PV021: Neural networks

Tomáš Brázdil

Course organization

Course materials:

- **Main:** The lecture
- Neural Networks and Deep Learning by Michael Nielsen

  `http://neuralnetworksanddeeplearning.com/`

  (Extremely well written modern online textbook.)
- Deep learning by Ian Goodfellow, Yoshua Bengio and Aaron Courville

  `http://www.deeplearningbook.org/`

  (A very good overview of the state-of-the-art in neural networks.)

Suggested: deeplearning.ai courses by Andrew Ng

Course organization

Evaluation:

- Project
  - teams of two students
  - implementation of a selected model + analysis of given data
  - implementation either in C, C++ **without use of any specialized libraries for data analysis and machine learning**
  - need to get over a given accuracy threshold (a gentle one, just to eliminate non-functional implementations)

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- Oral exam
  - I may ask about anything from the lecture!

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Q: Why should you attend this course when there are infinitely many great reasources elsewhere?

A: There are at least two reasons:

- You may discuss issues with me, my colleagues and other students.
- I will make you truly learn fundamentals by heart.

Notable features of the course

- Use of mathematical notation and reasoning (contains several proofs that are mandatory for the exam)
- Sometimes goes deeper into statistical underpinnings of neural networks learning
- The project demands a complete working solution which must satisfy a prescribed performance specification

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An example of an instruction email (from another course with the same system):

```
It is typically not sufficient to devote a single
afternoon to the preparation for the exam.
You have to know _everything_ (which means every
single thing) starting with the slide 42
and ending with the slide 245 with notable exceptions
of slides: 121 - 123, 137 - 140, 165, 167.
Proofs presented on the whiteboard are also mandatory.
```

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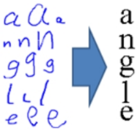

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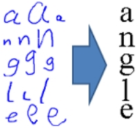

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  - and lots of much much more sophisticated applications ...

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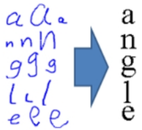

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- Basic attributes of learning algorithms:
  - **representation**: ability to capture the inner structure of training data
  - **generalization**: ability to work properly on new data

Machine learning in general

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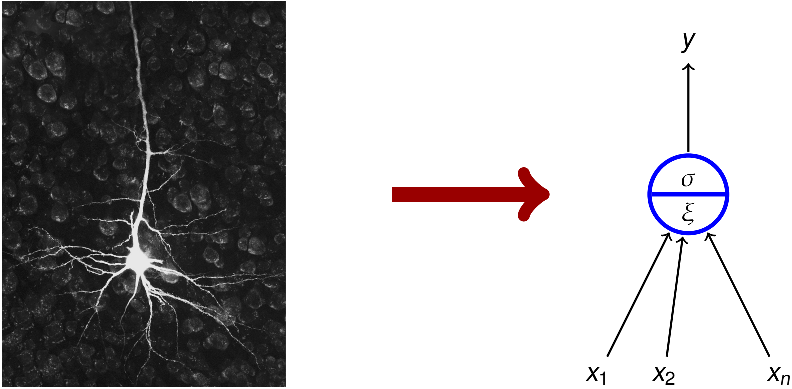
There are many types of models:

- decision trees
- support vector machines
- hidden Markov models
- Bayes networks and other graphical models
- **neural networks**
- ...

Neural networks, based on models of a (human) brain, form a natural basis for learning algorithms!

Artificial neural networks

- **Artificial neuron** is a *rough mathematical approximation* of a biological neuron.
- **(Aritificial) neural network (NN)** consists of a number of interconnected artificial neurons. "Behavior" of the network is encoded in connections between neurons.



Zdroj obrázku: `http://tulane.edu/sse/cmb/people/schrader/`

Why artificial neural networks?

Modelling of biological neural networks (computational neuroscience).

- simplified mathematical models help to identify important mechanisms
  - How a brain receives information?
  - How the information is stored?
  - How a brain develops?
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- neuroscience is strongly multidisciplinary; precise mathematical descriptions help in communication among experts and in design of new experiments.

I will not spend much time on this area!

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Neural networks in machine learning.

- Typically primitive models, far from their biological counterparts (but often inspired by biology).
- Strongly oriented towards concrete application domains:
  - decision making and control - autonomous vehicles, manufacturing processes, control of natural resources
  - games - backgammon, poker, GO, Starcraft, ...
  - finance - stock prices, risk analysis
  - medicine - diagnosis, signal processing (EKG, EEG, ...), image processing (MRI, roentgen, WSI ...)
  - text and speech processing - automatic translation, text generation, speech recognition
  - other signal processing - filtering, radar tracking, noise reduction
  - ...

I will concentrate on this area!

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  - a blurred photo of a rabbit may still be classified as an image of a rabbit
- Graceful degradation
  - Experiments have shown that damaged neural network is still able to work quite well
  - Damaged network may re-adapt, remaining neurons may take on functionality of the damaged ones

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- We will concentrate on
  - basic techniques and principles of neural networks,
  - fundamental models of neural networks and their applications.
- You should learn
  - basic models
    (multilayer perceptron, convolutional networks, recurrent network (LSTM), Hopfield and Boltzmann machines and their use in pre-training of deep nets, autoencoders and generative adversarial networks)

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  - Basic information about current implementations
    (TensorFlow, Keras)

Biological neural network

- Human neural network consists of approximately 10^{11} (100 billion on the short scale) neurons; a single cubic centimeter of a human brain contains almost 50 million neurons.
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- Afterwards, the output signal is transfered via PNS to *effectors* (e.g. muscle cells).

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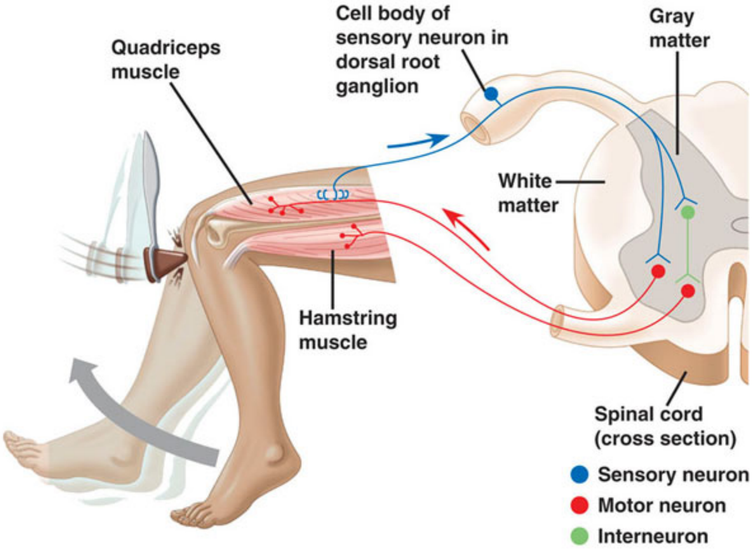


Zdroj: N. Campbell and J. Reece; Biology, 7th Edition; ISBN: 080537146X

Summation

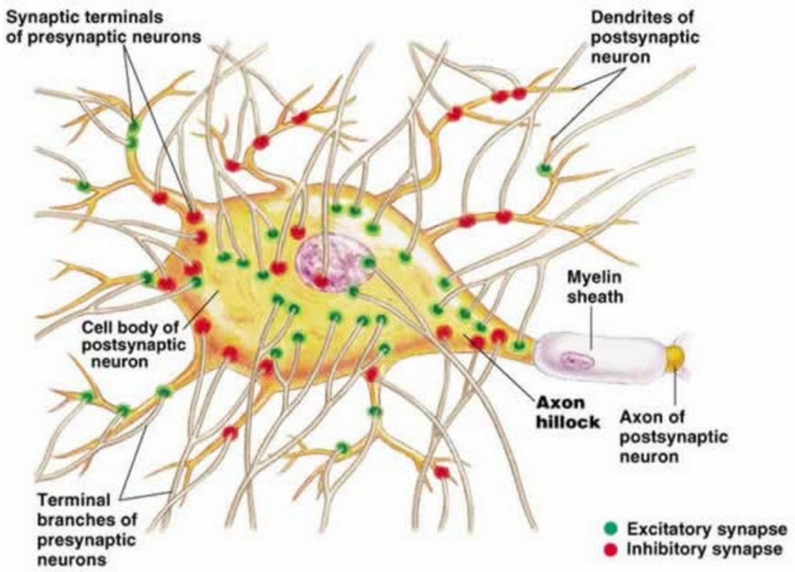
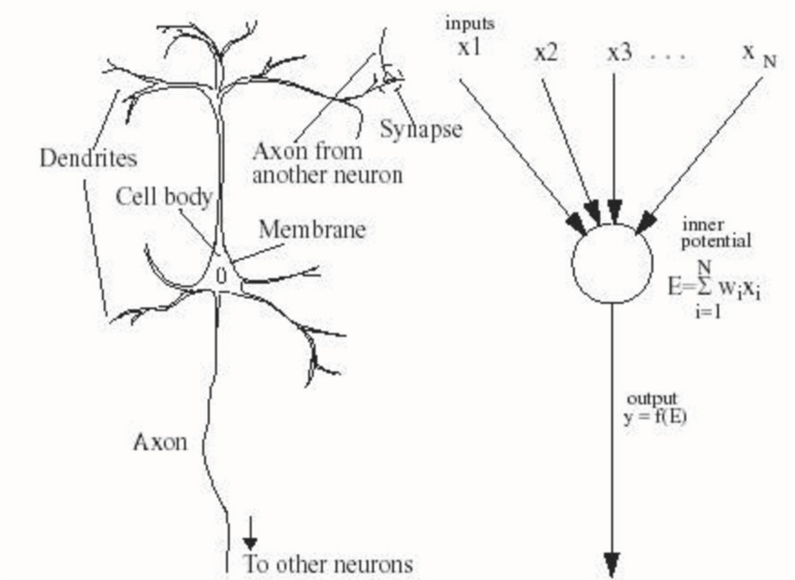
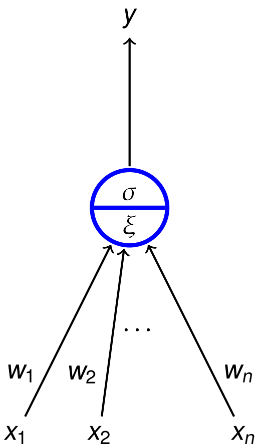


Figure 48.11(a), page 972, Campbell's *Biology, 5th Edition*

Biological and Mathematical neurons



Formal neuron (without bias)



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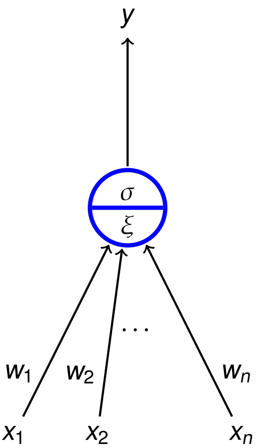

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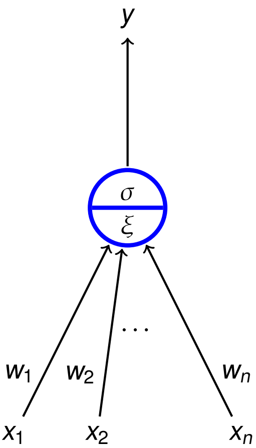

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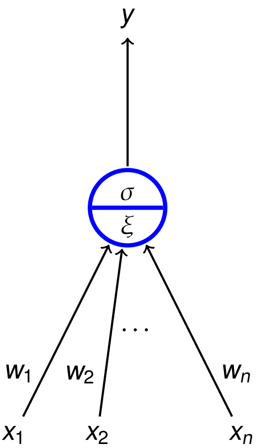

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  where σ is an **activation function**;

  e.g. a *unit step function*

$$\sigma(\xi) = \begin{cases} 1 & \xi \geq h\,; \\ 0 & \xi < h. \end{cases}$$

where $h \in \mathbb{R}$ is a *threshold*.

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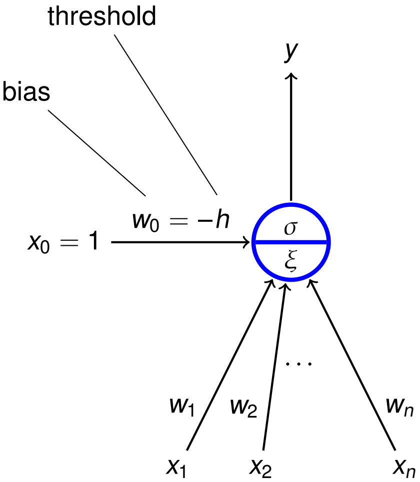

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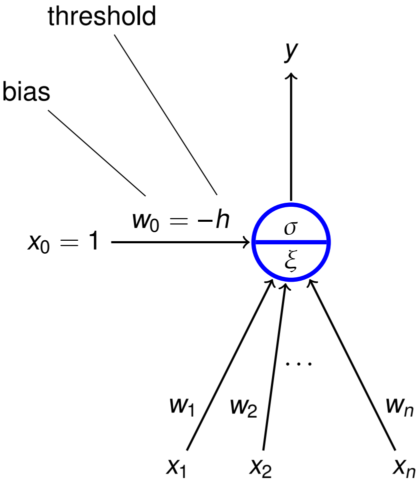

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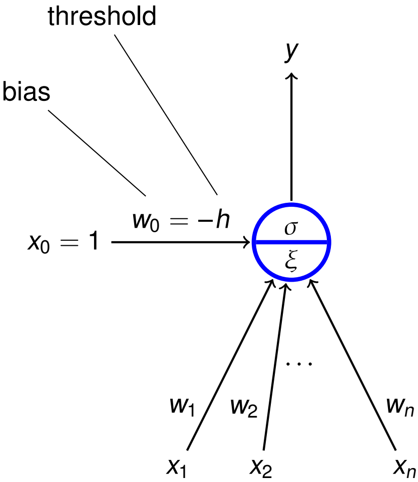

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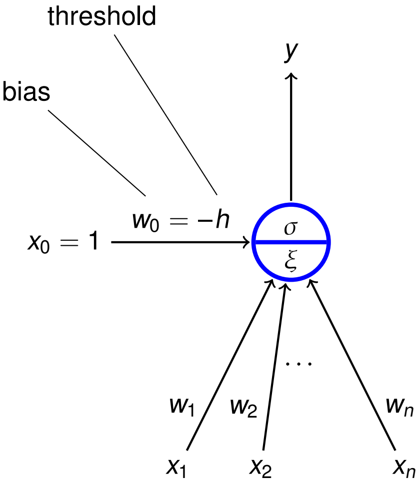

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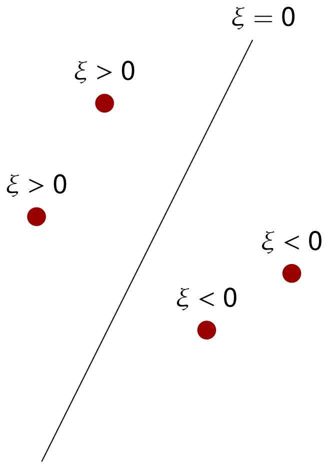
(The threshold h has been substituted with the new input $x_0 = 1$ and the weight $w_0 = -h$.)

Neuron and linear separation



- inner potential

$$\xi = w_0 + \sum_{i=1}^{n} w_i x_i$$

determines a separation hyperplane in the *n*-dimensional **input space**
  - in 2d line
  - in 3d plane
  - …

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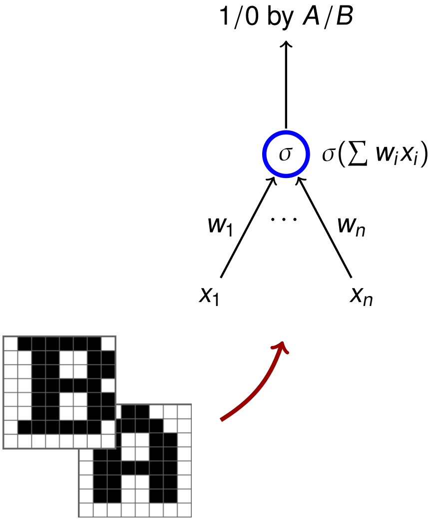

$n = 8 \cdot 8$, i.e. the number of pixels in the images. Inputs are binary vectors of dimension n (black pixel ≈ 1, white pixel ≈ 0).

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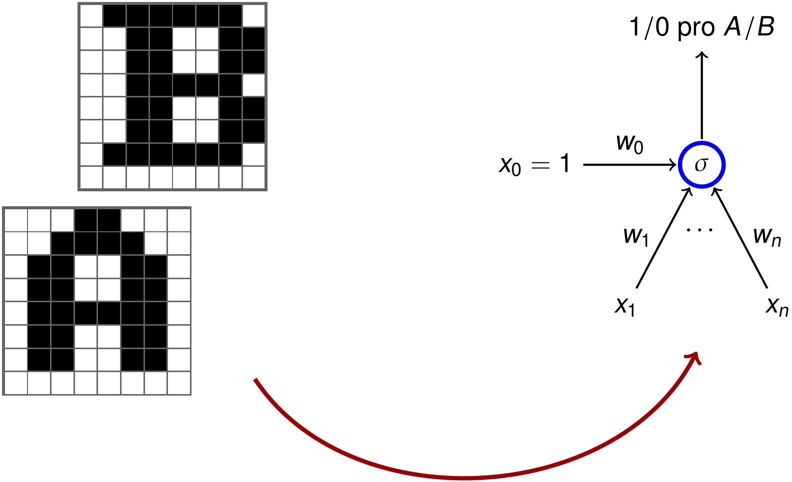

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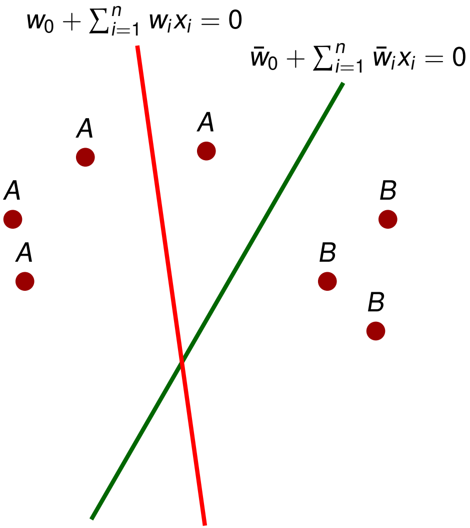
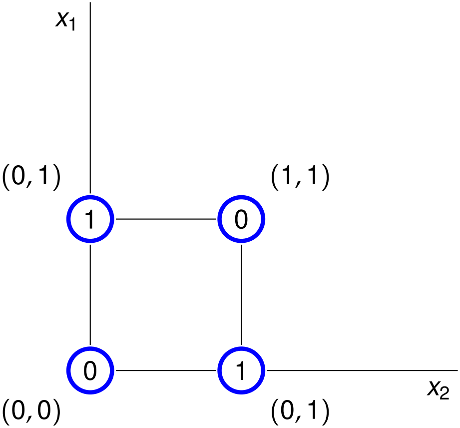


- Red line classifies incorrectly
- Green line classifies correctly (may be a result of a correction by a learning algorithm)

Neuron and linear separation (XOR)



- No line separates ones from zeros.

