

# Lecture 4: Artificial Neural Networks

Perceptrons, Multi-Layer Perceptrons, Delta-Rule, Backpropagation

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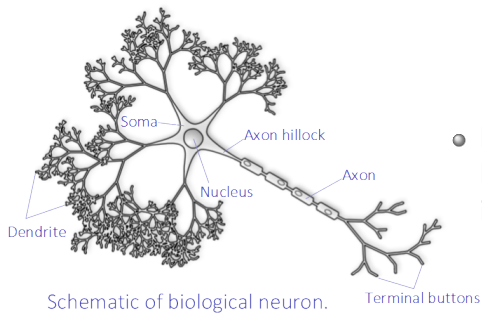


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# Outline

- Perceptron
- Delta Rule
- Backpropagation
- Multi-layer Perceptron (feed forwards netowrk)
- Inductive Bias

# Biological Motivation



- biological learning systems are built of complex webs of interconnected neurons

## Artificial Neural Networks

- realize highly parallel computation
- are based on distributed representation
- are highly performant but data intensive machine learning algorithms
- typically are only very roughly related to biological processes

# Computer vs. Brain

	Computer	Brain
computation units	1 CPU ( $> 10^7$ transistors)	$10^{11}$ neurons
memory units	64 GB RAM 10 TB HDD	$10^{11}$ neurons $10^{14}$ synapses
clock	$10^{-10}$ sec	$10^{-3}$ sec
transmission	$> 10^{11}$ bits/sec	$> 10^{14}$ bits/sec

- Computer: typically serial, fast
- Brain: parallel, slow, robust wrt noisy data

(Magnitudes given for computers are open to change.)

# Appropriate Problems – Perceptron

The perceptron algorithm is an early neuro-inspired approach to machine learning

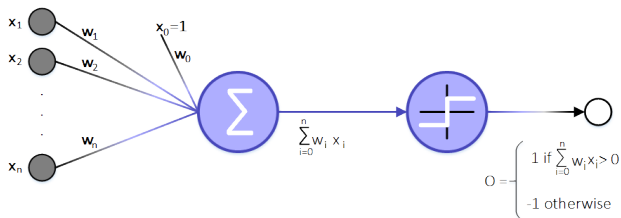
- instances are represented as many attribute-value pairs
  - ▶ input values can be any real values
- target function output is binary
- Hypotheses are linear, that is, hyper-planes which partition the hypothesis space in two areas (concept/not concept)
- When Minsky and Papert showed in their book *Perceptrons* (1969) that perceptrons cannot learn XOR problems, research in neuro-inspired approaches was mainly given up until it re-emerged end of the 1980ies.
- Support Vector Machines also rely on learning hyper-planes, but use the kernel trick to deal with data sets which are not linearly separable.

# Appropriate Problems – Backpropagation

The backpropagation algorithm is the most commonly used ANN learning technique with the following characteristics:

- instances are represented as many attribute-value pairs
  - ▶ input values can be any real values
- target function output may be discrete-, real- or vector- valued
- training examples may contain errors
- long training times are acceptable
- fast evaluation of the learned target function may be required
  - ▶ many iterations may be necessary to converge to a good approximation
- ability of humans to understand the learned target function is not important
  - ▶ learned weights are not intuitively understandable

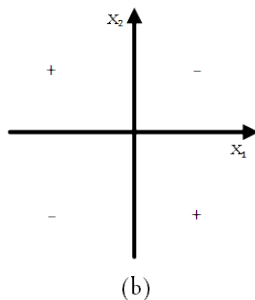
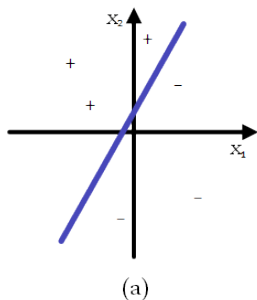
# Perceptrons



- takes a vector of real-valued inputs  $(x_1, \dots, x_n)$  weighted with  $(w_1, \dots, w_n)$
- calculates the linear combination of these inputs
  - ▶  $\sum_{i=0}^n w_i x_i = w_0 x_0 + w_1 x_1 + \dots + w_n x_n$
  - ▶  $-w_0$  denotes a threshold value, i.e. that value which must be reached by the linear combination of inputs to cause the perceptron to output 1
  - ▶  $x_0$  is always 1
- outputs 1 if the result is greater than 0, otherwise  $-1$

