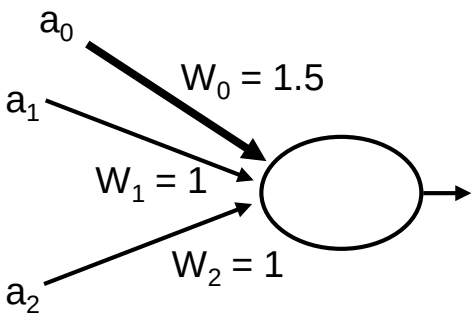
- Threshold perceptrons can represent only linearly separable functions (i.e. functions for which such a separation hyperplane exists)

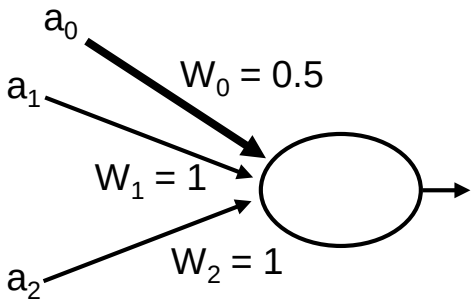


- Such perceptrons have limited expressivity.
- There exists an algorithm that can fit a threshold perceptron to any linearly separable training set.

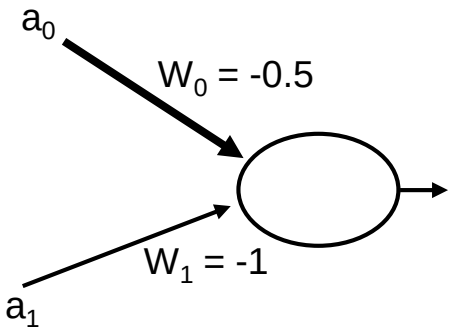
Example: Logical Functions



AND



OR



NOT

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

Example: Finding Weights for AND Operation

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- There are two input weights W_1 and W_2 and a treshold W_0. For each training pattern the perceptron needs to satisfay the following equation:

$$out = g(W_1*a_1 + W_2*a_2 - W_0) = sign(W_1*a_1 + W_2*a_2 - W_0)$$

- For a binary AND there are four training data items available that lead to four inequalities:
  - $W_1*0 + W_2*0 - W_0 < 0 \quad \Rightarrow W_0 > 0$
  - $W_1*0 + W_2*1 - W_0 < 0 \quad \Rightarrow W_2 < W_0$
  - $W_1*1 + W_2*0 - W_0 < 0 \quad \Rightarrow W_1 < W_0$
  - $W_1*1 + W_2*1 - W_0 \geq 0 \quad \Rightarrow W_1 + W_2 \geq W_0$

- There is an obvious infinite number of solutions that realize a logical AND; e.g. $W_1 = 1$, $W_2 = 1$ and $W_0 = 1.5$.

Limitations of Simple Perceptrons

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- XOR:
  - $W_1*0 + W_2*0 - W_0 < 0 \quad \Rightarrow W_0 > 0$
  - $W_1*0 + W_2*1 - W_0 \geq 0 \quad \Rightarrow W_2 \geq W_0$
  - $W_1*1 + W_2*0 - W_0 \geq 0 \quad \Rightarrow W_1 \geq W_0$
  - $W_1*1 + W_2*1 - W_0 < 0 \quad \Rightarrow W_1 + W_2 < W_0$

- 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.

Artificial Neural Network Structures

Neural Network Structures

- 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

Single-Layer Feed-Forward

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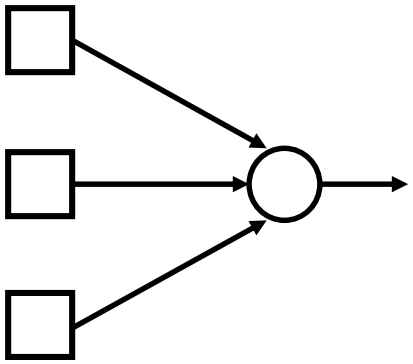
- A Single-Layer Feed-Forward Structure is a simple perceptron, and has thus
  - one input layer
  - one output layer
  - NO feed-back connections



- Feed-forward networks implement functions, have no internal state (of course also valid for multi-layer perceptrons).