Neural networks

Neural network consists of formal neurons interconnected in such a way that the output of one neuron is an input of several other neurons.

In order to describe a particular type of neural networks we need to specify:

- Architecture

  How the neurons are connected.
- Activity

  How the network transforms inputs to outputs.
- Learning

  How the weights are changed during training.

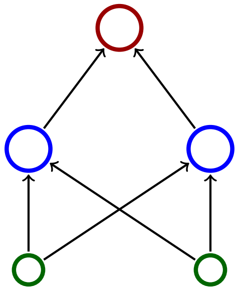
Architecture

Network architecture is given as a digraph whose nodes are neurons and edges are connections.

We distinguish several categories of neurons:

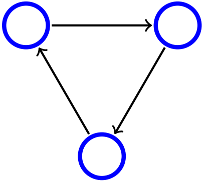
- Output neurons
- Hidden neurons
- Input neurons

(In general, a neuron may be both input and output; a neuron is hidden if it is neither input, nor output.)



Architecture – Cycles

- A network is **cyclic** (recurrent) if its architecture contains a directed cycle.



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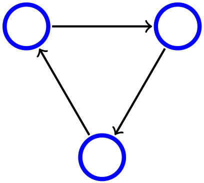
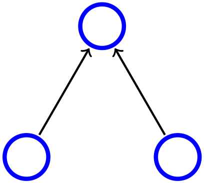
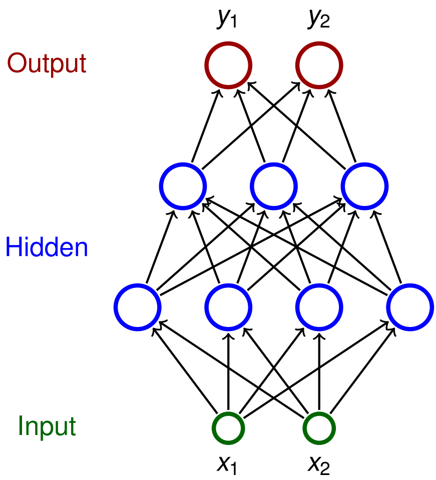


- Otherwise it is **acyclic** (feed-forward)



Architecture – Multilayer Perceptron (MLP)



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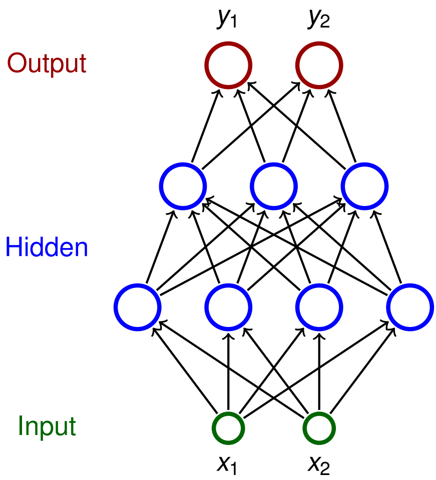

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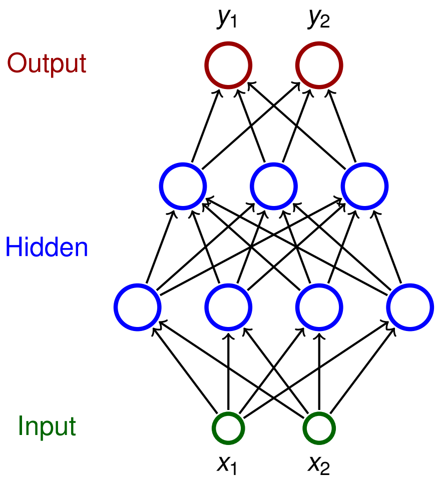

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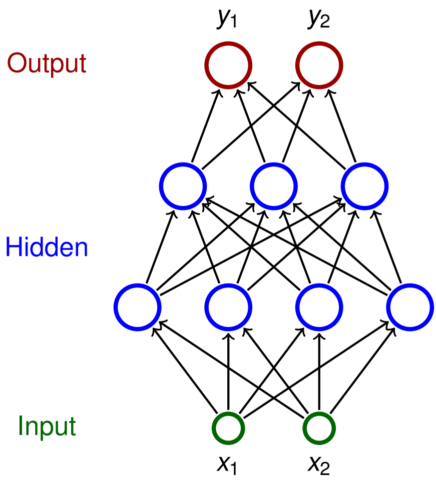

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- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

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- **Initial state**

  Input neurons set to values from the network input
  (each component of the network input corresponds to an input neuron)

  Values of the remaining neurons set to 0.

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MLP uses the following selection rule:

In the i-th step evaluate all neurons in the i-th layer.

Activity – semantics of a network

Definition

Consider a network with n neurons, k input, ℓ output.
Let $A \subseteq \mathbb{R}^k$ and $B \subseteq \mathbb{R}^\ell$. Suppose that the network stops on every input of A.
Then we say that the network computes a function $F : A \rightarrow B$ *if for every network input $\vec{x}$ the vector $F(\vec{x}) \in B$ is the output of the network after the computation on $\vec{x}$ stops.*

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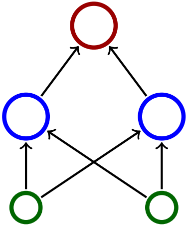
Example 1

This network computes a function from $\mathbb{R}^2$ to $\mathbb{R}$.



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We assume (unless otherwise specified) that

$$\xi = w_0 + \sum_{i=1}^{n} w_i \cdot x_i$$

here $\vec{x} = (x_1, \ldots, x_n)$ are inputs of the neuron and $\vec{w} = (w_1, \ldots, w_n)$ are weights.

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There are special types of neural network where the inner potential is computed differently, e.g. as a "distance" of an input from the weight vector:

$$\xi = \left\| \vec{x} - \vec{w} \right\|$$

here $\|\cdot\|$ is a vector norm, typically Euclidean.

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- (Logistic) sigmoid

$$\sigma(\xi) = \frac{1}{1 + e^{-\lambda \cdot \xi}}$$ here $\lambda \in \mathbb{R}$ is a *steepness* parameter.

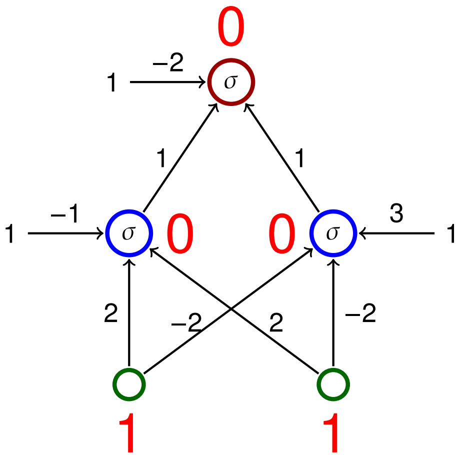
- Hyperbolic tangens

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

- ReLU

$$\sigma(\xi) = \max(\xi, 0)$$

Activity – XOR



- Activation function is a unit step function

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- The network computes $XOR(x_1, x_2)$

x_1	x_2	y
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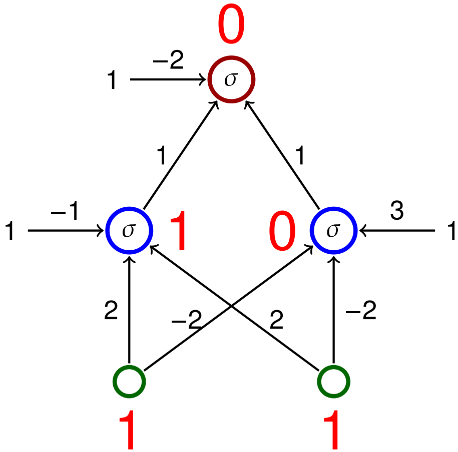

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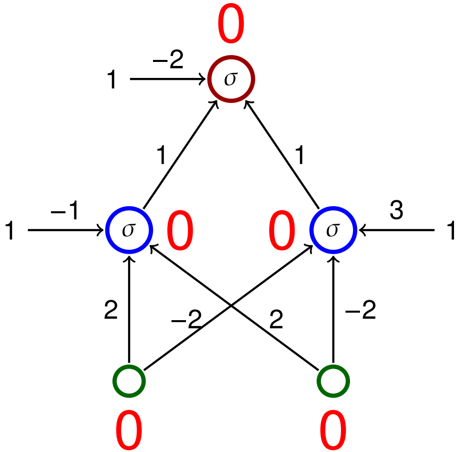

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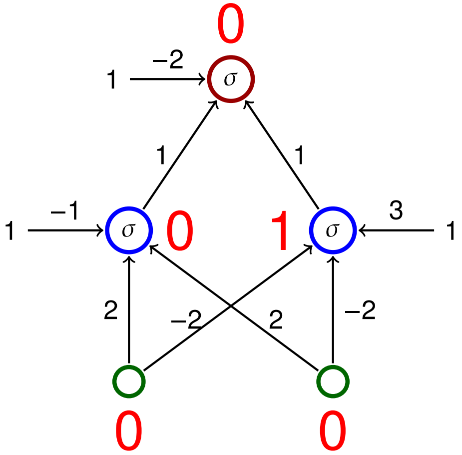

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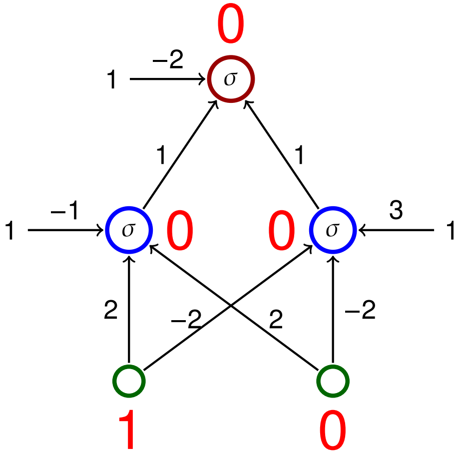

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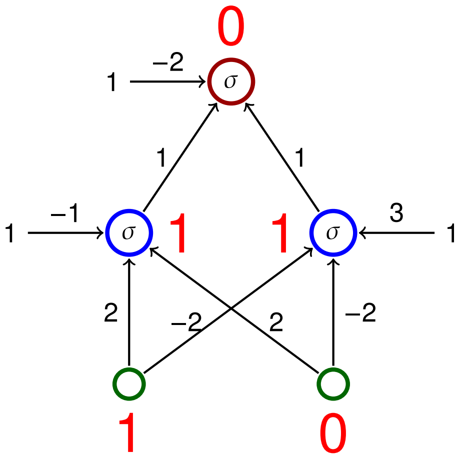

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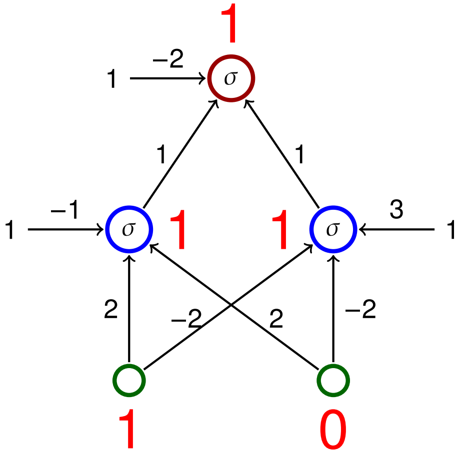

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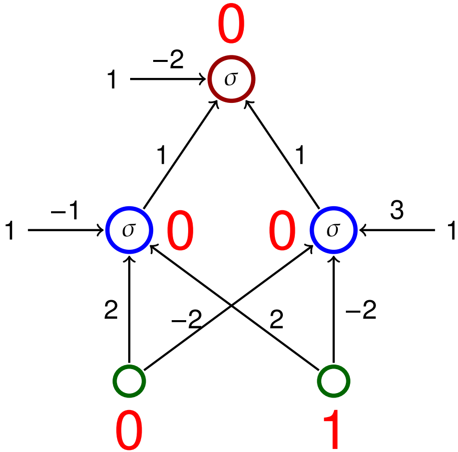

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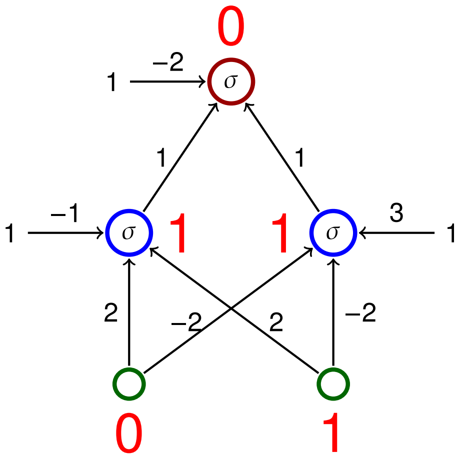

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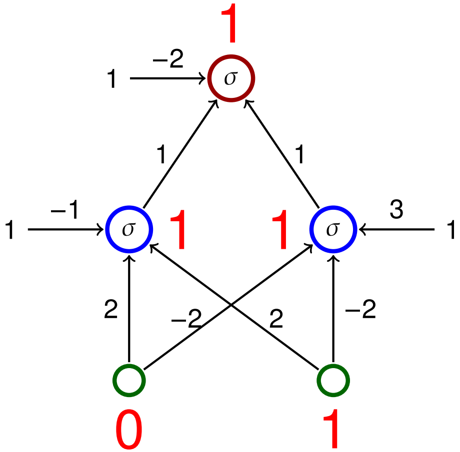

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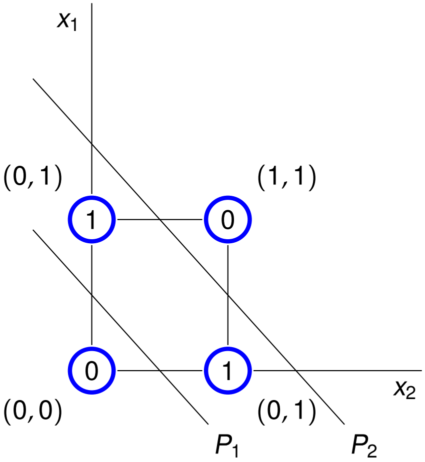
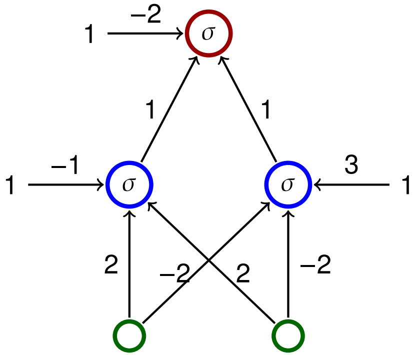
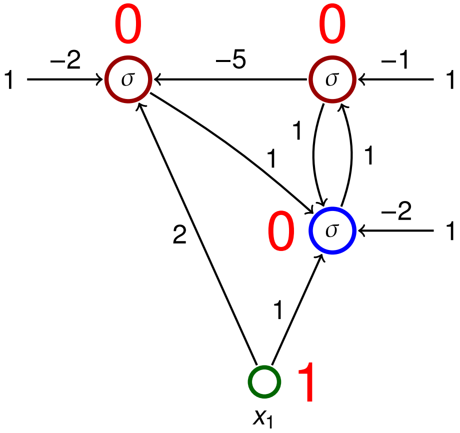




- The line P_1 is given by $-1 + 2x_1 + 2x_2 = 0$
- The line P_2 is given by $3 - 2x_1 - 2x_2 = 0$

Activity – example



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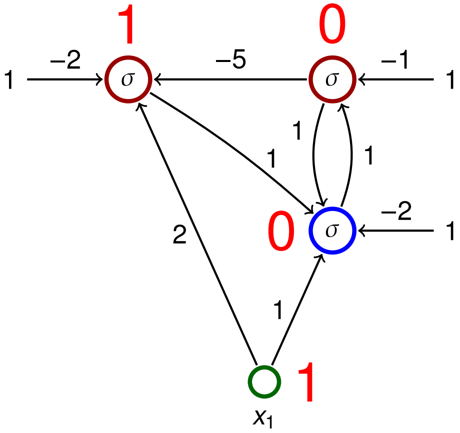

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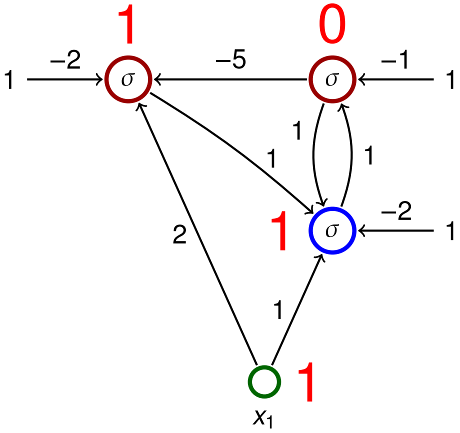

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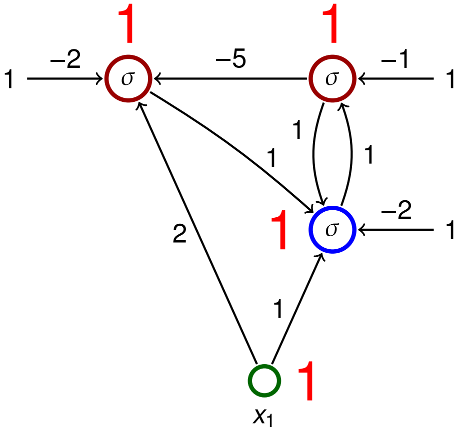

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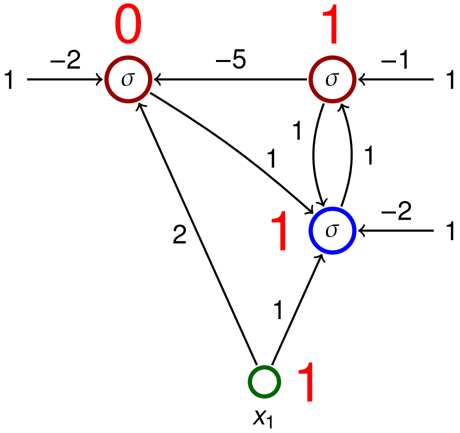

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  weights can be initialized randomly or using some sophisticated algorithm

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Learning rule for weight adaptation.