# Representational Power

- a perceptron represents a **hyperplane decision surface** in the  $n$ -dimensional space of instances
- some sets of examples cannot be separated by any hyperplane, those that can be separated are called **linearly separable**
- many boolean functions can be represented by a perceptron: AND, OR, NAND, NOR





# Perceptron Training Rule

- **problem:** determine a weight vector  $\vec{w}$  that causes the perceptron to produce the correct output for each training example

- **perceptron training rule:**

$$w_i = w_i + \Delta w_i \text{ where } \Delta w_i = \eta(t - o)x_i$$

$t$  target output

$o$  perceptron output

$\eta$  learning rate (usually some small value, e.g. 0.1)

## Algorithm

- ① initialize  $\vec{w}$  to random weights
  - ② repeat, until each training example is classified correctly
    - ⇒ apply perceptron training rule to each training example
- convergence guaranteed provided *linearly separable* training examples and sufficiently small  $\eta$

# Delta Rule

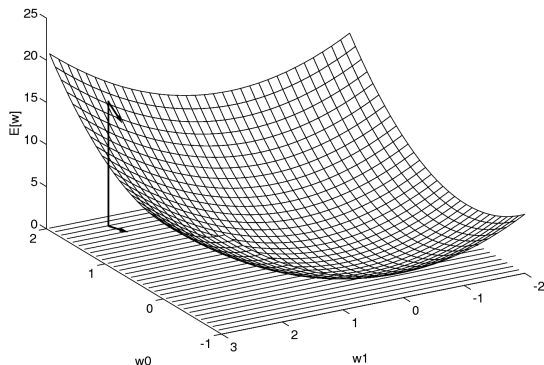
- perceptron rule fails if data is not linearly separable
- delta rule converges toward a **best-fit approximation**
- uses **gradient descent** to search the hypothesis space
  - ▶ perceptron cannot be used, because it is not differentiable
  - ▶ hence, a **unthresholded linear unit** is appropriate
  - ▶ error measure (instead of perceptron training rule):

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

- to understand gradient descent, it is helpful to visualize the entire hypothesis space with
  - ▶ all possible weight vectors and
  - ▶ associated  $E$  values

# Error Surface

- the axes  $w_0, w_1$  represent possible values for the two weights of a simple linear unit



⇒ error surface must be **parabolic** with a **single global minimum**

# Derivation of Gradient Descent

- **problem:** How calculate the steepest descent along the error surface?
- derivative of  $E$  with respect to each component of  $\vec{w}$
- this vector derivative is called *gradient* of  $E$ , written  $\nabla E(\vec{w})$  (the nabla operator)

$$\nabla E(\vec{w}) \equiv \left[ \frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \dots, \frac{\partial E}{\partial w_n} \right]$$

- $\nabla E(\vec{w})$  specifies the steepest ascent, so  $-\nabla E(\vec{w})$  specifies the steepest descent
- **training rule:**  $w_i = w_i + \Delta w_i$

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i} \quad \text{and} \quad \frac{\partial E}{\partial w_i} = \sum_{d \in D} (t_d - o_d)(-x_{id})$$
$$\Rightarrow \Delta w_i = \eta \sum_{d \in D} (t_d - o_d)x_{id}$$

# Differentiating E

$$\frac{\partial E}{\partial w_i} =$$

$$\frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2 =$$

$$\frac{1}{2} \sum_{d \in D} \frac{\partial}{\partial w_i} (t_d - o_d)^2 =$$

$$\frac{1}{2} \sum_{d \in D} 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) =$$

$$\sum_{d \in D} (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \vec{x}_d) =$$

$$\sum_{d \in D} (t_d - o_d) (-x_{id})$$

Remember:

Outer and inner derivation for  $y = u^2$ :  $\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}$  with  $u = t_d - o_d$

# Incremental Gradient Descent

- application difficulties of gradient descent
  - ▶ convergence may be quite slow
  - ▶ in case of many local minima, the global minimum may not be found
- **idea:** approximate gradient descent search by updating weights *incrementally*, following the calculation of the error for *each* individual example

$$\Delta w_i = \eta(t - o)x_i \text{ where } E_d(\vec{w}) = \frac{1}{2}(t_d - o_d)^2$$

- **key differences:**
  - ▶ weights are not summed up over all examples before updating
  - ▶ requires less computation
  - ▶ better for avoidance of local minima

# Gradient Descent

## Algorithm

GRADIENT-DESCENT(*training\_examples*,  $\eta$ )

Each training example is a pair of the form  $\langle \vec{x}, t \rangle$ , where  $\vec{x}$  is the vector of input values, and  $t$  is the target output value.  $\eta$  is the learning rate.