Single-Layer Feed-Forward: Example

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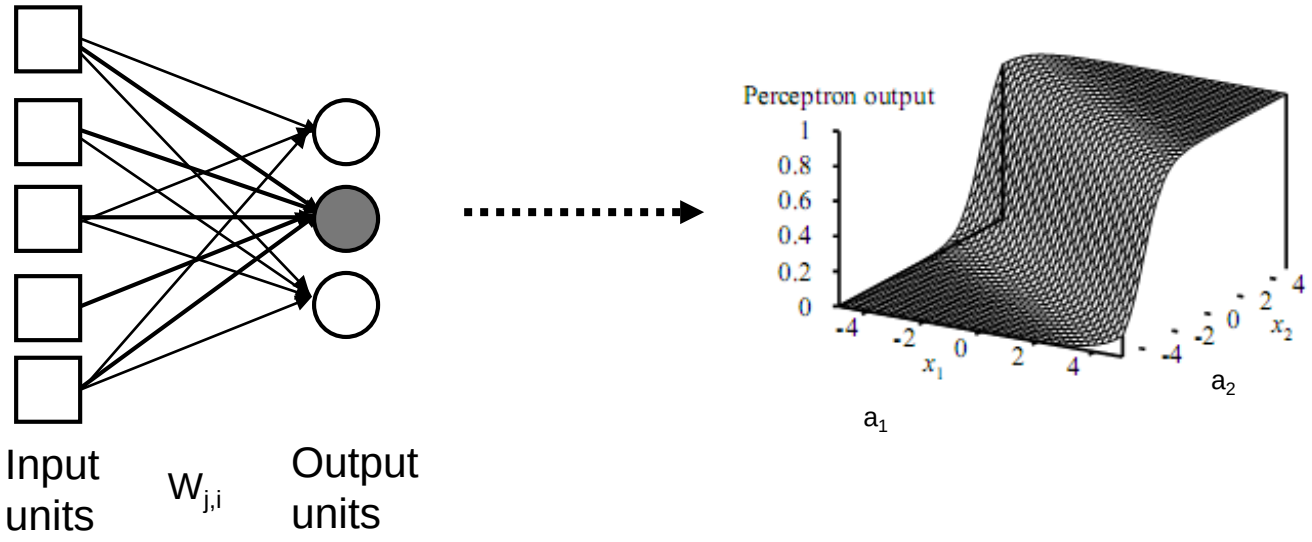
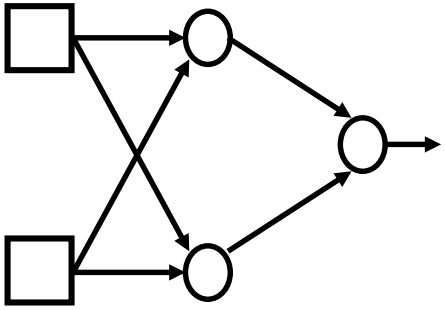
- Output units all operate separately – no shared weights
- Adjusting weights moves the location, orientation, and steepness of cliff (i.e., the separation hyperplane).



Multi-Layer Feed-Forward

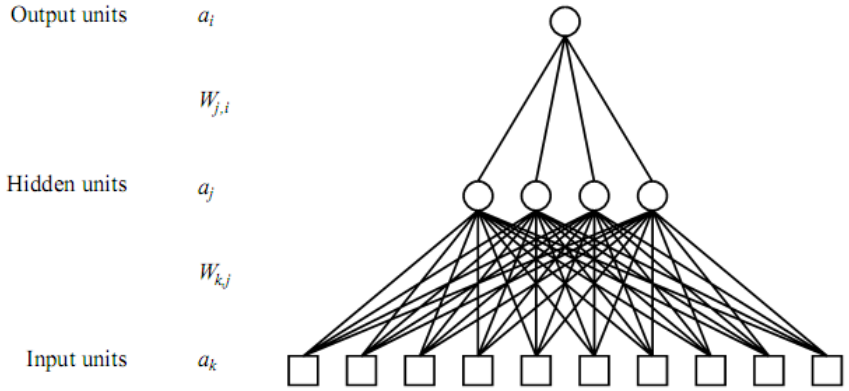


- Multi-Layer Feed-Forward Structures have:
  - one input layer
  - one output layer
  - one or many hidden layers of processing units