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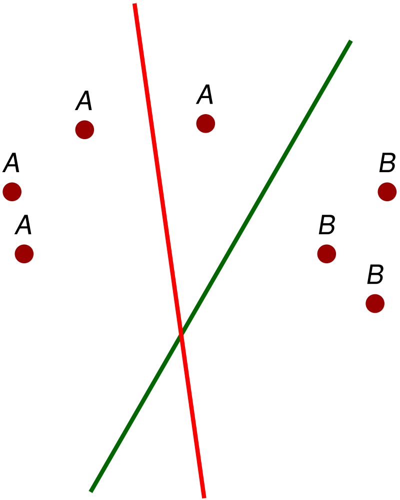
- Unsupervised learning
  - The training set contains only inputs.
  - The goal is to determine distribution of the inputs (clustering, deep belief networks, etc.)

Supervised learning – illustration



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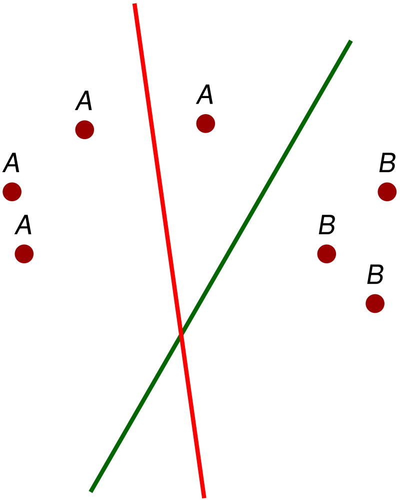

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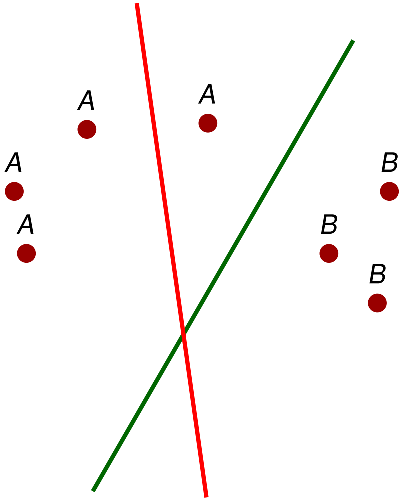

- classification in the plane using a single neuron
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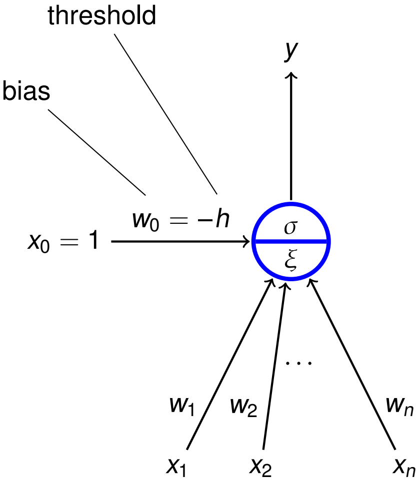
  - "close" inputs typicaly get similar values
- Graceful degradation
  - damage typically causes only a decrease in precision of results

Expressive power of neural networks

Formal neuron (with bias)



- $x_0 = 1, x_1, \ldots, x_n \in \mathbb{R}$ are **inputs**
- $w_0, w_1, \ldots, w_n \in \mathbb{R}$ are **weights**
- ξ is an **inner potential**;
  almost always $\xi = w_0 + \sum_{i=1}^{n} w_i x_i$
- y is an **output** given by $y = \sigma(\xi)$
  where σ is an **activation function**;

  e.g. a *unit step function*

$$\sigma(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

Boolean functions

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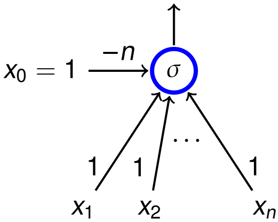
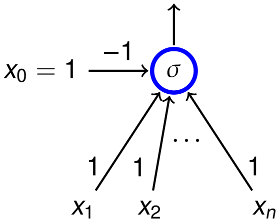
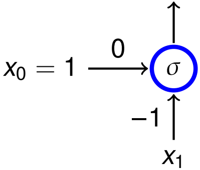


$y = OR(x_1, \ldots, x_n)$



$y = NOT(x_1)$



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Let σ *be the unit step function. Two layer MLPs, where each neuron has* σ *as the activation function, are able to compute all functions of the form* $F : \{0, 1\}^n \rightarrow \{0, 1\}$.

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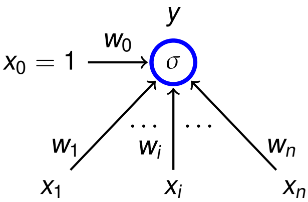
Proof.

- Given a vector $\vec{v} = (v_1, \ldots, v_n) \in \{0,1\}^n$, consider a neuron $N_{\vec{v}}$ whose output is 1 iff the input is $\vec{v}$:

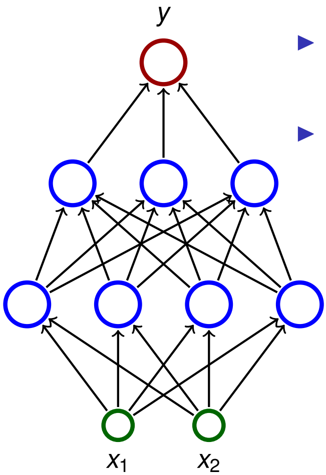


$$w_0 = -\sum_{i=1}^{n} v_i$$

$$w_i = \begin{cases} 1 & v_i = 1 \\ -1 & v_i = 0 \end{cases}$$

- Now let us connect all outputs of all neurons $N_{\vec{v}}$ satisfying $F(\vec{v}) = 1$ using a neuron implementing *OR*. □

Non-linear separation



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- The network divides the input space in two subspaces according to the output (0 or 1).

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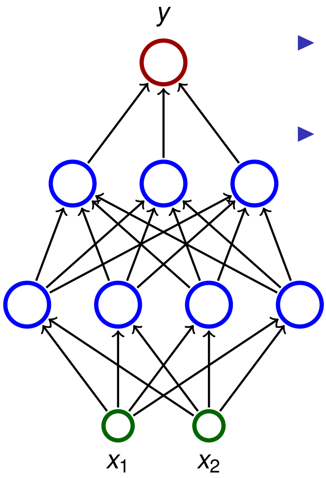
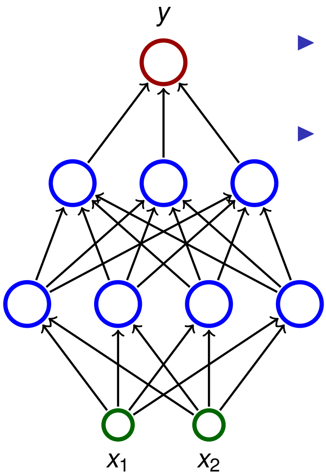


- Consider a three layer network; each neuron has the unit step activation function.
- The network divides the input space in two subspaces according to the output (0 or 1).
  - The first (hidden) layer divides the input space into half-spaces.

Non-linear separation



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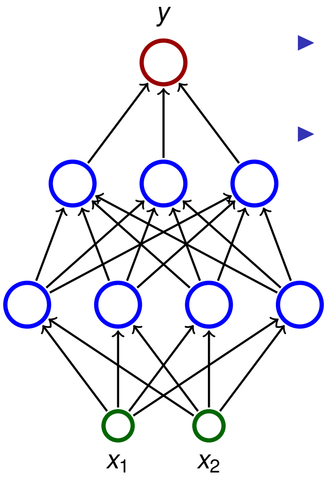

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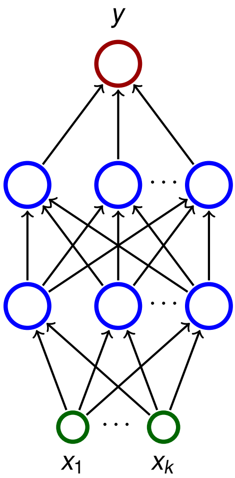
  - The third layer may e.g. make unions of some convex sets.

Non-linear separation – illustration



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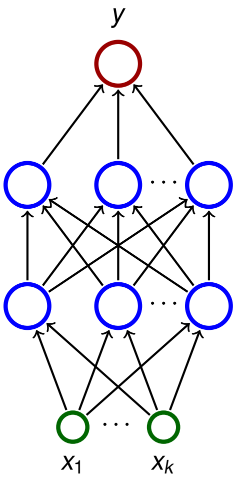

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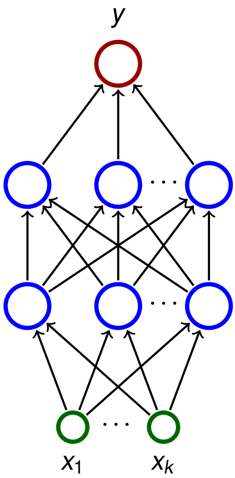

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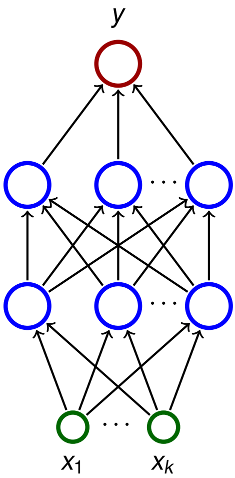

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    (i.e. a function computed by N_K gives 1 for points in K and 0 for the rest).
  - Finally, connect outputs of the nets N_K satisfying $K \cap A \neq \emptyset$ using a neuron implementing OR.

Non-linear separation - sigmoid

Theorem (Cybenko 1989 - informal version)

Let σ be a continuous function which is sigmoidal, i.e. satisfies

$$\sigma(x) = \begin{cases} 1 & \text{for } x \to +\infty \\ 0 & \text{for } x \to -\infty \end{cases}$$

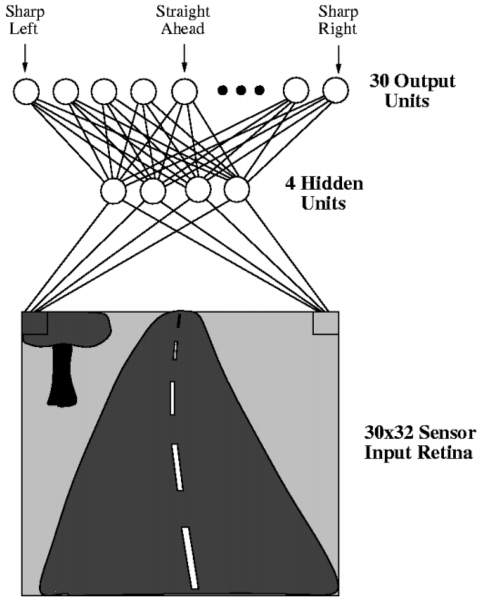
For every "reasonable" set $A \subseteq [0,1]^n$, there is a **two layer network** *where each hidden neuron has the activation function σ (output neurons are linear), that satisfies the following:*

For "most" vectors $\vec{v} \in [0,1]^n$ we have that $\vec{v} \in A$ iff the network output is > 0 for the input $\vec{v}$.

For mathematically oriented:

- "reasonable" means Lebesgue measurable
- "most" means that the set of incorrectly classified vectors has the Lebesgue measure smaller than a given $\varepsilon > 0$

Non-linear separation - practical illustration



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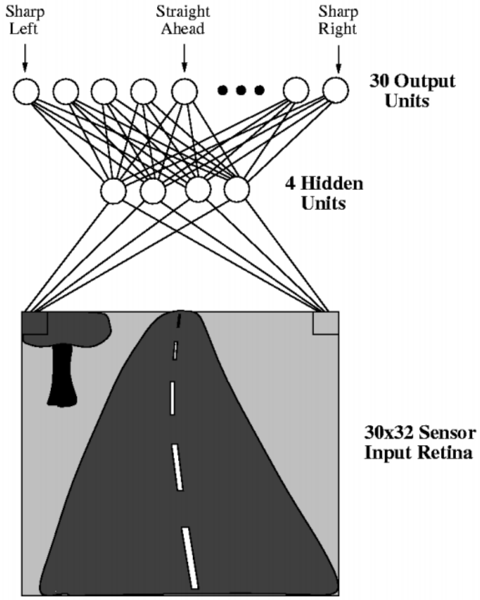

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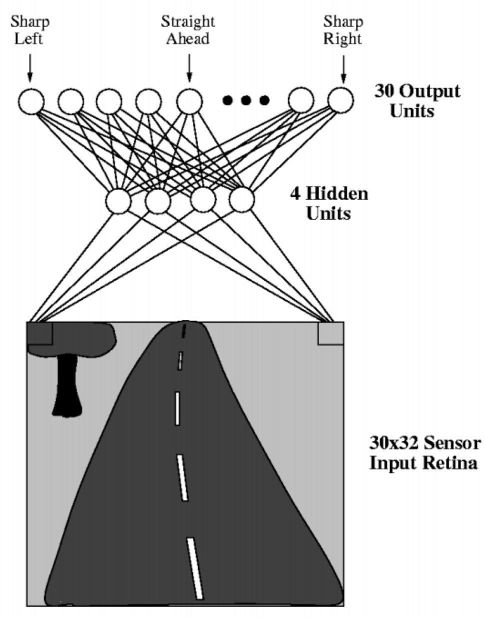

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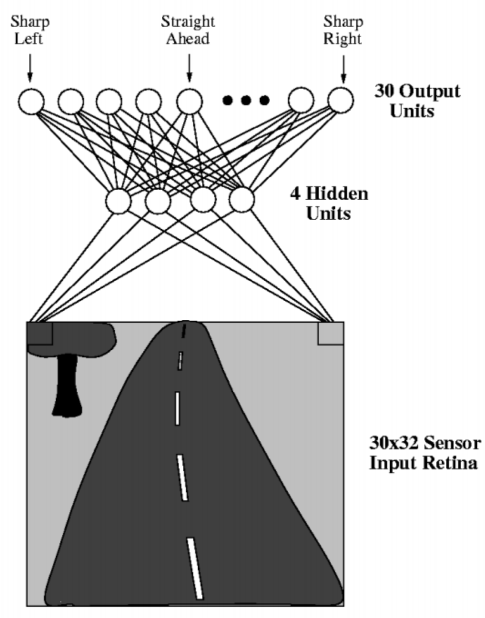

- ALVINN drives a car
- The net has $30 \times 32 = 960$ inputs (the input space is thus $\mathbb{R}^{960}$)
- Input values correspond to shades of gray of pixels.
- Output neurons "classify" images of the road based on their "curvature".

Zdroj obrázku: `http://jmvidal.cse.sc.edu/talks/ann/alvin.html`

Function approximation - three layers

Let σ be a logistic sigmoid, i.e.

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

For every continuous function $f : [0, 1]^n \rightarrow [0, 1]$ and $\varepsilon > 0$ there is a three-layer network computing a function $F : [0, 1]^n \rightarrow [0, 1]$ such that

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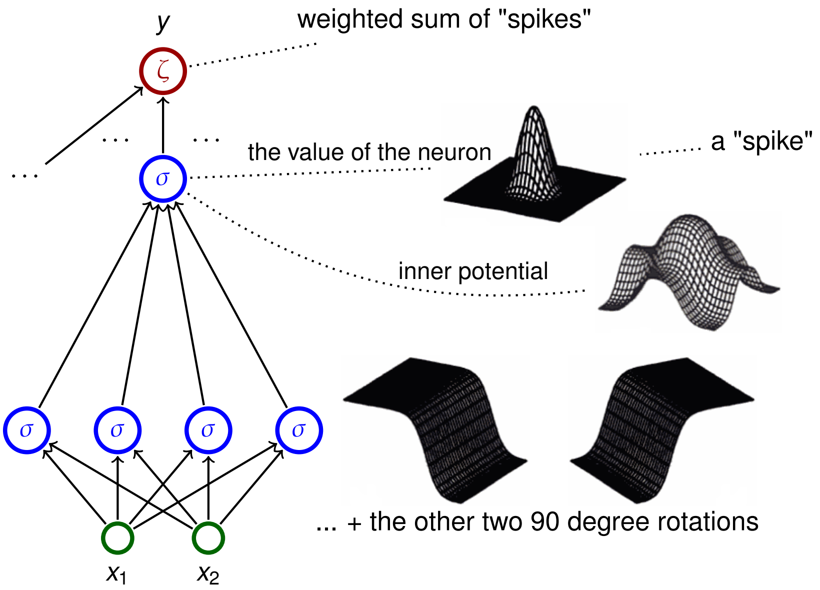
Function approximation – three layer networks



Function approximation - two-layer networks

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$$|f(\vec{v}) - F(\vec{v})| < \varepsilon \qquad \textit{pro každé } \vec{v} \in [0,1]^n.$$

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- We encode words $\omega \in \{0,1\}^+$ into numbers as follows:

$$\delta(\omega) = \sum_{i=1}^{|\omega|} \frac{\omega(i)}{2^i} + \frac{1}{2^{|\omega|+1}}$$

E.g. $\omega = 11001$ gives $\delta(\omega) = \frac{1}{2} + \frac{1}{2^2} + \frac{1}{2^5} + \frac{1}{2^6}$ $(= 0.110011$ in binary form).