- Initialize each  $w_i$  to some small random value
- Until the **termination condition** is met, Do
  - ▶ Initialize each  $\Delta w_i$  to zero
  - ▶ For each  $\langle \vec{x}, t \rangle$  in *training\_examples*, Do
    - Input the instance  $\vec{x}$  to the unit and compute the output  $o$
    - For each linear unit weight  $w_i$ , Do  $\Delta w_i = \Delta w_i + \eta(t - o)x_i^*$
  - ▶ For each linear unit weight  $w_i$ , Do  $w_i \leftarrow w_i + \Delta w_i^{**}$

To implement *incremental approximation*, equation  $**$  is deleted and equation  $*$  is replaced by  $w_i \leftarrow w_i + \eta(t - o)x_i$ .

# Perceptron vs. Delta Rule

- **perceptron training rule:**

- ▶ uses thresholded unit
- ▶ converges after a finite number of iterations
- ▶ output hypothesis classifies training data perfectly
- ▶ linearly separability necessary

- **delta rule:**

- ▶ uses unthresholded linear unit
- ▶ converges asymptotically toward a minimum error hypothesis
- ▶ termination is not guaranteed
- ▶ linear separability not necessary



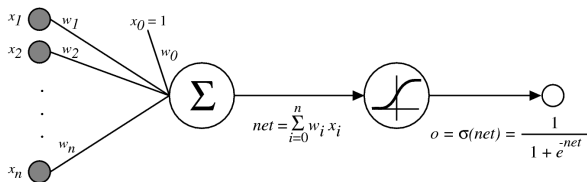
# Multi-layer Networks (ANNs)

- capable of learning **non-linear decision surfaces**
- normally **directed** and **acyclic**  $\Rightarrow$  Feed-forward Network
- based on **sigmoid unit**
  - ▶ much like a perceptron
  - ▶ but based on a smoothed, **differentiable threshold function**

$$\sigma(\text{net}) = \frac{1}{1 + e^{-\text{net}}}$$

$$\lim_{\text{net} \rightarrow +\infty} \sigma(\text{net}) = 1$$

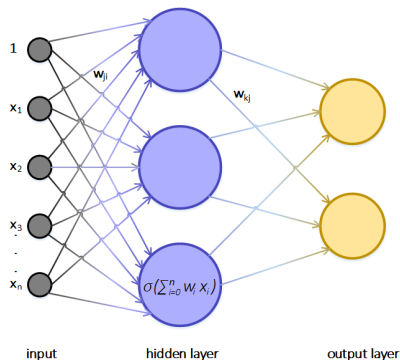
$$\lim_{\text{net} \rightarrow -\infty} \sigma(\text{net}) = 0$$



# Backpropagation

- learns weights for a feed-forward multilayer network with a fixed set of neurons and interconnections
- employs gradient descent to minimize error
- redefinition of  $E$ 
  - ▶ has to sum the errors over all units
  - ▶  $E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in \text{outputs}} (t_{kd} - o_{kd})^2$

- **problem:**  
search through a large  $H$  defined over all possible weight values for all units in the network



# Backpropagation - Algorithm

## BACKPROPAGATION(*training\_examples*, $\eta$ , $n_{in}$ , $n_{out}$ , $n_{hidden}$ )

The input from unit  $i$  to unit  $j$  is denoted  $x_{ji}$  and the weight from unit  $i$  to unit  $j$  is denoted  $w_{ji}$ .

- Create a feed-forward network with  $n_{in}$  inputs,  $n_{hidden}$  hidden units, and  $n_{out}$  output units
- Initialize all network weights to small random numbers
- Until the **termination condition** is met, Do (EPOCHE)
  - ▶ For each  $\langle \vec{x}, \vec{t} \rangle$  in *training\_examples*, Do