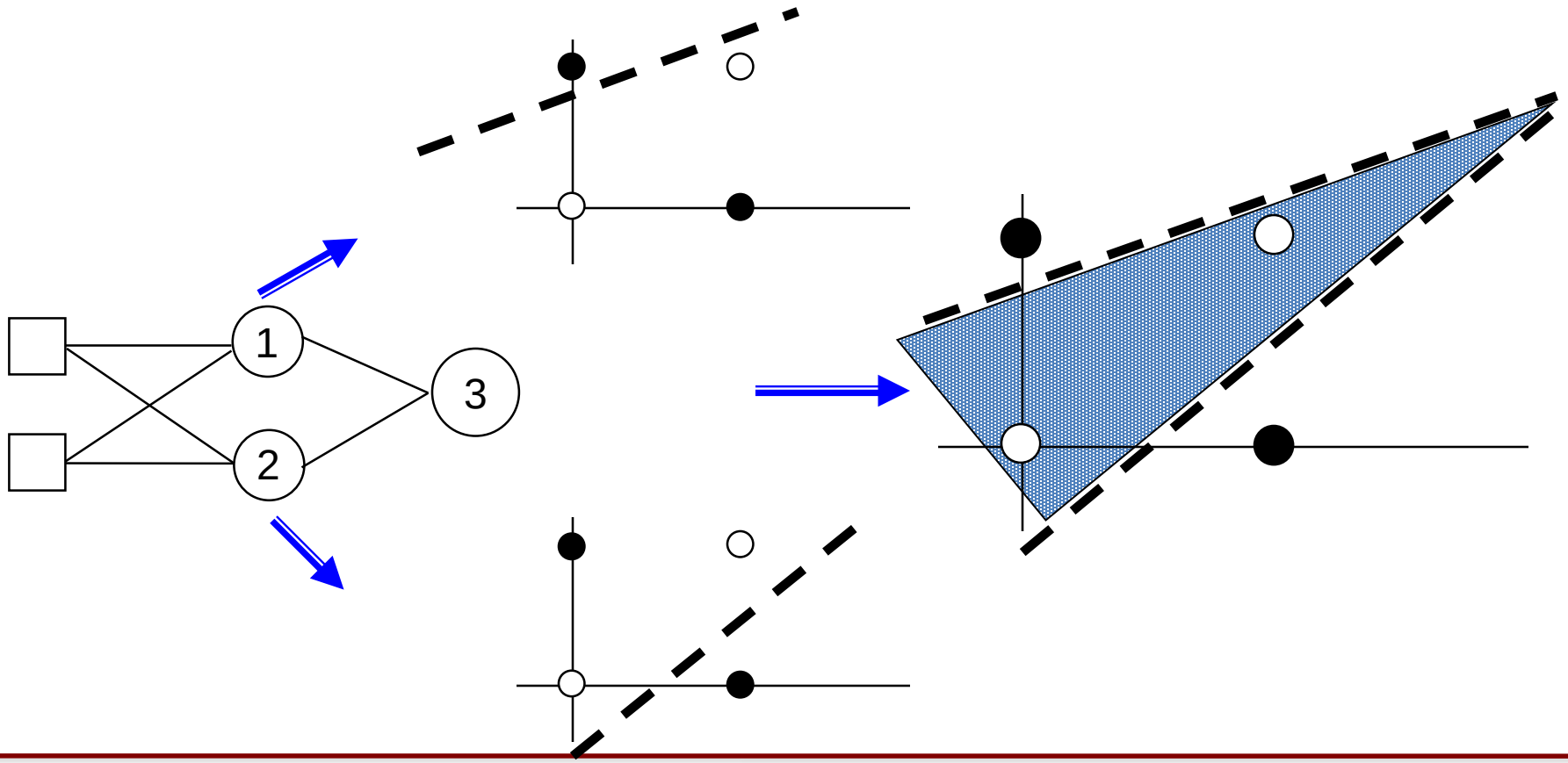
- The hidden layers are between the input and the output layer, and thus hidden from the outside world: no input from the world, not output to the world.

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.