Neural networks and computability

A network **recognizes** a language $L \subseteq \{0,1\}^+$ if it computes a function $F : A \to \mathbb{R}$ ($A \subseteq \mathbb{R}$) such that

$$\omega \in L \text{ iff } \delta(\omega) \in A \text{ and } F(\delta(\omega)) > 0.$$

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- Recurrent networks with rational weights are equivalent to Turing machines
  - For every recursively enumerable language $L \subseteq \{0,1\}^+$ there is a recurrent network with rational weights and less than 1000 neurons, which recognizes L.
  - The halting problem is undecidable for networks with at least 25 neurons and rational weights.
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- Recurrent networks are super-Turing powerful
  - For **every** language $L \subseteq \{0,1\}^+$ there is a recurrent network with less than 1000 nerons which recognizes L.

Summary of theoretical results

- Neural networks are very strong from the point of view of theory:
  - All Boolean functions can be expressed using two-layer networks.
  - Two-layer networks may approximate any continuous function.
  - Recurrent networks are at least as strong as Turing machines.

Summary of theoretical results

- Neural networks are very strong from the point of view of theory:
  - All Boolean functions can be expressed using two-layer networks.
  - Two-layer networks may approximate any continuous function.
  - Recurrent networks are at least as strong as Turing machines.
- These results are purely theoretical!
  - "Theoretical" networks are extremely huge.
  - It is very difficult to handcraft them even for simplest problems.
- From practical point of view, the most important advantage of neural networks are: learning, generalization, robustness.

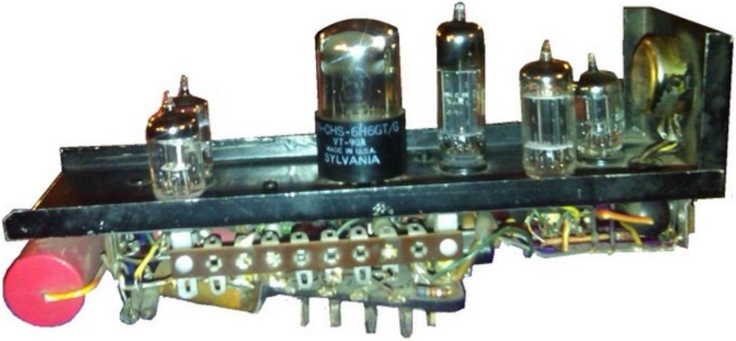
Neural networks vs classical computers

	Neural networks	"Classical" computers
Data	implicitly in weights	explicitly
Computation	naturally parallel	sequential, localized
Robustness	robust w.r.t. input corruption & damage	changing one bit may completely crash the computation
Precision	imprecise, network recalls a training example "similar" to the input	(typically) precise
Programming	learning	manual

History & implementations

History of neurocomputers

- 1951: SNARC (Minski et al)
  - the first implementation of neural network
  - a rat strives to exit a maze
  - 40 artificial neurons (300 vacuum tubes, engines, etc.)



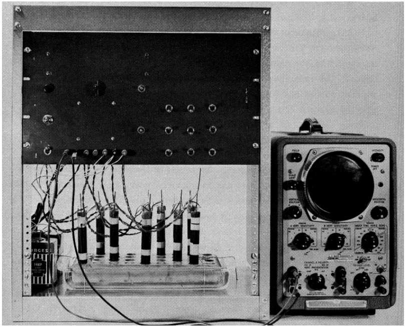
History of neurocomputers

- 1957: Mark I Perceptron (Rosenblatt et al) - the first successful network for image recognition

  - single layer network
  - image represented by 20×20 photocells
  - intensity of pixels was treated as the input to a perceptron (basically the formal neuron), which recognized figures
  - weights were implemented using potentiometers, each set by its own engine
  - it was possible to arbitrarily reconnect inputs to neurons to demonstrate adaptability

History of neurocomputers

- 1960: ADALINE (Widrow & Hof)



  - single layer neural network
  - weights stored in a newly invented electronic component **memistor**, which remembers history of electric current in the form of resistance.
  - Widrow founded a company Memistor Corporation, which sold implementations of neural networks.
- 1960-66: several companies concerned with neural networks were founded.

History of neurocomputers

- 1967-82: dead still after publication of a book by Minski & Papert (published 1969, title *Perceptrons*)
- 1983-end of 90s: revival of neural networks
  - many attempts at hardware implementations
    - application specific chips (ASIC)
    - programmable hardware (FPGA)
  - hw implementations typically not better than "software" implementations on universal computers (problems with weight storage, size, speed, cost of production etc.)

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- end of 90s-cca 2005: NN suppressed by other machine learning methods (support vector machines (SVM))
- 2006-now: The boom of neural networks!
  - deep networks – often better than any other method
  - GPU implementations
  - ... some specialized hw implementations (Google's TPU)

Some highlights

- Breakthrough in image recognition.
  Accuracy of image recognition improved by an order of magnitude in 5 years.
- Breakthrough in game playing.
  Superhuman results in Go and Chess almost without any human intervention. Master level in Starcraft, poker, etc.
- Breakthrough in machine translation.
  Switching to deep learning produced a 60% increase in translation accuracy compared to the phrase-based approach previously used in Google Translate (in human evaluation)
- Breakthrough in speech processing.

History in waves ...

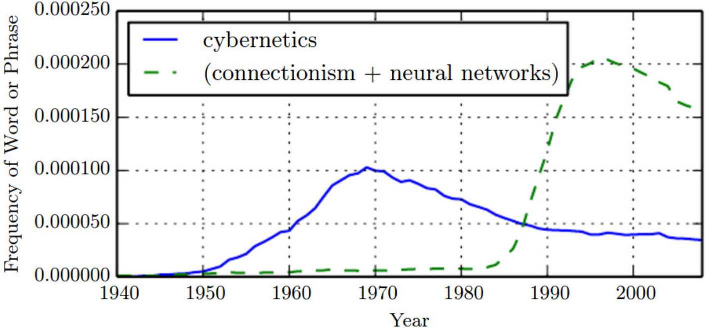
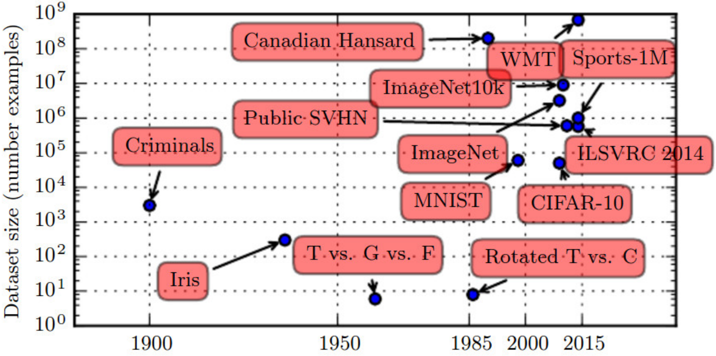


Figure: The figure shows two of the three historical waves of artificial neural nets research, as measured by the frequency of the phrases "cybernetics" and "connectionism" or "neural networks" according to Google Books (the third wave is too recent to appear).

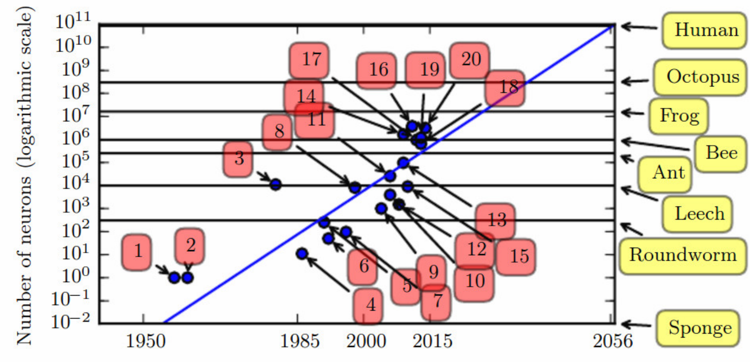
Current hardware – What do we face?

Increasing dataset size ...



Current hardware – What do we face?

... and thus increasing size of neural networks ...



2. ADALINE
4. Early back-propagation network (Rumelhart et al., 1986b)
8. Image recognition: LeNet-5 (LeCun et al., 1998b)
10. Dimensionality reduction: Deep belief network (Hinton et al., 2006)
    ... here the third "wave" of neural networks started
15. Digit recognition: GPU-accelerated multilayer perceptron (Ciresan et al., 2010)
18. Image recognition (AlexNet): Multi-GPU convolutional network (Krizhevsky et al., 2012)
20. Image recognition: GoogLeNet (Szegedy et al., 2014a)

Current hardware – What do we face?

... as a reward we get this ...

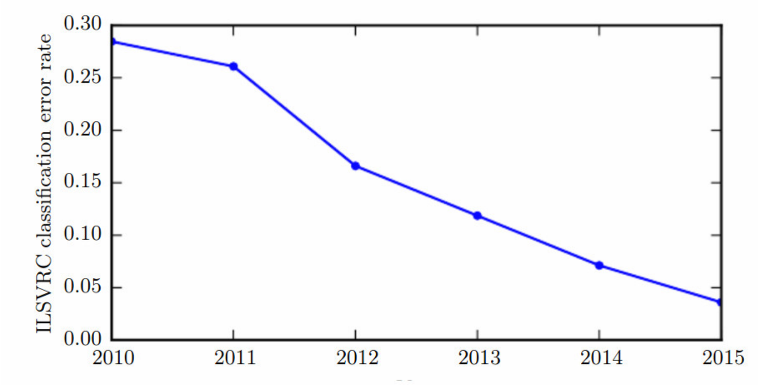


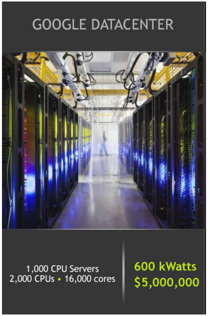
Figure: Since deep networks reached the scale necessary to compete in the ImageNetLarge Scale Visual Recognition Challenge, they have consistently won the competition every year, and yielded lower and lower error rates each time. Data from Russakovsky et al. (2014b) and He et al. (2015).

Current hardware

In 2012, Google trained a large network of 1.7 billion weights and 9 layers

The task was image recognition (10 million youtube video frames)

The hw comprised a 1000 computer network (16 000 cores), computation took three days.



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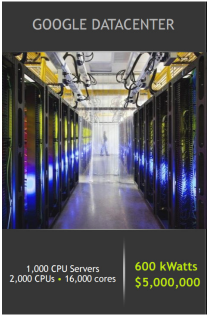
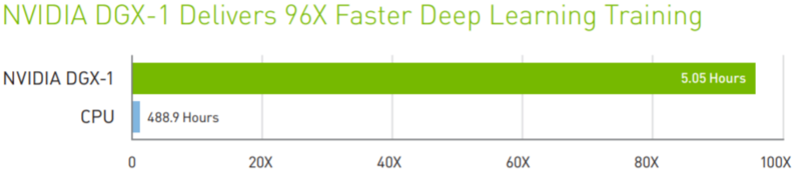
In 2014, similar task performed on Commodity Off-The-Shelf High Performance Computing (COTS HPC) technology: a cluster of GPU servers with Infiniband interconnects and MPI.

Able to train 1 billion parameter networks on just 3 machines in a couple of days.
Able to scale to 11 billion weights (approx. 6.5 times larger than the Google model) on 16 GPUs.



Current hardware – NVIDIA DGX-1 Station

- 8x GPU (Tesla V100)
- TFLOPS = 1000
- GPU memory 256GB total
- NVIDIA Tensor Cores: 5,120
- NVIDIA CUDA Cores: 40,960
- System memory: 512 GB
- Network: Dual 10 Gb LAN
- NVIDIA Deep Learning SDK



Deep learning in clouds

Several companies offer cloud services for deep learning:

- Amazon Web Services
- Google Cloud
- Deep Cognition
- ...

Advantages:

- Do not have to care (too much) about technical problems.
- Do not have to buy and optimize highend hw/sw, networks etc.
- Scaling & virtually limitless storage.

Disadvatages:

- Do not have full control.
- Performance can vary, connectivity problems.
- Have to pay for services.
- Privacy issues.

Current software

- **TensorFlow** (Google)
  - open source software library for numerical computation using data flow graphs
  - allows implementation of most current neural networks
  - allows computation on multiple devices (CPUs, GPUs, ...)
  - Python API
  - **Keras**: a part of TensorFlow that allows easy description of most modern neural networks
- **PyTorch** (Facebook)
  - similar to TensorFlow
  - object oriented
- **Theano (dead)**:
  - The "academic" grand-daddy of deep-learning frameworks, written in Python. Strongly inspired TensorFlow (some people developing Theano moved on to develop TensorFlow).
- There are others: Caffe, Deeplearning4j, ...

Current software – Keras

```
from keras.models import Sequential
from keras.layers import Dense, Dropout, Activation
from keras.optimizers import SGD

model = Sequential()
# Dense(64) is a fully-connected layer with 64 hidden units.
# in the first layer, you must specify the expected input data shape
# here, 20-dimensional vectors.
model.add(Dense(64, input_dim=20, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(64, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(10, init='uniform'))
model.add(Activation('softmax'))

sgd = SGD(lr=0.1, decay=1e-6, momentum=0.9, nesterov=True)
model.compile(loss='categorical_crossentropy',
              optimizer=sgd,
              metrics=['accuracy'])

model.fit(X_train, y_train,
          nb_epoch=20,
          batch_size=16)
score = model.evaluate(X_test, y_test, batch_size=16)
```

Current software – Keras functional API

```python
from keras.layers import Input, Dense
from keras.models import Model

# This returns a tensor
inputs = Input(shape=(784,))

# a layer instance is callable on a tensor, and returns a tensor
output_1 = Dense(64, activation='relu')(inputs)
output_2 = Dense(64, activation='relu')(output_1)
predictions = Dense(10, activation='softmax')(output_2)

# This creates a model that includes
# the Input layer and three Dense layers
model = Model(inputs=inputs, outputs=predictions)
model.compile(optimizer='rmsprop',
              loss='categorical_crossentropy',
              metrics=['accuracy'])
model.fit(data, labels)  # starts training
```

Current software – TensorFlow

```
# tf Graph input
X = tf.placeholder("float", [None, n_input])
Y = tf.placeholder("float", [None, n_classes])

# Store layers weight & bias
weights = {
    'h1': tf.Variable(tf.random_normal([n_input, n_hidden_1])),
    'h2': tf.Variable(tf.random_normal([n_hidden_1, n_hidden_2])),
    'out': tf.Variable(tf.random_normal([n_hidden_2, n_classes]))
}
biases = {
    'b1': tf.Variable(tf.random_normal([n_hidden_1])),
    'b2': tf.Variable(tf.random_normal([n_hidden_2])),
    'out': tf.Variable(tf.random_normal([n_classes]))
}
```

Current software – TensorFlow

```
# Create model
def multilayer_perceptron(x):
    # Hidden fully connected layer with 256 neurons
    layer_1 = tf.add(tf.matmul(x, weights['h1']), biases['b1'])
    # Hidden fully connected layer with 256 neurons
    layer_2 = tf.add(tf.matmul(layer_1, weights['h2']), biases['b2'])
    # Output fully connected layer with a neuron for each class
    out_layer = tf.matmul(layer_2, weights['out']) + biases['out']
    return out_layer

# Construct model
logits = multilayer_perceptron(X)
```

Current software – PyTorch

```
class Net(nn.Module):
    def __init__(self, input_size, hidden_size, num_classes):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU()
        self.fc2 = nn.Linear(hidden_size, num_classes)

    def forward(self, x):
        out = self.fc1(x)
        out = self.relu(out)
        out = self.fc2(out)
        return out

net = Net(input_size, hidden_size, num_classes)
```

Other software implementations

Most "mathematical" software packages contain some support of neural networks:

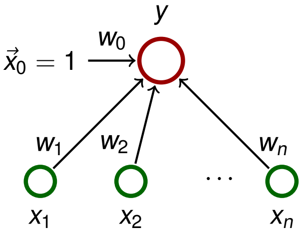
- MATLAB
- R
- STATISTICA
- Weka
- ...

The implementations are typically not on par with the previously mentioned dedicated deep-learning libraries.

Training linear models

Linear regression (ADALINE)

Architecture:



$\vec{w} = (w_0, w_1, \ldots, w_n)$ and $\vec{x} = (x_0, x_1, \ldots, x_n)$ where $x_0 = 1$.

Activity:

- inner potential: $\xi = w_0 + \sum_{i=1}^{n} w_i x_i = \sum_{i=0}^{n} w_i x_i = \vec{w} \cdot \vec{x}$
- activation function: $\sigma(\xi) = \xi$
- network function: $y[\vec{w}](\vec{x}) = \sigma(\xi) = \vec{w} \cdot \vec{x}$

Linear regression (ADALINE)

Learning:

- Given a **training dataset**

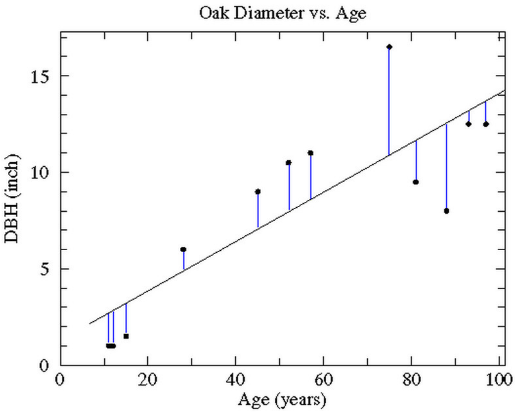
$$\mathcal{T} = \left\{\left(\vec{x}_1, d_1\right), \left(\vec{x}_2, d_2\right), \dots, \left(\vec{x}_p, d_p\right)\right\}$$

Here $\vec{x}_k = (x_{k0}, x_{k1} \dots, x_{kn}) \in \mathbb{R}^{n+1}$, $x_{k0} = 1$, is the k-th input, and $d_k \in \mathbb{R}$ is the expected output.

Intuition: The network is supposed to compute an affine approximation of the function (some of) whose values are given in the training set.