*Propagate the input forward through the network:*

1. Input  $\vec{x}$  to the network and compute  $o_u$  of every unit  $u$

*Propagate the errors back through the network:*

2. For each network **output unit**  $k$ , calculate its error term  $\delta_k$

$$\delta_k \leftarrow o_k(1 - o_k)(t_k - o_k)$$

3. For each **hidden unit**  $h$ , calculate its error term  $\delta_h$

$$\delta_h \leftarrow o_h(1 - o_h) \sum_{k \in \text{outputs}} w_{kh} \delta_k$$

4. Update each weight  $w_{ji}$

$$w_{ji} \leftarrow w_{ji} + \Delta w_{ji} \text{ where } \Delta w_{ji} = \eta \delta_j x_{ji}$$

# Termination conditions

- fixed number of iterations
- error falls below some threshold
- error on a separate validation set falls below some threshold
- **important:**
  - ▶ too few iterations reduce error insufficiently
  - ▶ too many iterations can lead to overfitting the data

# Adding Momentum

- one way to avoid local minima in the error surface or flat regions
- make the weight update in the  $n^{\text{th}}$  iteration depend on the update in the  $(n - 1)^{\text{th}}$  iteration

$$\Delta w_{ji}(n) = \eta \delta_j x_{ji} + \alpha \Delta w_{ji}(n - 1)$$

Note:  $\Delta w_{ji}(n - 1)$  represents the cumulative updates for this weight in the complete last epoch.

$$0 \leq \alpha \leq 1$$

# Representational Power

- *boolean functions*:
  - ▶ every boolean function can be represented by a two-layer network
- *continuous functions*:
  - ▶ every continuous function can be approximated with arbitrarily small error by a two-layer network (sigmoid units at the hidden layer and linear units at the output layer)
- *arbitrary functions*:
  - ▶ each arbitrary function can be approximated to arbitrary accuracy by a three-layer network

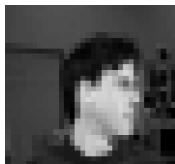
# Inductive Bias

- every possible assignment of network weights represents a syntactically different hypothesis

$$H = \{\vec{w} \mid \vec{w} \in \mathfrak{R}^{(n+1)}\}$$

- inductive bias:** smooth interpolation between data points
  - ▶ **Multilayer Networks:** smooth interpolation between data points  
⇒ **Preference bias**
  - ▶ **Perceptron:** linear separability necessary  
⇒ **Restriction bias**

# Illustrative Example - Face Recognition



## Task:

- ▶ classifying camera image of faces of various people
- ▶ images of 20 people were made, including approximately 32 different images per person
- ▶ image resolution  $120 \times 128$  with each pixel described by a grey-scale intensity between 0 and 255
- ▶ identifying the direction in which the persons are looking (i.e., left, right, up, ahead)



# Illustrative Example - Design Choices

- **input encoding:**

- ▶ image encoded as a set of  $30 \times 32$
- ▶ pixel intensity values ranging from 0 to 255 linearly scaled from 0 to 1
- ⇒ reduces the number of inputs and network weights
- ⇒ reduces computational demands

- **output encoding:**

- ▶ network must output one of four values indicating the face direction
- ▶ *1-of-n* output encoding: 1 output unit for each direction
- ⇒ more degrees of freedom
- ⇒ difference between highest and second-highest output can be used as a measure of classification confidence

# Illustrative Example - Design Choices

- **network graph structure:**

- ▶ BACKPROPAGATION works with any DAG of sigmoid units
- ▶ question of how many units and how to interconnect them
- ▶ using *standard design*: hidden layer and output layer where every unit in the hidden layer is connected with every unit in the output layer

⇒ 30 hidden units

⇒ test accuracy of 90%

# Further Topics

- hidden layer representations
- alternative error functions
- recurrent networks
- dynamically modifying network structure
- different variants of Deep Learning Networks

# Summary

- able to learn discrete-, real- and vector-valued target functions
- noise in the data is allowed
- perceptrons learn hyperplane decision surfaces (linear separability)
- multilayer networks can learn non-linear decision surfaces
- Backpropagation works on all feed-forward networks and uses gradient-descent to minimize the squared error over the set of training examples
- an arbitrary function can be approximated to arbitrary accuracy by a three-layer network

## Perceptrons / Multilayer Perceptrons

<b>Supervised Learning</b>	unsupervised learning
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Approaches:

<b>Concept / Classification</b>	Policy Learning
symbolic	statistical / <b>neuronal network</b>
<b>inductive</b>	analytical

Learning Strategy:	<b>learning from examples</b>
Data:	<b>categorical/metric features</b>
Target Values:	<b>arbitrary (concept, class, value, vector)</b>