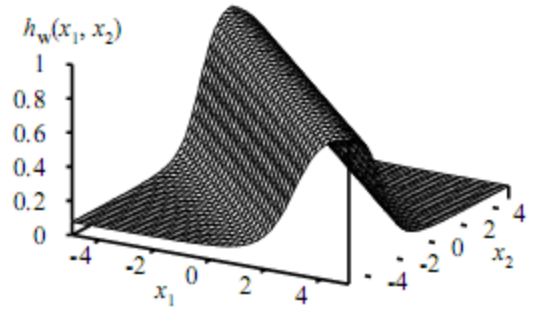


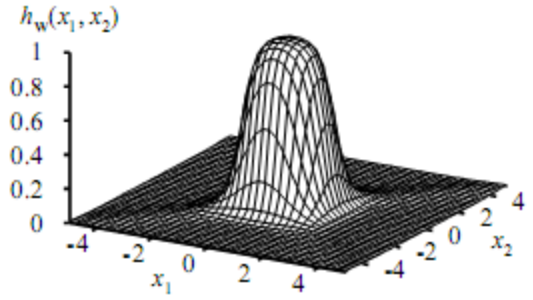
- XOR Problem: Recall that XOR cannot be modeled with a Single-Layer Feed-Forward perceptron.



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.

Number of Hidden Layers

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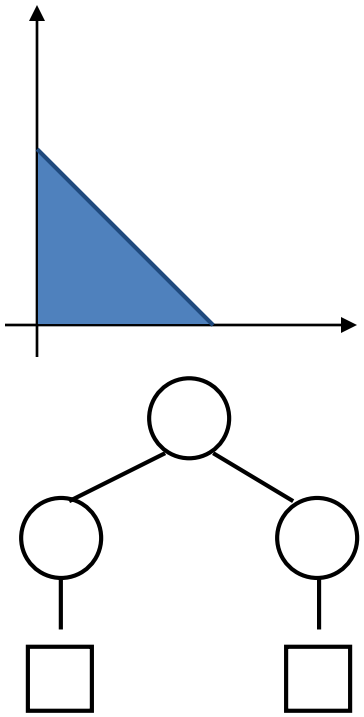
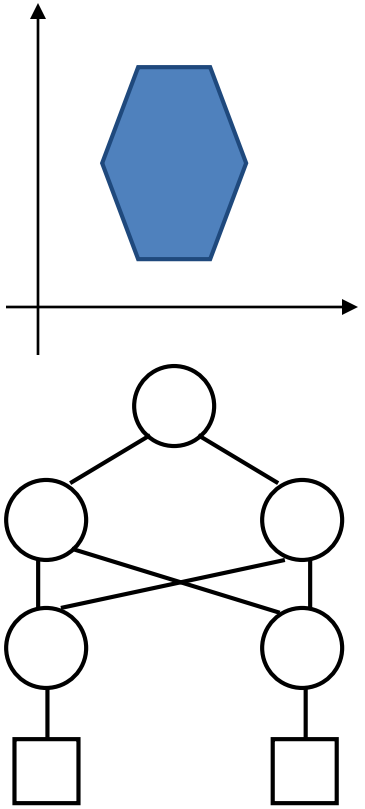
- Rule of Thumb 1
  Even if the function to learn is slightly non-linear, the generalization may be better with a simple linear model than with a complicated non-linear model; if there is too little data or too much noise to estimate the non-linearities accurately.

- 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.

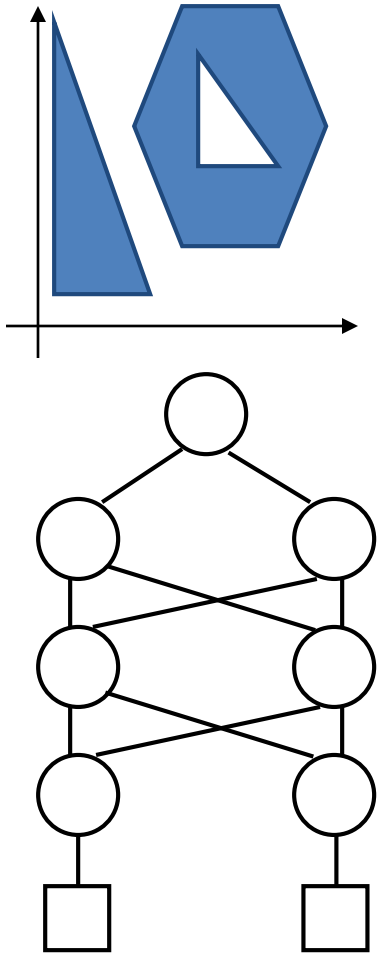
Example: Number of Hidden Layers



1st layer draws linear boundaries



2nd layer combines the boundaries.



3rd layer can generate arbitrarily boundaries.