Oaks in Wisconsin

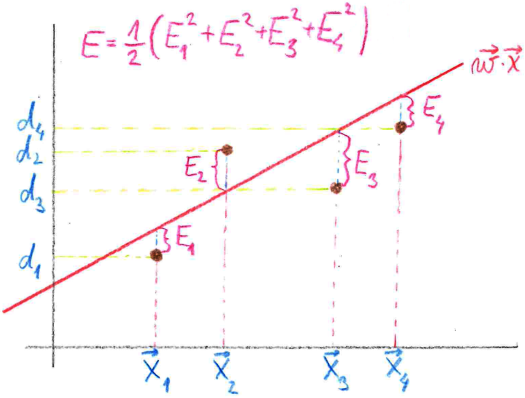
Age (years)	*DBH* (inch)
97	12.5
93	12.5
88	8.0
81	9.5
75	16.5
57	11.0
52	10.5
45	9.0
28	6.0
15	1.5
12	1.0
11	1.0



Linear regression (ADALINE)

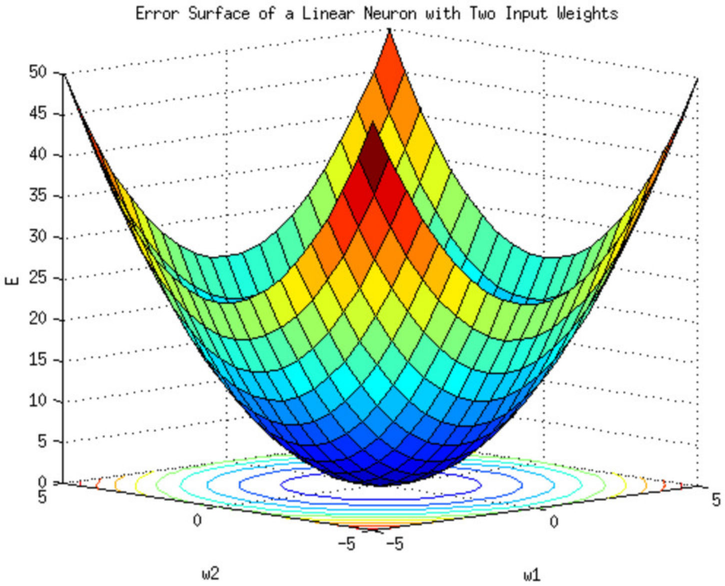
- **Error function:**

$$E(\vec{w}) = \frac{1}{2}\sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right)^2 = \frac{1}{2}\sum_{k=1}^{p}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)^2$$



- The goal is to find $\vec{w}$ which minimizes $E(\vec{w})$.

Error function



Gradient of the error function

Consider **gradient** of the error function:

$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \ldots, \frac{\partial E}{\partial w_n}(\vec{w}) \right)$$

Intuition: $\nabla E(\vec{w})$ is a vector in the **weight space** which points in the direction of the *steepest ascent* of the error function.

Note that the vectors $\vec{x}_k$ are just parameters of the function E, and are thus fixed!

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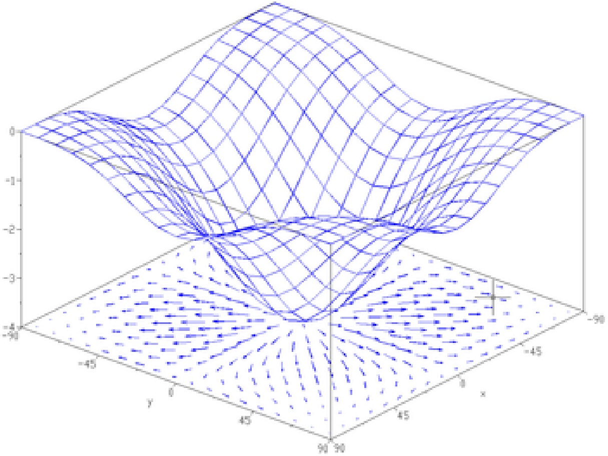
Fact

If $\nabla E(\vec{w}) = \vec{0} = (0, \ldots, 0)$, *then* $\vec{w}$ *is a global minimum of* E.

For ADALINE, the error function $E(\vec{w})$ is a convex paraboloid and thus has the unique global minimum.

Gradient - illustration



Caution! This picture just illustrates the notion of gradient ... it is not the convex paraboloid $E(\vec{w})$!

Gradient of the error function

First, consider $n = 1$.

Then the model is $y = w_0 + w_1 \cdot x$.

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$$\begin{aligned}\mathcal{T} &= \{((1,2),1),((1,3),2),((1,4),5)\} \\ &= ((x_{10},x_{11}),d_1),((x_{20},x_{21}),d_2),((x_{30},x_{31}),d_3)\end{aligned}$$

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$$E(w_0,w_1) = \tfrac{1}{2}[(w_0+w_1\cdot 2-1)^2+(w_0+w_1\cdot 3-2)^2+(w_0+w_1\cdot 4-5)^2]$$

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$$\frac{\delta E}{\delta w_0} = (w_0+w_1\cdot 2-1)\cdot 1+(w_0+w_1\cdot 3-2)\cdot 1+(w_0+w_1\cdot 4-5)\cdot 1$$

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$$\frac{\delta E}{\delta w_0} = (w_0 + w_1 \cdot 2 - 1) \cdot 1 + (w_0 + w_1 \cdot 3 - 2) \cdot 1 + (w_0 + w_1 \cdot 4 - 5) \cdot 1$$

$$\frac{\delta E}{\delta w_1}$$

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$$\frac{\delta E}{\delta w_0} = (w_0+w_1\cdot 2-1)\cdot 1+(w_0+w_1\cdot 3-2)\cdot 1+(w_0+w_1\cdot 4-5)\cdot 1$$

$$\frac{\delta E}{\delta w_1} = (w_0+w_1\cdot 2-1)\cdot 2+(w_0+w_1\cdot 3-2)\cdot 3+(w_0+w_1\cdot 4-5)\cdot 4$$

Gradient of the error function

$$\frac{\partial E}{\partial w_\ell}(\vec{w}) \quad = \quad \frac{1}{2}\sum_{k=1}^{p} \frac{\delta}{\delta w_\ell}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)^2$$

Gradient of the error function

$$
\begin{aligned}
\frac{\partial E}{\partial w_\ell}(\vec{w}) &= \frac{1}{2}\sum_{k=1}^{p} \frac{\delta}{\delta w_\ell}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)^2 \\
&= \frac{1}{2}\sum_{k=1}^{p} 2\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)\frac{\delta}{\delta w_\ell}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)
\end{aligned}
$$

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$$
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&= \frac{1}{2}\sum_{k=1}^{p} 2\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)\left(\sum_{i=0}^{n}\left(\frac{\delta}{\delta w_\ell} w_i x_{ki}\right) - \frac{\delta E}{\delta w_\ell} d_k\right)
\end{aligned}
$$

Gradient of the error function

$$
\begin{aligned}
\frac{\partial E}{\partial w_\ell}(\vec{w}) &= \frac{1}{2}\sum_{k=1}^{p} \frac{\delta}{\delta w_\ell}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)^2 \\
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&= \sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right) x_{k\ell}
\end{aligned}
$$

Gradient of the error function

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&= \sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right) x_{k\ell}
\end{aligned}
$$

Thus

$$
\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \ldots, \frac{\partial E}{\partial w_n}(\vec{w})\right) = \sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right)\vec{x}_k
$$

Linear regression - learning

Batch algorithm (gradient descent):

Idea: In every step "move" the weights in the direction *opposite* to the gradient.

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Here $0 < \varepsilon \leq 1$ is a *learning rate*.

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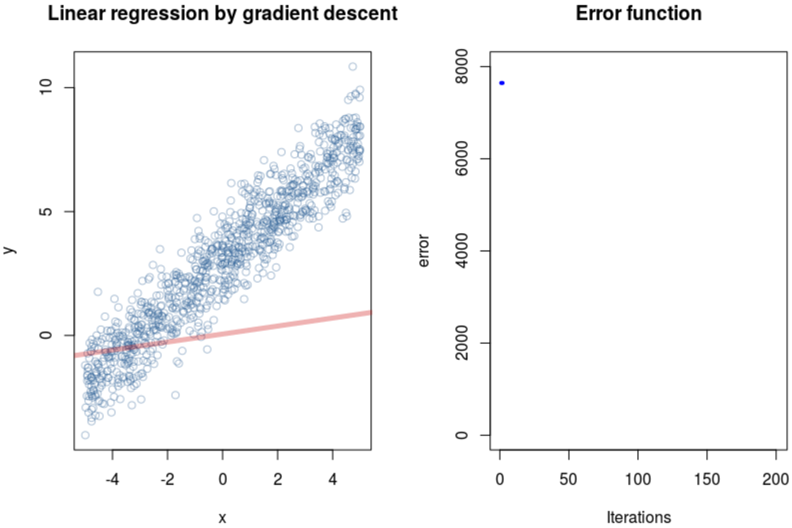
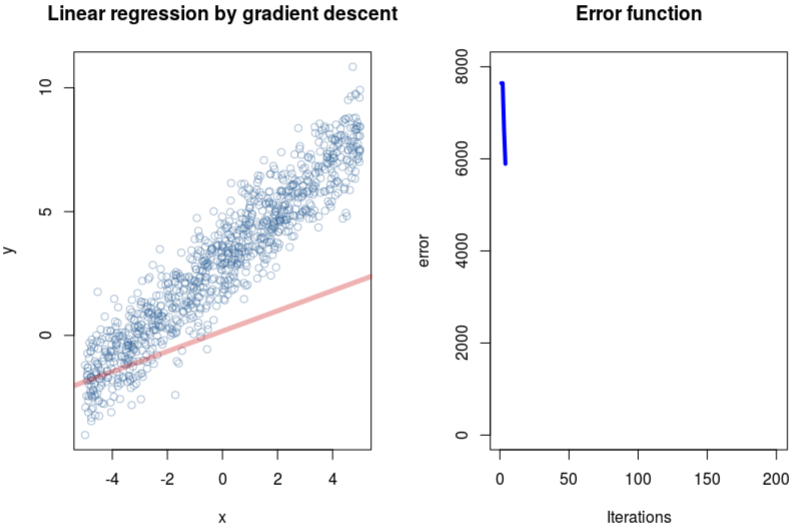
Proposition

For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (componentwise) to the global minimum of E (i.e. to the vector $\vec{w}$ satisfying $\nabla E(\vec{w}) = \vec{0}$).

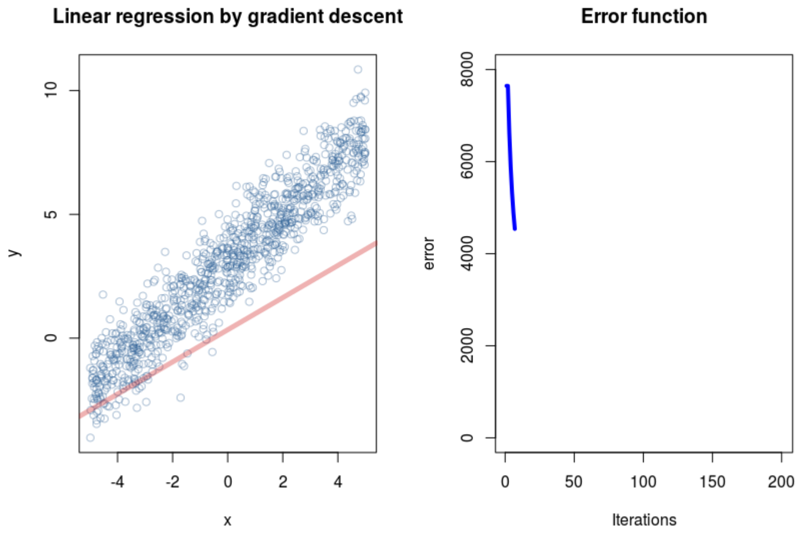
Linear regression - animation



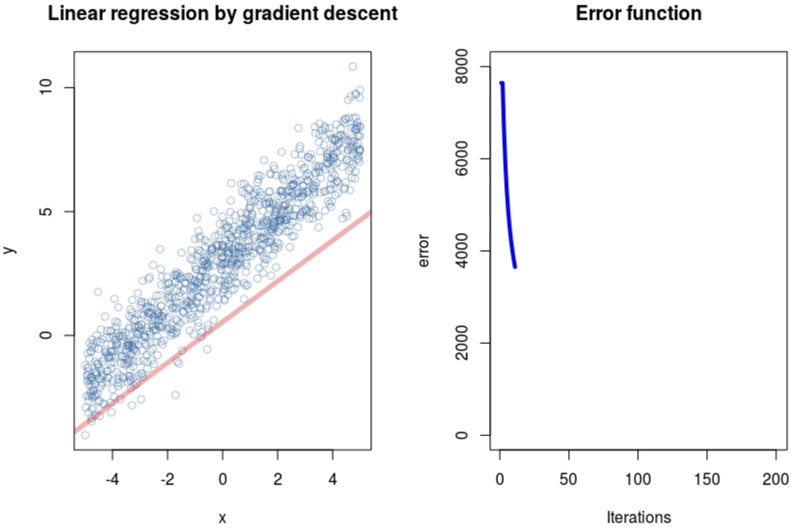
Linear regression - animation



Linear regression - animation



Linear regression - animation



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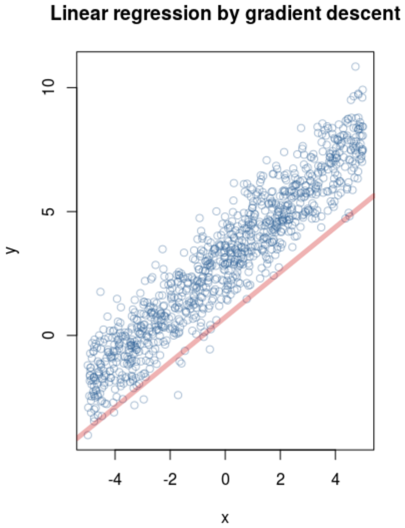

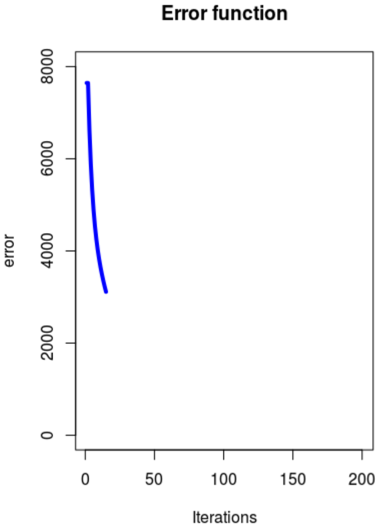

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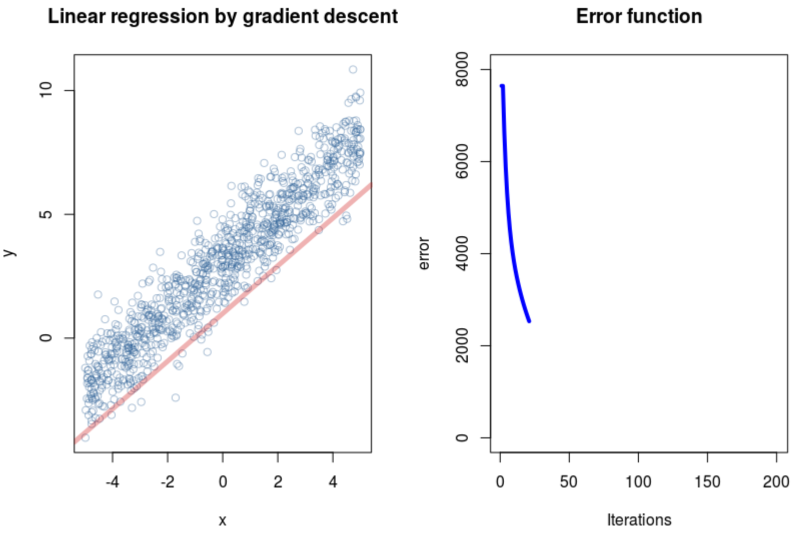

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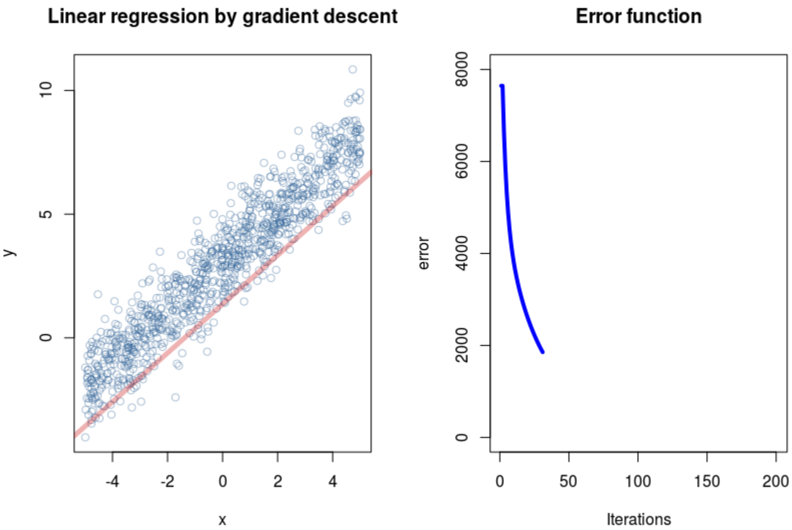

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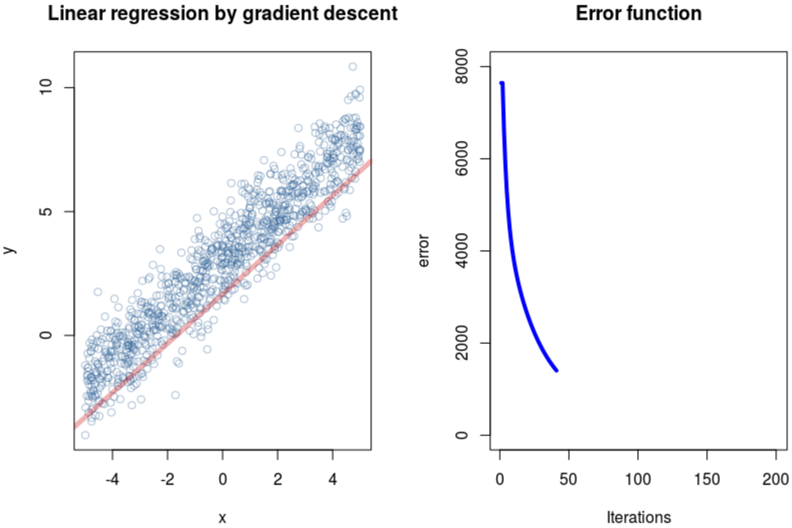

