Lecture 4: Artificial Neural Networks

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

Ute Schmid

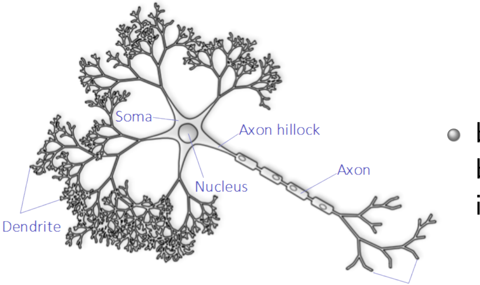
Cognitive Systems, Applied Computer Science, University of Bamberg
www.uni-bamberg.de/cogsys

Last change: November 21, 2020

Outline

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

Biological Motivation



Schematic of biological neuron.

- 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^{11} neurons
	10 TB HDD	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

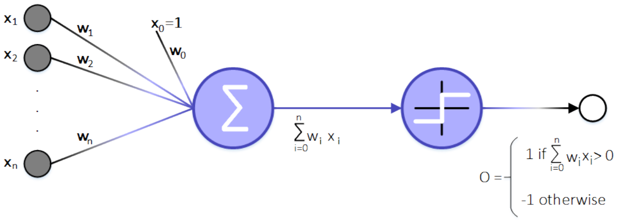
- instances are represented as many attribute-value pairs
  - input values can be any real values
- target function output is binary
- Hypotheses are linear, that is, hyper-planes which partition the hypothesis space in two areas (concept/not concept)
- When Minsky and Papert showed in their book *Perceptrons* (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

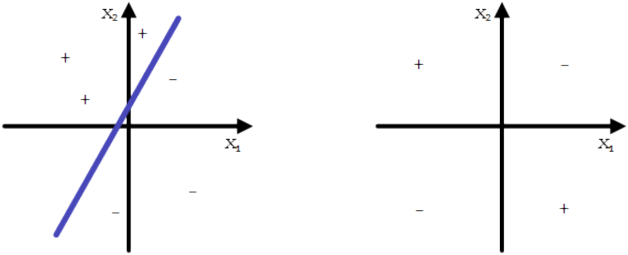
Perceptrons



- takes a vector of real-valued inputs $(x_1, \ldots, x_n)$ weighted with $(w_1, \ldots, w_n)$
- calculates the linear combination of these inputs
  - $\sum_{i=0}^{n} w_i x_i = w_0 x_0 + w_1 x_1 + \ldots + w_n x_n$
  - $-w_0$ 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



(a) (b)

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:**

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

t target output
o perceptron output
η 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
   $\Rightarrow$ apply perceptron training rule to each training example

- convergence guaranteed provided *linearly separable* training examples and sufficiently small η

Delta Rule

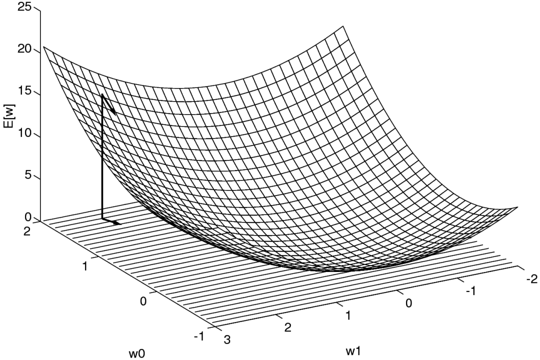
- perceptron rule fails if data is not linearly separable
- delta rule converges toward a **best-fit approximation**
- uses **gradient descent** to search the hypothesis space
  - perceptron cannot be used, because it is not differentiable
  - hence, a **unthresholded linear unit** is appropriate
  -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



$\Rightarrow$ 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)

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

- $\nabla E(\vec{w})$ 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.* η is the learning rate.

- Initialize each w_i to some small random value
- Until the **termination condition** is met, Do
  - Initialize each Δw_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 $w_i \leftarrow w_i + \eta(t - o)x_i$.

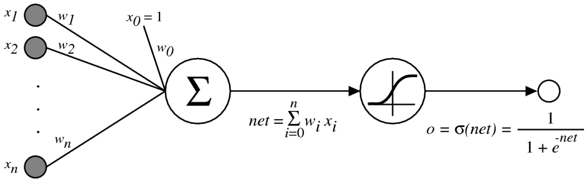
Perceptron vs. Delta Rule

- **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**

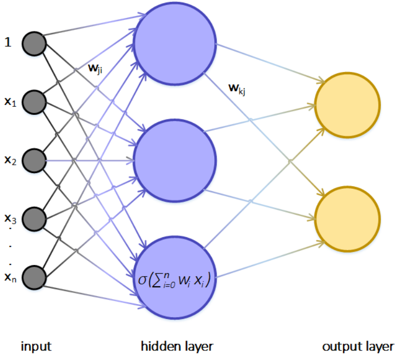
$$\sigma(net) = \frac{1}{1+e^{-net}}$$
$$\lim_{net \to +\infty} \sigma(net) = 1$$
$$\lim_{net \to -\infty} \sigma(net) = 0$$



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
  - $E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} - o_{kd})^2$

- **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 δ_k
       $$\delta_k \leftarrow o_k(1 - o_k)(t_k - o_k)$$
    3. For each **hidden unit** h, calculate its error term δ_h
       $$\delta_h \leftarrow o_h(1 - o_h) \sum_{k \in outputs} w_{kh}\delta_k$$
    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^{th} iteration depend on the update in the $(n-1)^{th}$ 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

  $H = \{\vec{w} | \vec{w} \in \Re^{(n+1)}\}$

- **inductive bias:** smooth interpolation between data points
  - **Multilayer Networks:** smooth interpolation between data points
    $\Rightarrow$ **Preference bias**
  - **Perceptron:** linear separability necessary
    $\Rightarrow$ **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 120×128 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 30×32
  - pixel intensity values ranging from 0 to 255 linearly scaled from 0 to 1

  $\Rightarrow$ reduces the number of inputs and network weights

  $\Rightarrow$ 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

  $\Rightarrow$ more degrees of freedom

  $\Rightarrow$ 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

$\Rightarrow$ 30 hidden units

$\Rightarrow$ 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

Supervised Learning	unsupervised learning

Approaches:

Concept / Classification	Policy Learning
symbolic	statistical / **neuronal network**
inductive	analytical

Learning Strategy: Data: Target Values:	**learning from examples** **categorial/metric features** **arbitrary (concept, class, value, vector)**