Recurrent Network

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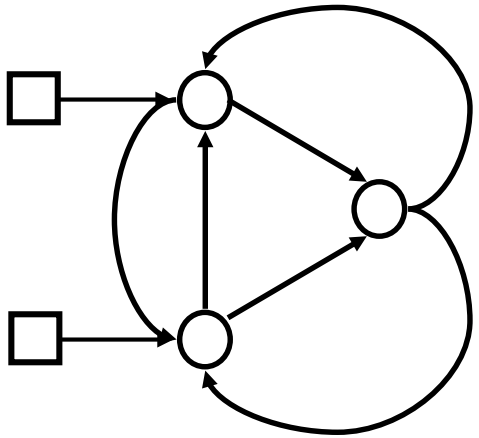
- Recurrent networks have at least one feedback connection:
  - They have directed cycles with delays: they have internal states (like flip flops), can oscillate, etc.
  - The response to an input depends on the initial state which may depend on previous inputs.
  - This creates an internal state of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



Building Neural Networks

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- 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.

Learning and Generalization

Learning and Generalization

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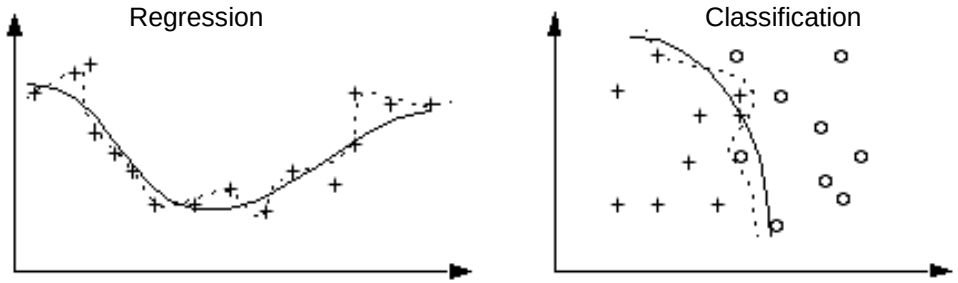
- Neural networks have two important aspects to fulfill:
  - They must learn decision surfaces from training data, so that training data (and test data) are classified correctly;
  - They must be able to generalize based on the learning process, in order to classify data sets it has never seen before.

- 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.

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!



„Perfect“ learning achieves the dotted separation, while the desired one is in fact given by the solid line.

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

Estimation of Generalization Error

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- 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.

Estimation of Generalization Error

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- 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.

Algorithm for ANN Learning

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- 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: $\mathbf{W_i(t+1) = W_i(t) + \Delta W_i(t)}$

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

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

- Perform optimization search by gradient descent:

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

- Simple weight update rule: $W_j \leftarrow W_j + \alpha \times Err \times g'(in) \times x_j$

- Positive error $\Rightarrow$ increase network output
  - increase weights on positive inputs,
  - decrease on negative inputs

Perceptron Learning (2)

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- 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 weighty 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.