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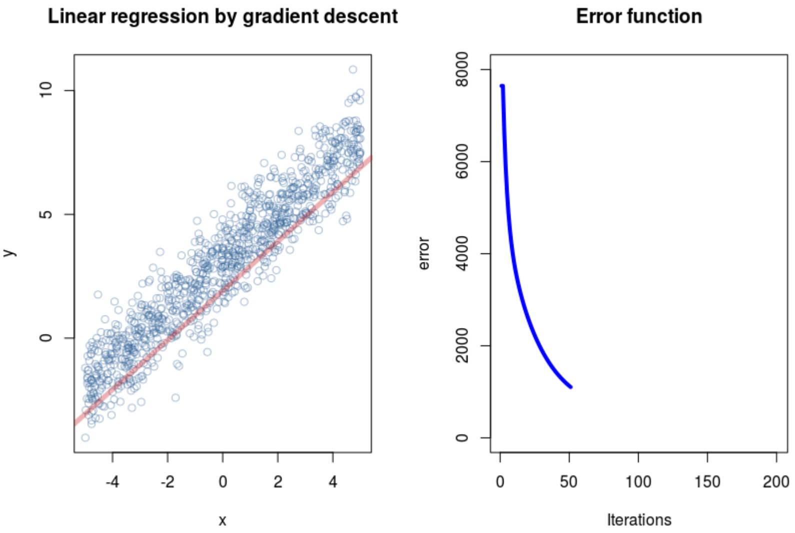

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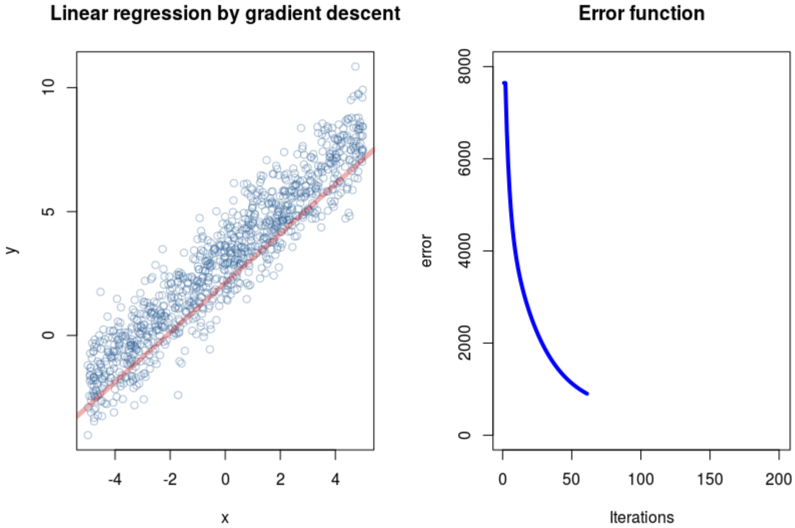

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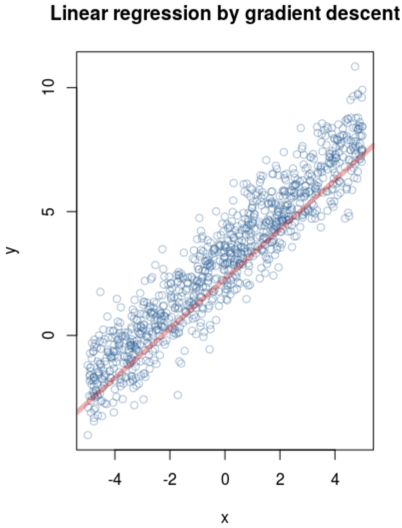

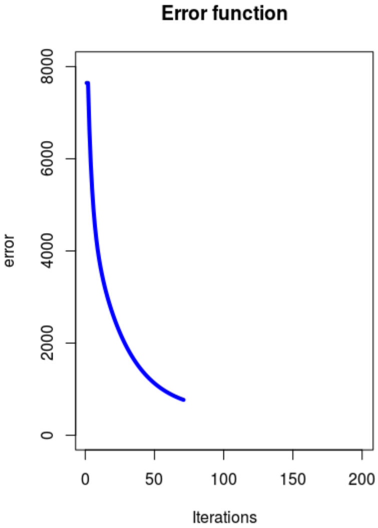

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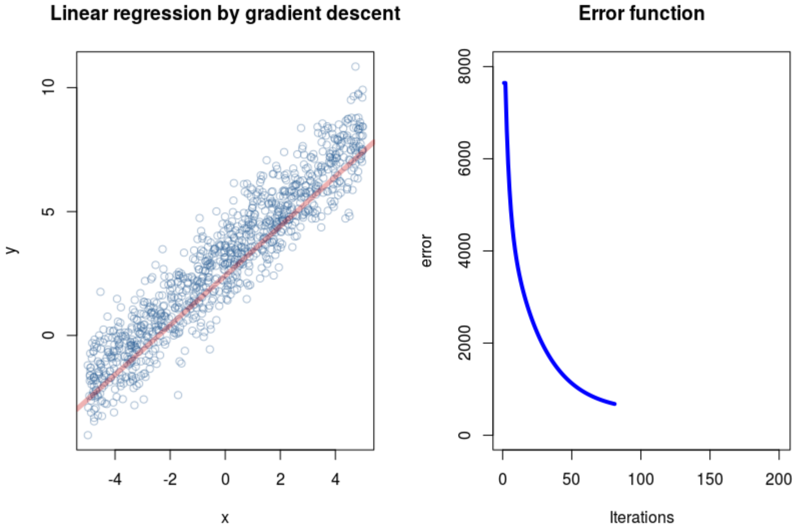

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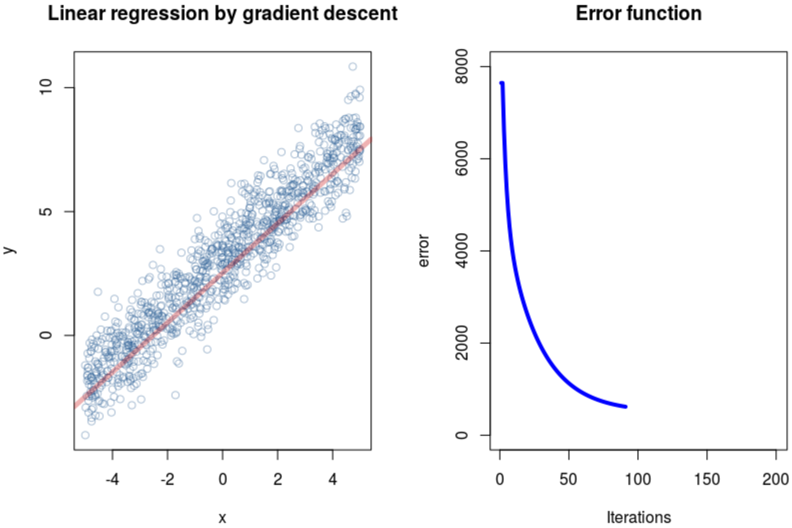

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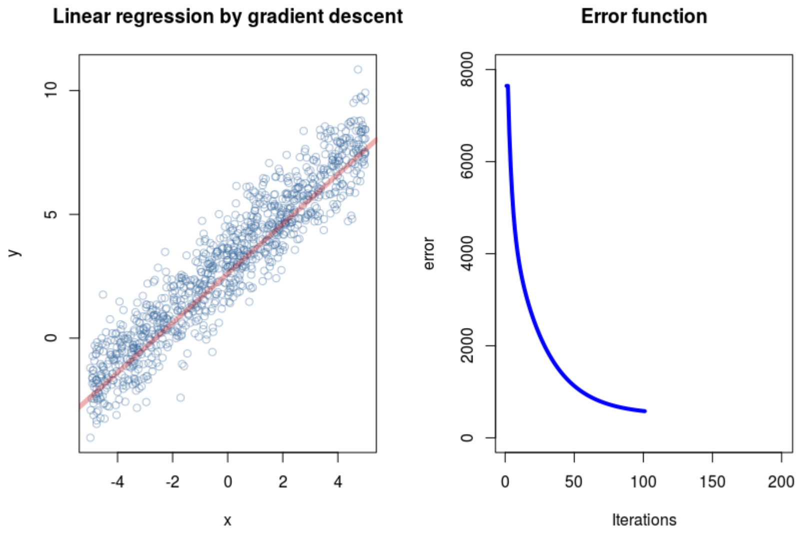

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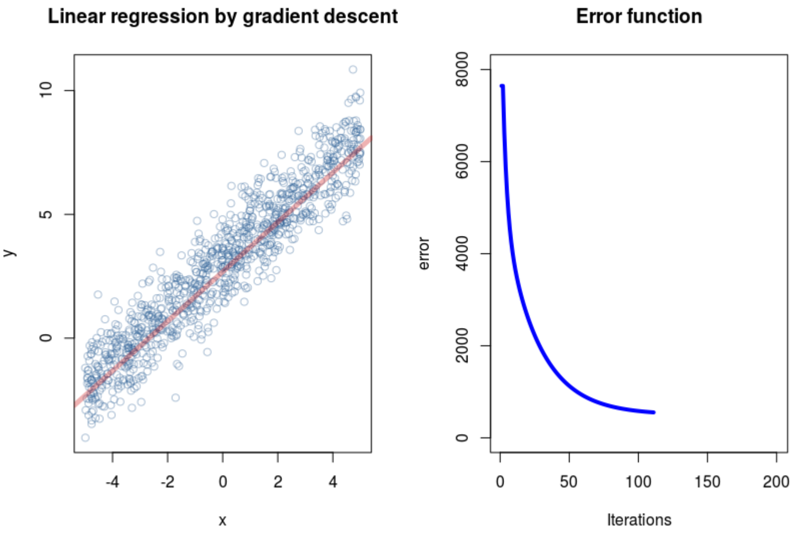
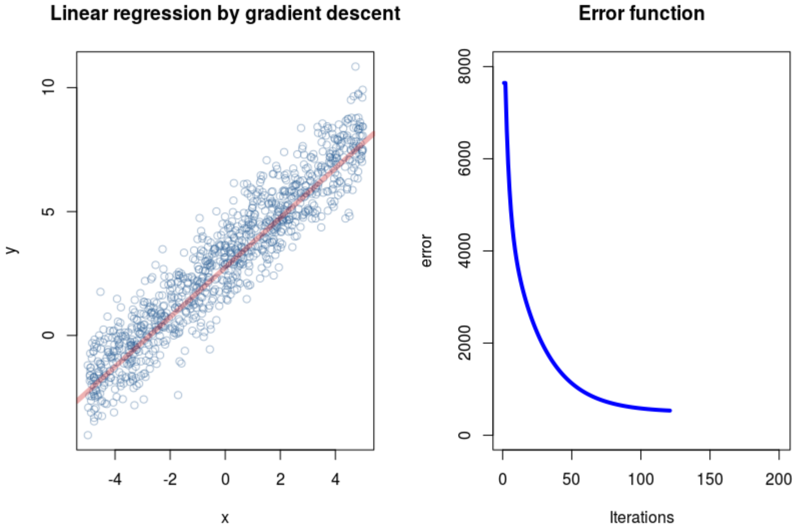


Linear regression - animation



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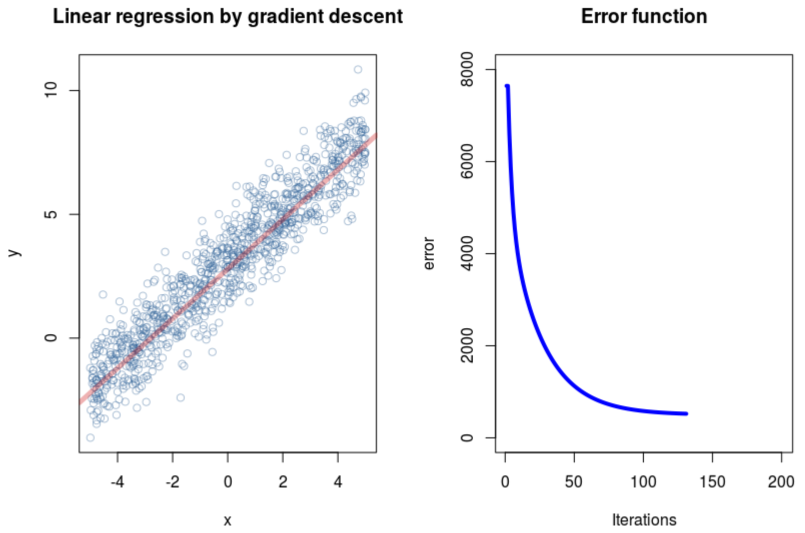

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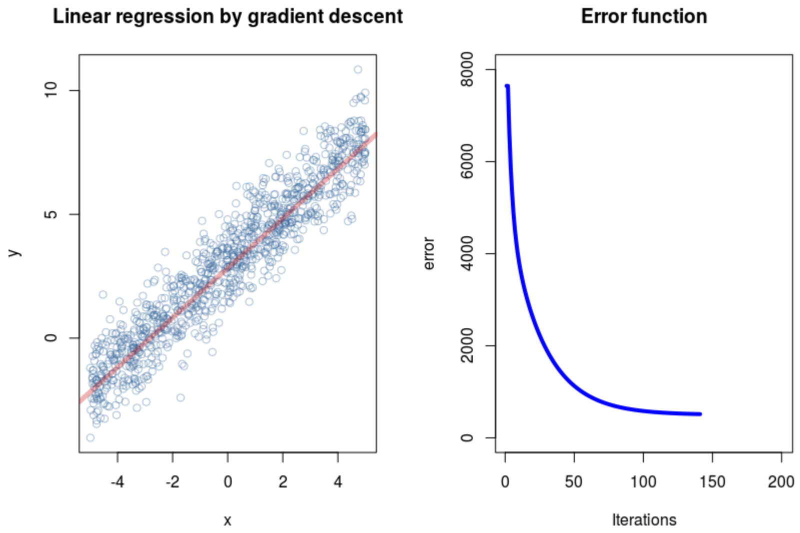

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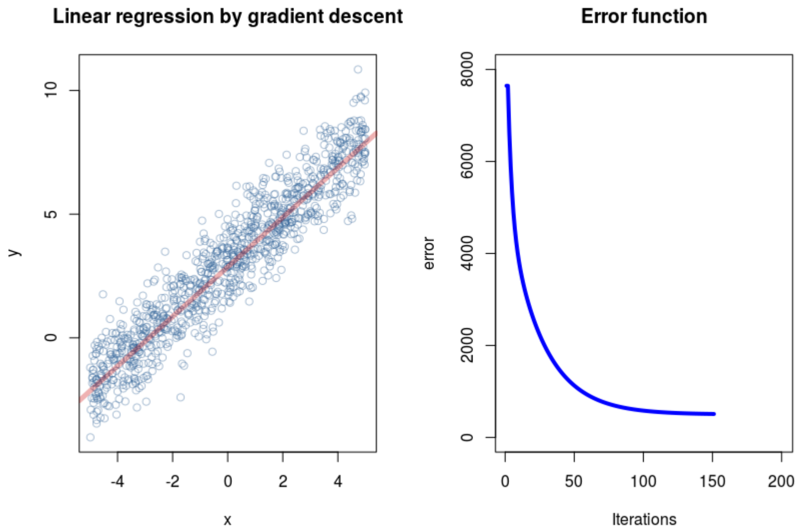

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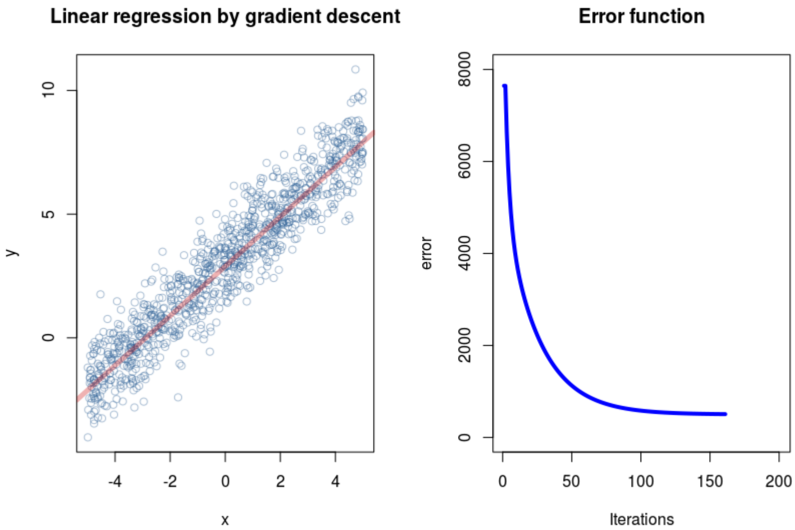
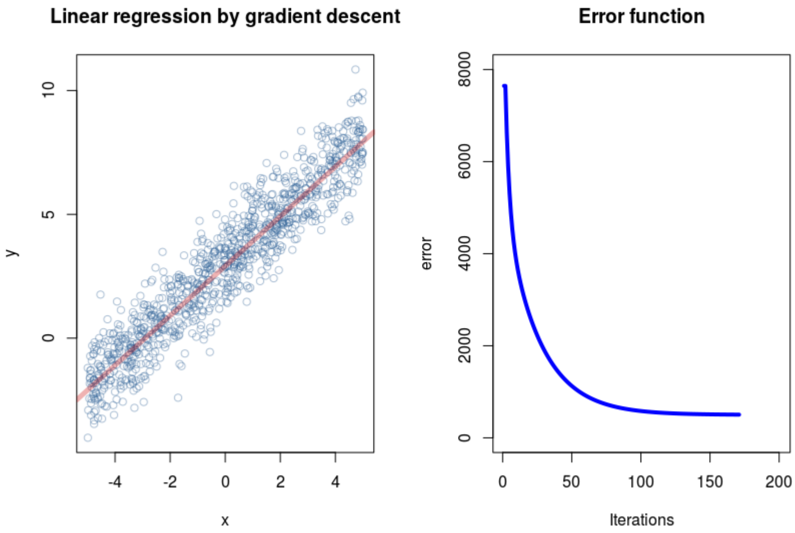


Linear regression - animation



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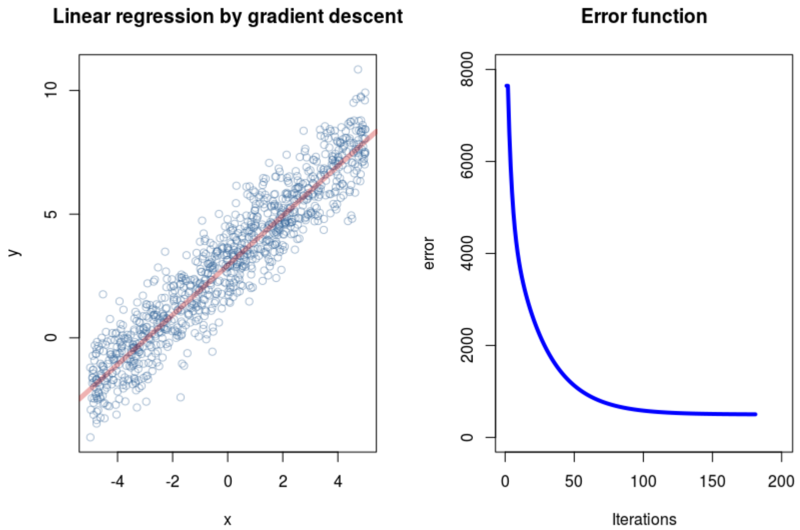

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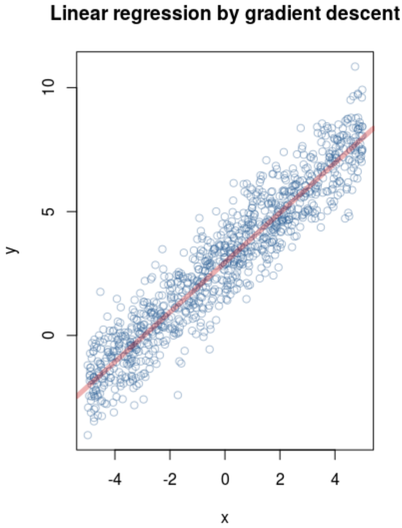

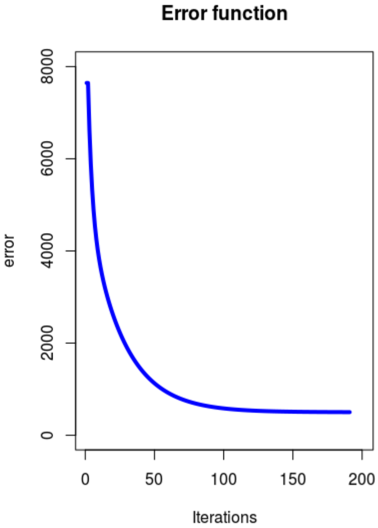

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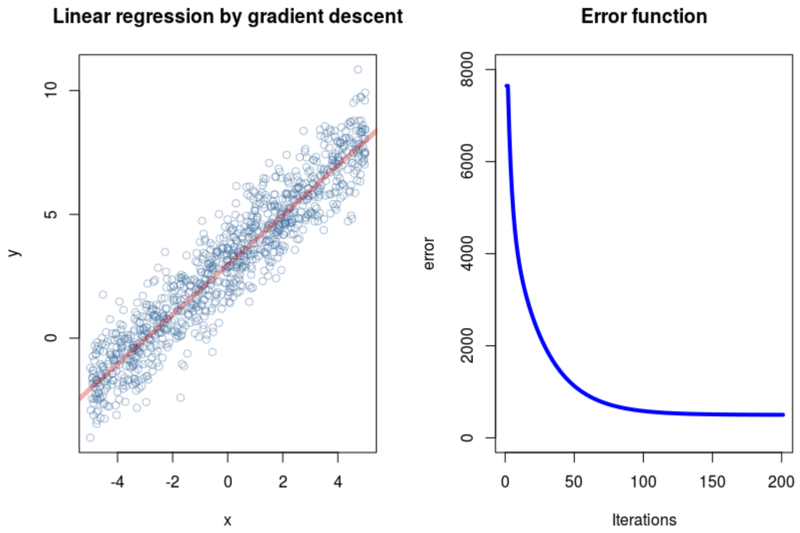


ADALINE - learning

Online algorithm (Delta-rule, Widrow-Hoff rule):

- weights in $\vec{w}^{(0)}$ initialized randomly close to 0
- in the step $t+1$, weights $\vec{w}^{(t+1)}$ are computed as follows:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \left(\vec{w}^{(t)} \cdot \vec{x}_k - d_k\right) \cdot \vec{x}_k$$

Here $k = t \mod p + 1$ and $0 < \varepsilon(t) \leq 1$ is a learning rate in the step $t+1$.

Note that the algorithm does not work with the complete gradient but only with its part determined by the currently considered training example.

ADALINE - learning

Online algorithm (Delta-rule, Widrow-Hoff rule):

- weights in $\vec{w}^{(0)}$ initialized randomly close to 0
- in the step $t+1$, weights $\vec{w}^{(t+1)}$ are computed as follows:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \left(\vec{w}^{(t)} \cdot \vec{x}_k - d_k\right) \cdot \vec{x}_k$$

Here $k = t \mod p + 1$ and $0 < \varepsilon(t) \leq 1$ is a learning rate in the step $t+1$.

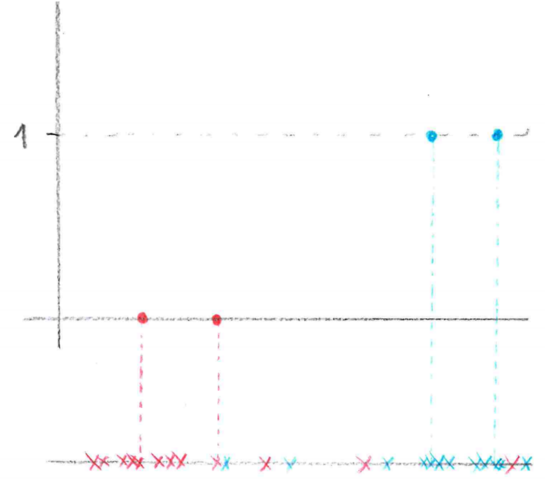
Note that the algorithm does not work with the complete gradient but only with its part determined by the currently considered training example.

Theorem (Widrow & Hoff)

If $\varepsilon(t) = \frac{1}{t}$, then $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges to the global minimum of E.

What about classification?

Binary classification: Desired outputs 0 and 1.



Ideally, capture the probability distribution of classes.

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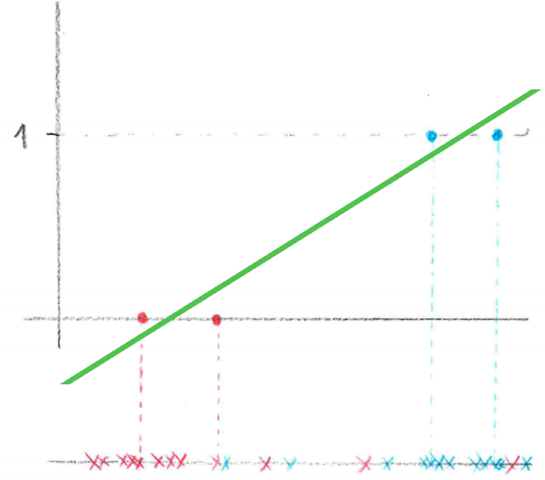

... does not capture probability well (it is not a probability at all)

What about classification?

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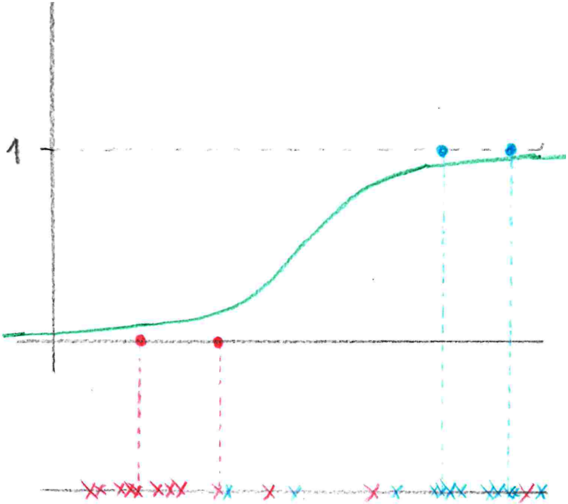
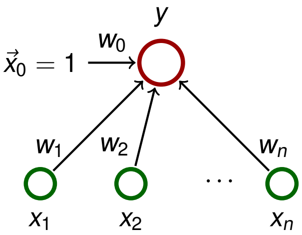


... logistic sigmoid $\frac{1}{1+e^{-(\vec{w}\cdot\vec{x})}}$ is much better!

Logistic regression



$\vec{w} = (w_0, w_1, \ldots, w_n)$ and $\vec{x} = (x_0, x_1, \ldots, x_n)$ where $x_0 = 1$.

Activity:

- inner potential: $\xi = w_0 + \sum_{i=1}^{n} w_i x_i = \sum_{i=0}^{n} w_i x_i = \vec{w} \cdot \vec{x}$
- activation function: $\sigma(\xi) = \frac{1}{1+e^{-\xi}}$
- network function: $y[\vec{w}](\vec{x}) = \sigma(\xi) = \frac{1}{1+e^{-(\vec{w}\cdot\vec{x})}}$

Intuition: The output y is now interpreted as the probability of the class 1 given the input $\vec{x}$.

But what is the meaning of the sigmoid?

The model gives a probability y of the class 1 given an input $\vec{x}$.
But why we model such a probability using $1/(1 + e^{-\vec{w}\cdot\vec{x}})$??

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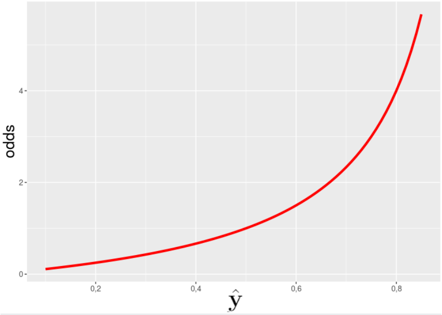
Let $\hat{y}$ be the "true" probability of the class 1 to be modeled.
What about odds of the class 1?

$$odds(\hat{y}) = \hat{y}/(1 - \hat{y})$$



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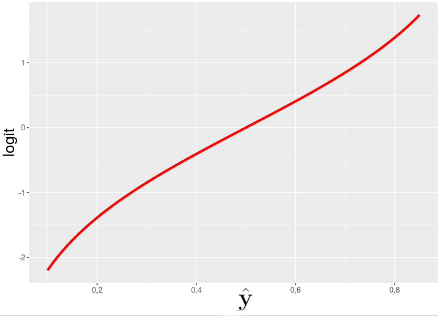
What about log odds (aka logit) of the class 1?

$$logit(\hat{y}) = \log(\hat{y}/(1-\hat{y}))$$



Looks almost linear ...

But what is the meaning of the sigmoid?

Assume that $\hat{y}$ is the probability of the class 1. Put

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and

$$\hat{y} = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}}$$

That is, if we model log odds using a linear function, the probability is obtained by applying the logistic sigmoid on the result of the linear function.

Logistic regression

Learning:

- Given a **training dataset**

$$\mathcal{T} = \left\{ \left(\vec{x}_1, d_1\right), \left(\vec{x}_2, d_2\right), \ldots, \left(\vec{x}_p, d_p\right) \right\}$$

Here $\vec{x}_k = (x_{k0}, x_{k1} \ldots, x_{kn}) \in \mathbb{R}^{n+1}$, $x_{k0} = 1$, is the k-th input, and $d_k \in \{0, 1\}$ is the expected output.

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What error function?

(Binary) cross-entropy:

$$E(\vec{w}) = \sum_{k=1}^{p} -(d_k \log(y_k) + (1 - d_k) \log(1 - y_k))$$

What?!?

Log likelihood is your friend!

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Answer: The one that generates the data with maximum probability!

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$$LL = log(L) = \log(y) + \log(y) + \log(1 - y) + \log(1 - y) + \log(y)$$

But then

$$-LL = -1 \cdot log(y) - 1 \cdot log(y) - (1 - 0) \cdot log(1 - y) - (1 - 0) \cdot \log(1 - y) - 1 \cdot \log(y)$$

i.e. $-LL$ is the cross-entropy.

Let the coin depend on the input

Consider our model:

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The likelihood:

$$L = \prod_{k=1}^{p} y_k^{d_k} \cdot (1 - y_k)^{(1-d_k)}$$

and $LL = \log(L) = \sum_{k=1}^{p} (d_k \log(y_k) + (1 - d_k) \log(1 - y_k))$ and thus $-LL$ = the cross-entropy.

Minimizing the cross-entropy maximizes the log-likelihood (and vice versa).

Normal Distribution

Distribution of continuous random variables.

Density (one dimensional, that is over $\mathbb{R}$):

$$p(x) \quad = \quad \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} \quad =: \quad N[\mu,\sigma^2](x)$$

μ is the expected value (the mean), σ^2 is the variance.

Maximum Likelihood vs Least Squares (Dim 1)

Fix a training set $D = \left\{ (x_1, d_1), (x_2, d_2), \ldots, \left(x_p, d_p\right) \right\}$

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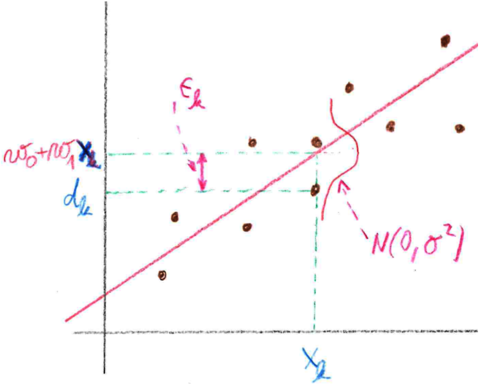
Assume that each d_k has been generated randomly by

$$d_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$$

- w_0, w_1 are **unknown numbers**
- ϵ_k are normally distributed with mean 0 and an unknown variance σ^2



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Denote by $p(d_1, \ldots, d_p \mid w_0, w_1, \sigma^2)$ the probability density according to which the values $d_1, \ldots, d_n$ were generated assuming fixed $w_0, w_1, \sigma^2, x_1, \ldots, x_p$.

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The independence and normality imply

$$\begin{aligned} p(d_1, \ldots, d_p \mid w_0, w_1, \sigma^2) &= \prod_{k=1}^{p} N[w_0 + w_1 x_k, \sigma^2](d_k) \\ &= \prod_{k=1}^{p} \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(d_k - w_0 - w_1 x_k)^2}{2\sigma^2}\right\} \end{aligned}$$

Maximum Likelihood vs Least Squares

Our goal is to find (w_0, w_1) that maximizes the likelihood that the training set D with **fixed** values $d_1, \ldots, d_n$ has been generated:

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Theorem

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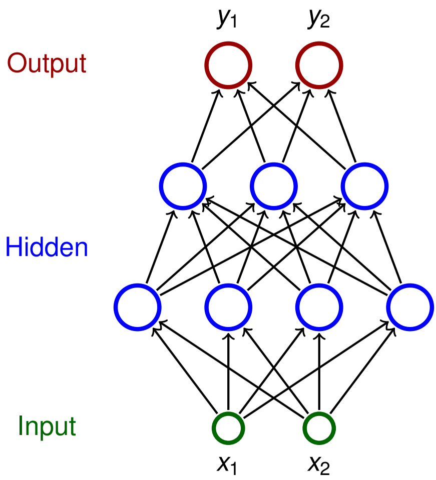
Maximizing σ^2 satisfies $\sigma^2 = \frac{1}{p}\sum_{k=1}^{p}(d_k - w_0 - w_1 \cdot x_k)^2$.

MLP training – theory

Architecture – Multilayer Perceptron (MLP)



- Neurons partitioned into **layers**; one input layer, one output layer, possibly several hidden layers
- layers numbered from 0; the input layer has number 0
  - E.g. three-layer network has two hidden layers and one output layer
- Neurons in the *i*-th layer are connected with all neurons in the $i + 1$-st layer
- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

MLP – architecture

Notation:

- Denote
  - X a set of *input* neurons
  - Y a set of *output* neurons
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- The network computes a function $\mathbb{R}^{|X|}$ do $\mathbb{R}^{|Y|}$. Layer-wise computation: First, all input neurons are assigned values of the input. In the ℓ-th step, all neurons of the ℓ-th layer are evaluated.

MLP – learning

Learning:

- Given a **training set** $\mathcal{T}$ of the form

$$\left\{ \left(\vec{x}_k, \vec{d}_k\right) \;\middle|\; k = 1, \ldots, p \right\}$$

Here, every $\vec{x}_k \in \mathbb{R}^{|X|}$ is an *input vector* end every $\vec{d}_k \in \mathbb{R}^{|Y|}$ is the desired network output. For every $j \in Y$, denote by d_{kj} the desired output of the neuron j for a given network input $\vec{x}_k$ (the vector $\vec{d}_k$ can be written as $\left(d_{kj}\right)_{j \in Y}$).

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- **Error function:**

$$E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$$

where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} \left(y_j(\vec{w}, \vec{x}_k) - d_{kj}\right)^2$$

MLP – learning algorithm

Batch algorithm (gradient descent):

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:

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

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- in the step $t + 1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:

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

  where

  $$\Delta w_{ji}^{(t)} = -\varepsilon(t) \cdot \frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$$

  is a *weight update* of w_{ji} in step $t + 1$ and $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t + 1$.

MLP – learning algorithm

Batch algorithm (gradient descent):

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t + 1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:

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  is a *weight update* of w_{ji} in step $t + 1$ and $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t + 1$.

Note that $\frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$ is a component of the gradient ∇E, i.e. the weight update can be written as $\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \nabla E(\vec{w}^{(t)})$.

MLP – error function gradient

For every w_{ji} we have

$$\frac{\partial E}{\partial w_{ji}} = \sum_{k=1}^{p} \frac{\partial E_k}{\partial w_{ji}}$$

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and for every $j \in Z \smallsetminus X$ we get

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj} \qquad \text{for } j \in Y$$

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(Here all y_j are in fact $y_j(\vec{w}, \vec{x}_k)$).