Example Functions

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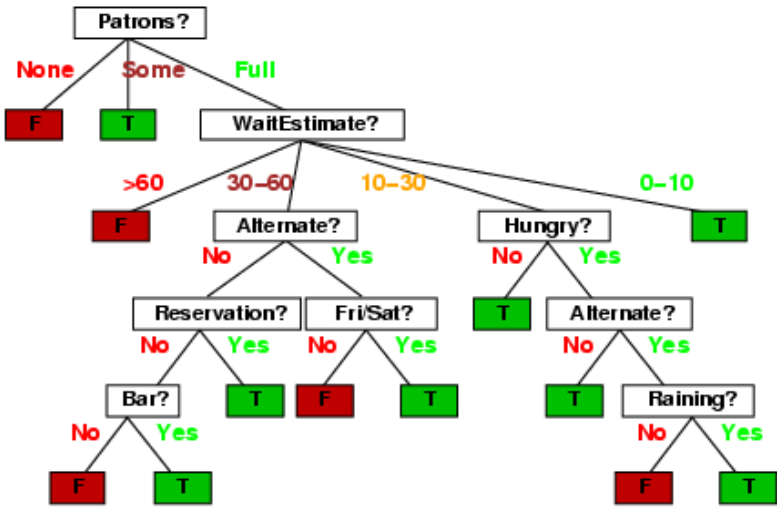
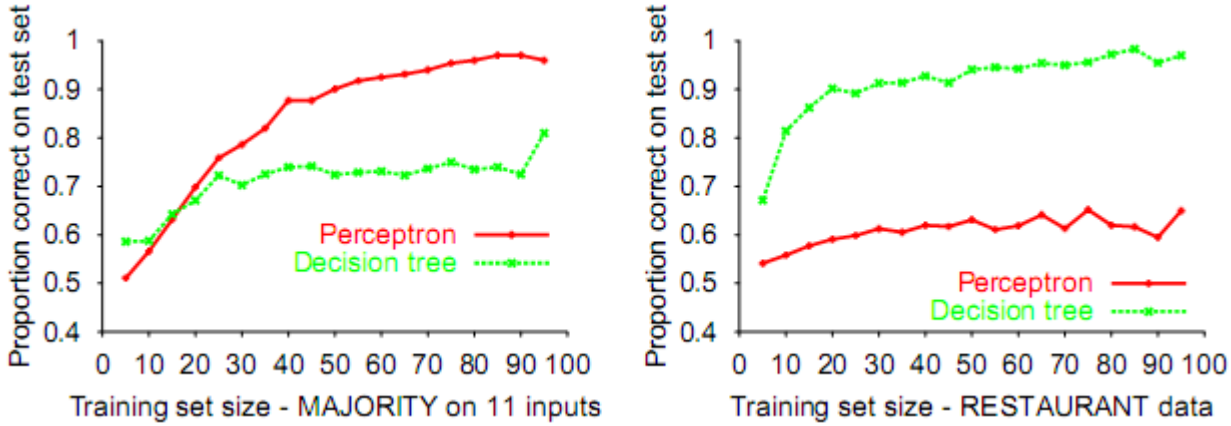
- Majority Function: the output is false when n/2 or more inputs are false, and true otherwise.

- 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?



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.

Back-Propagation Learning

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- 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.

Back-Propagation Learning (2)

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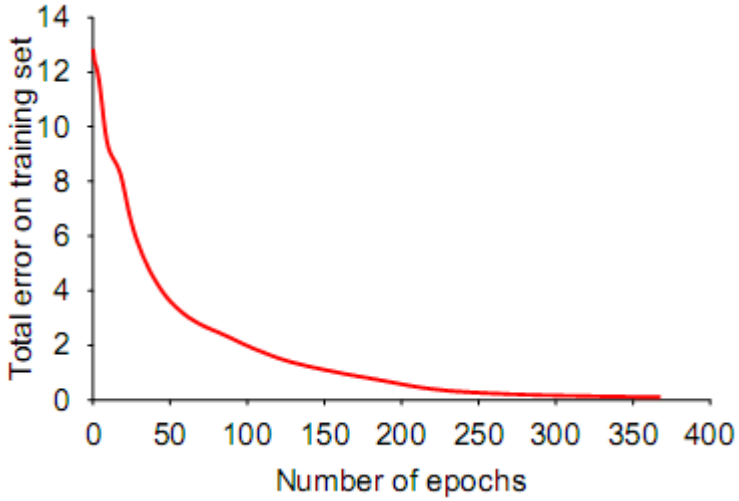
- Training curve for 100 restaurant examples converges to a perfect fit to the training data



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

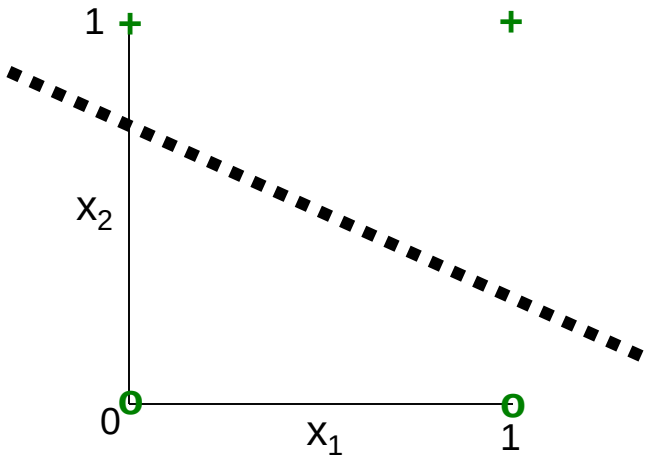
ILLUSTRATION BY AN EXAMPLE

Perceptron Learning Example

- The applied algorithm is as follows
  - Initialize the weights and threshold to small random numbers.
  - Present a vector **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



Perceptron Learning Example

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- 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 = sign(0.92*0 + 0.62*0 – 0.22) = sign(-0.22) = 0 ✓

  out2 = sign(0.92*1 + 0.62*0 – 0.22) = sign(0.7) = 1 ✗

  $W_1(1) = 0.92 + 0.1 * (0 – 1) * 1 \quad = 0.82$

  $W_2(1) = 0.62 + 0.1 * (0 – 1) * 0 \quad = 0.62$

  $W_0(1) = 0.22 + 0.1 * (0 – 1) * (-1) = 0.32$ ✓

  out3 = sign(0.82*0 + 0.62*1 – 0.32) = sign(0.5) = 1 ✓

  out4 = sign(0.82*1 + 0.62*1 – 0.32) = 1

Perceptron Learning Example

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- Training – epoch 2:

  out1 = sign(0.82*0 + 0.62*0 – 0.32) = sign(0.32) = 0

  out2 = sign(0.82*1 + 0.62*0 – 0.32) = sign(0.5) = 1

  $W_1(2) = 0.82 + 0.1 * (0 – 1) * 1 \quad = 0.72$

  $W_2(2) = 0.62 + 0.1 * (0 – 1) * 0 \quad = 0.62$

  $W_0(2) = 0.32 + 0.1 * (0 – 1) * (-1) = 0.42$

  out3 = sign(0.72*0 + 0.62*1 – 0.42) = sign(0.3) = 1

  out4 = sign(0.72*1 + 0.62*1 – 0.42) = 1

- Training – epoch 3:

  out1 = sign(0.72*0 + 0.62*0 – 0.42) = 0

  out2 = sign(0.72*1 + 0.62*0 – 0.42) = 1

  $W_1(3) = 0.72 + 0.1 * (0 – 1) * 1 \quad = 0.62$

  $W_2(3) = 0.62 + 0.1 * (0 – 1) * 0 \quad = 0.62$

  $W_0(3) = 0.42 + 0.1 * (0 – 1) * (-1) = 0.52$

Perceptron Learning Example

out3 = sign(0.62*0 + 0.62*1 – 0.52) = 1 ✓

out4 = sign(0.62*1 + 0.62*1 – 0.52) = 1 ✓

- Training – epoch 4:

out1 = sign(0.62*0 + 0.62*0 – 0.52) = 0 ✓

out2 = sign(0.62*1 + 0.62*0 – 0.52) = 1 X

$W_1(4) = 0.62 + 0.1 * (0 – 1) * 1 \quad = 0.52$

$W_2(4) = 0.62 + 0.1 * (0 – 1) * 0 \quad = 0.62$

$W_0(4) = 0.52 + 0.1 * (0 – 1) * (-1) = 0.62$

out3 = sign(0.52*0 + 0.62*1 – 0.62) = 0 X

$W_1(4) = 0.52 + 0.1 * (1 – 0) * 0 \quad = 0.52$

$W_2(4) = 0.62 + 0.1 * (1 – 0) * 1 \quad = 0.72$

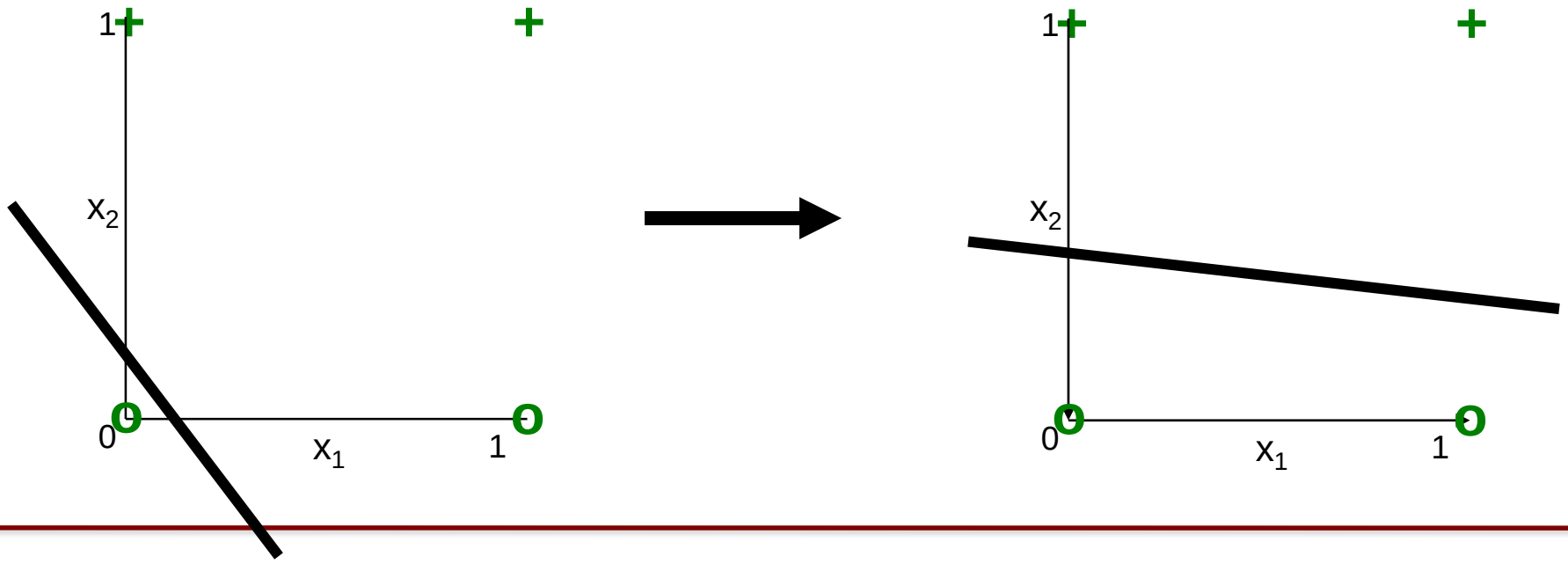
$W_0(4) = 0.62 + 0.1 * (1 – 0) * (-1) = 0.52$

out4 = sign(0.52*1 + 0.72*1 – 0.52) = 1 ✓

Perceptron Learning Example

- Finally:

out1 = sign(0.12*0 + 0.82*0 – 0.42) = 0
out2 = sign(0.12*1 + 0.82*0 – 0.42) = 0
out3 = sign(0.12*0 + 0.82*1 – 0.42) = 1
out4 = sign(0.12*1 + 0.82*1 – 0.42) = 1



Further Application Examples

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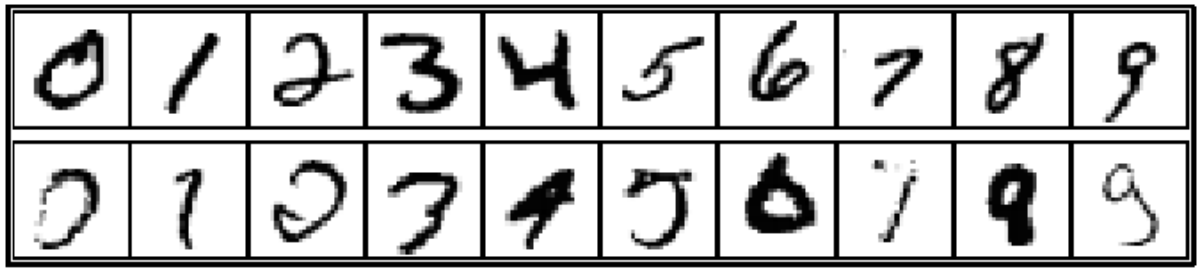
- There are endless further examples: :
  - Handwriting Recognition
  - Time Series Prediction
  - Kernel Machines (Support Vectore Machines)
  - Data Compression
  - Financial Predication
  - Speech Recognition
  - Computer Vision
  - Protein Structures
  - ...



SUMMARY

Summary

- 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...

REFERENCES

References

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- http://en.wikipedia.org/wiki/Artificial_neural_network
- http://en.wikipedia.org/wiki/Perceptron
- http://en.wikipedia.org/wiki/Feedforward_neural_network
- http://en.wikipedia.org/wiki/Recurrent_neural_networks
- http://en.wikipedia.org/wiki/Back_propagation

Next lecture

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#	Title
1	Introduction
2	Propositional Logic
3	Predicate Logic
4	Reasoning
5	Search Methods
6	CommonKADS
7	Problem-Solving Methods
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10	Rule Learning
11	Inductive Logic Programming
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13	**Neural Networks**
14	**Semantic Web and Services**

Questions?

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