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- If $\sigma_j(\xi) = \frac{1}{1+e^{-\lambda_j \xi}}$ for all $j \in Z$, then

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- If $\sigma_j(\xi) = a \cdot \tanh(b \cdot \xi_j)$ for all $j \in Z$, then

  $$\sigma'_j(\xi_j) = \frac{b}{a}(a - y_j)(a + y_j)$$

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$$\frac{\partial E_k}{\partial w_{ji}} := \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$$

4. $\mathcal{E}_{ji} := \mathcal{E}_{ji} + \frac{\partial E_k}{\partial w_{ji}}$

The resulting $\mathcal{E}_{ji}$ equals $\frac{\partial E}{\partial w_{ji}}$.

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- if $j \in Y$, then $\frac{\partial E_k}{\partial y_j} = y_j - d_{kj}$
- if $j \in Z \setminus Y \cup X$, then assuming that j is in the ℓ-th layer and assuming that $\frac{\partial E_k}{\partial y_r}$ has already been computed for all neurons in the $\ell + 1$-st layer, compute

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj}$$

(This works because all neurons of $r \in j^{\rightarrow}$ belong to the $\ell + 1$-st layer.)

Complexity of the batch algorithm

Computation of $\frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t-1)})$ stops in time linear in the size of the network plus the size of the training set.

(assuming unit cost of operations including computation of $\sigma'_r(\xi_r)$ for given ξ_r)

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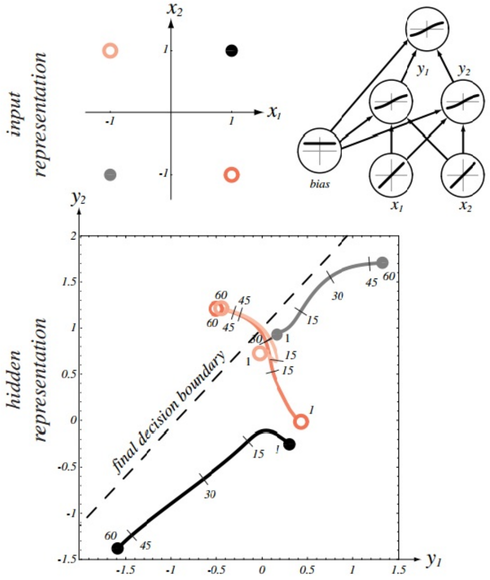
The steps 1. - 3. take linear time.

Note that the speed of convergence of the gradient descent cannot be estimated ...

Illustration of the gradient descent – XOR



Source: Pattern Classification (2nd Edition); Richard O. Duda, Peter E. Hart, David G. Stork

MLP – learning algorithm

Online algorithm:

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:

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  where

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  is the *weight update* of w_{ji} in the step $t+1$ and $0 < \varepsilon(t) \leq 1$ is the *learning rate* in the step $t+1$.

There are other variants determined by selection of the training examples used for the error computation (more on this later).

SGD

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:
  - Choose (randomly) a set of training examples $T \subseteq \{1, \ldots, p\}$
  - Compute

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

    where

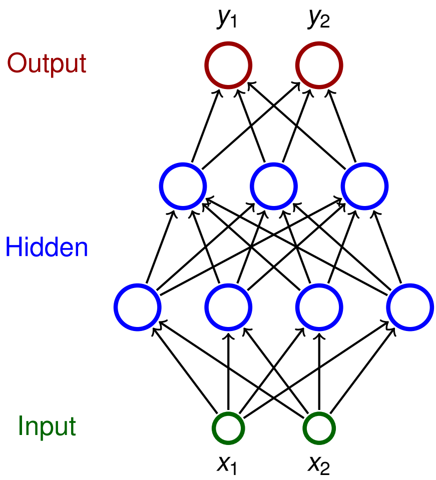
$$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \sum_{k \in T} \nabla E_k(\vec{w}^{(t)})$$

- $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$
- $\nabla E_k(\vec{w}^{(t)})$ is the gradient of the error of the example k

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially.

MLP training – practical issues

Architecture – Multilayer Perceptron (MLP)



- Neurons partitioned into **layers**; one input layer, one output layer, possibly several hidden layers
- layers numbered from 0; the input layer has number 0
  - E.g. three-layer network has two hidden layers and one output layer
- Neurons in the *i*-th layer are connected with all neurons in the $i+1$-st layer
- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

MLP – architecture

Notation:

- Denote
  - X a set of *input* neurons
  - Y a set of *output* neurons
  - Z a set of *all* neurons ($X, Y \subseteq Z$)
- individual neurons denoted by indices i, j etc.
  - ξ_j is the inner potential of the neuron j *after the computation stops*
  - y_j is the output of the neuron j *after the computation stops*

  (define $y_0 = 1$ is the value of the formal unit input)
- w_{ji} is the weight of the connection **from** i **to** j

  (in particular, w_{j0} is the weight of the connection from the formal unit input, i.e. $w_{j0} = -b_j$ where b_j is the bias of the neuron j)
- $j_{\leftarrow}$ is a set of all i such that j is adjacent from i
  (i.e. there is an arc **to** j from i)
- $j^{\rightarrow}$ is a set of all i such that j is adjacent to i
  (i.e. there is an arc **from** j to i)

MLP – learning

Learning:

- Given a **training set** $\mathcal{T}$ of the form

$$\left\{ \left(\vec{x}_k, \vec{d}_k \right) \;\middle|\; k = 1, \ldots, p \right\}$$

Here, every $\vec{x}_k \in \mathbb{R}^{|X|}$ is an *input vector* end every $\vec{d}_k \in \mathbb{R}^{|Y|}$ is the desired network output. For every $j \in Y$, denote by d_{kj} the desired output of the neuron j for a given network input $\vec{x}_k$ (the vector $\vec{d}_k$ can be written as $\left(d_{kj}\right)_{j \in Y}$).

- **Error function:** $E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$

SGD

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2\ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:
  - Choose (randomly) a set of training examples $T \subseteq \{1, \ldots, p\}$
  - Compute

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

where

$$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \sum_{k \in T} \nabla E_k(\vec{w}^{(t)})$$

- $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$
- $\nabla E_k(\vec{w}^{(t)})$ is the gradient of the error of the example k

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially.

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$$\frac{\partial E_k}{\partial w_{ji}} = \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$$

and for every $j \in Z \smallsetminus X$ we get (for squared error)

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj} \qquad \text{for } j \in Y$$

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj} \qquad \text{for } j \in Z \smallsetminus (Y \cup X)$$

(Here all y_j are in fact $y_j(\vec{w}, \vec{x}_k)$).

(Some) error functions

- **squared error:**

$$E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$$

where $E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} \left(y_j(\vec{w}, \vec{x}_k) - d_{kj} \right)^2$

- **mean squared error (mse):**

$$E(\vec{w}) = \frac{1}{p} \sum_{k=1}^{p} E_k(\vec{w})$$

- **(categorical) cross entropy:**

$$E(\vec{w}) = -\frac{1}{p} \sum_{k=1}^{p} \sum_{j \in Y} d_{kj} \ln(y_j)$$

Practical issues of gradient descent

- Training efficiency:
  - What size of a minibatch?
  - How to choose the learning rate $\varepsilon(t)$ and control SGD ?
  - How to pre-process the inputs?
  - How to initialize weights?
  - How to choose desired output values of the network?

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  - How to initialize weights?
  - How to choose desired output values of the network?
- Quality of the resulting model:
  - When to stop training?
  - Regularization techniques.
  - How large network?

For simplicity, I will illustrate the reasoning on MLP + mse. Later we will see other topologies and error functions with different but always somewhat related issues.

Issues in gradient descent

- Small networks: Lots of local minima where the descent gets stuck.
- The model identifiability problem: Swapping incoming weights of neurons *i* and *j* leaves the same network topology – **weight space symmetry**.
- Recent studies show that for sufficiently large networks all local minima have low values of the error function.

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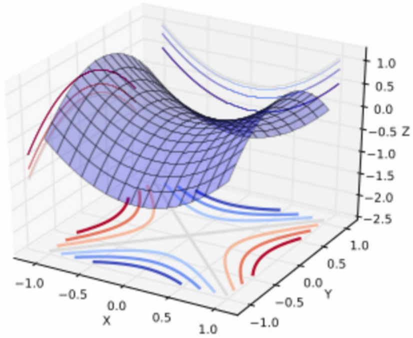
Saddle points

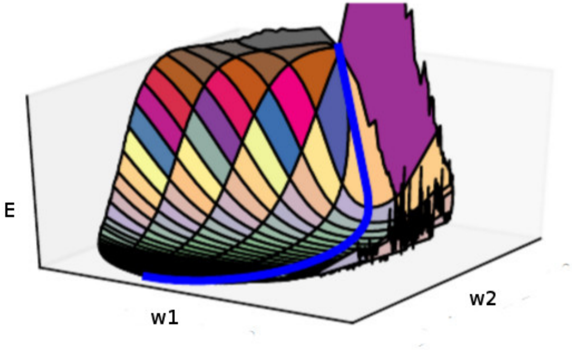
One can show (by a combinatorial argument) that larger networks have exponentially more saddle points than local minima.



Issues in gradient descent – too slow descent

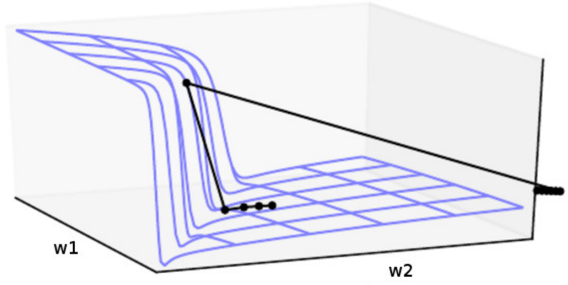
- flat regions

  E.g. if the inner potentials are too large (in abs. value), then their derivative is extremely small.

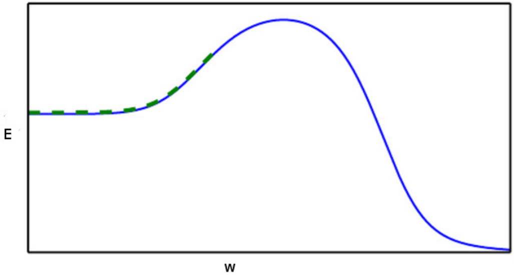


Issues in gradient descent – too fast descent

- steep cliffs: the gradient is extremely large, descent skips important weight vectors



Issues in gradient descent – local vs global structure



What if we initialize on the left?

Gradient Descent in Large Networks

Theorem

Assume (roughly),

- *activation functions: "smooth" ReLU (softplus)*

  $$\sigma(z) = \log(1 + \exp(z))$$

  In general: Smooth, non-polynomial, analytic, Lipschitzs.

- *inputs $\vec{x}_k$ of Euclidean norm equal to 1, desired values d_k satisfying $|d_k| \in O(1)$,*
- *the number of hidden neurons per layer sufficiently large (polynomial in certain numerical characteristics of inputs roughly measuring their similarity, and exponential in the depth of the network),*
- *the learning rate constant and sufficiently small.*

The gradient descent converges (with high probability) to a global minimum with zero error at linear rate.

Later we get to a special type of networks called ResNet where the above result demands only polynomially many neurons per layer (w.r.t. depth).

Issues in computing the gradient

- vanishing and exploding gradients

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj} \qquad \text{for } j \in Y$$

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma'_r(\xi_r) \cdot w_{rj} \qquad \text{for } j \in Z \setminus (Y \cup X)$$

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- inexact gradient computation:
  - Minibatch gradient is only an estimate of the true gradient.
  - Note that the variance of the estimate is (roughly) $\sigma/\sqrt{m}$ where m is the size of the minibatch and σ is the variance of the gradient estimate for a single training example.
    (E.g. minibatch size 10 000 means 100 times more computation than the size 100 but gives only 10 times less variance.)

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- Multicore architectures are usually underutilized by extremely small batches.
- If all examples in the batch are to be processed in parallel (as is the typical case), then the amount of memory scales with the batch size. For many hardware setups this is the limiting factor in batch size.
- It is common (especially when using GPUs) for power of 2 batch sizes to offer better runtime. Typical power of 2 batch sizes range from 32 to 256, with 16 sometimes being attempted for large models.

Minibatch size

- Larger batches provide a more accurate estimate of the gradient, but with less than linear returns.
- Multicore architectures are usually underutilized by extremely small batches.
- If all examples in the batch are to be processed in parallel (as is the typical case), then the amount of memory scales with the batch size. For many hardware setups this is the limiting factor in batch size.
- It is common (especially when using GPUs) for power of 2 batch sizes to offer better runtime. Typical power of 2 batch sizes range from 32 to 256, with 16 sometimes being attempted for large models.
- Small batches can offer a regularizing effect, perhaps due to the noise they add to the learning process.

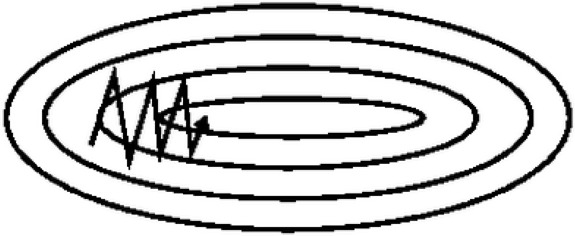
  It has been observed in practice that when using a larger batch there is a degradation in the quality of the model, as measured by its ability to generalize.

("On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima". Keskar et al, ICLR'17)

Momentum

Issue in the gradient descent:

- $\nabla E(\vec{w}^{(t)})$ constantly changes direction (but the error steadily decreases).



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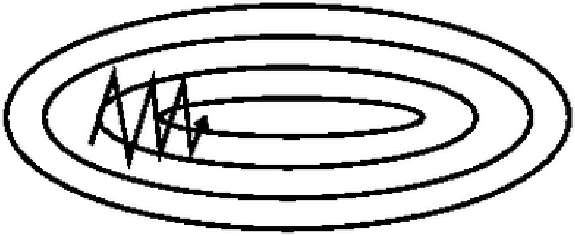
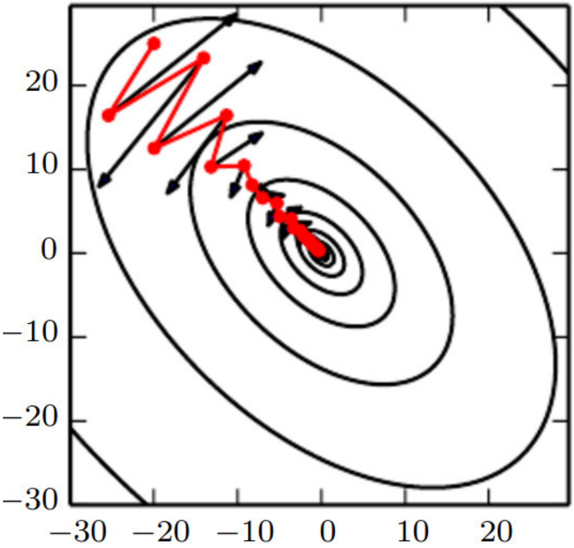


Solution: In every step add the change made in the previous step (weighted by a factor α):

$$\Delta \vec{w}^{(t)} = -\varepsilon(t) \cdot \sum_{k \in T} \nabla E_k(\vec{w}^{(t)}) + \alpha \cdot \Delta w_{ji}^{(t-1)}$$

where $0 < \alpha < 1$.

Momentum – illustration



SGD with momentum

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:
  - Choose (randomly) a set of training examples $T \subseteq \{1, \ldots, p\}$
  - Compute

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

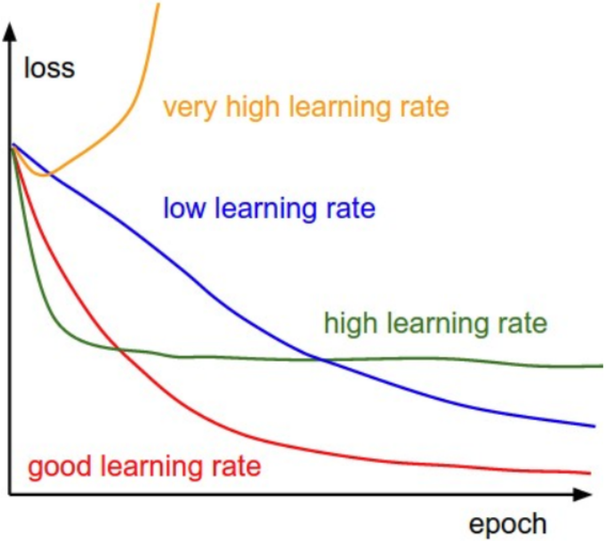
    where

    $$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \sum_{k \in T} \nabla E_k(\vec{w}^{(t)}) + \alpha\Delta\vec{w}^{(t-1)}$$

- $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$
- $0 < \alpha < 1$ measures the "influence" of the momentum
- $\nabla E_k(\vec{w}^{(t)})$ is the gradient of the error of the example k

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially.

Learning rate



Adaptive learning rate

- Power scheduling: Set $\epsilon(t) = \epsilon_0/(1 + t/s)$ where ϵ_0 is an initial learning rate and s a number of steps

  (after s steps the learning rate is $\epsilon_0/2$, after $2s$ it is $\epsilon_0/3$ etc.)

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- Piecewise constant scheduling: A constant learning rate for a number of steps/epochs, then a smaller learning rate, and so on.

- 1cycle scheduling: Start by increasing the initial learning rate from ϵ_0 linearly to ϵ_1 (approx. $\epsilon_1 = 10\epsilon_0$) halfway through training. Then decrease from ϵ_1 linearly to ϵ_0. Finish by dropping the learning rate by several orders of magnitude (still linearly).

  According to a 2018 paper by Leslie Smith this may converge much faster (100 epochs vs 800 epochs on CIFAR10 dataset).

For comparison of some methods see: AN EMPIRICAL STUDY OF LEARNING RATES IN DEEP NEURAL NETWORKS FOR SPEECH RECOGNITION, Senior et al

AdaGrad

So far we have considered fixed schedules for learning rates.

It is better to have

- larger rates for weights with smaller updates,
- smaller rates for weights with larger updates.

AdaGrad uses individually adapting learning rate for each weight.

SGD with AdaGrad

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t + 1$ (here $t = 0, 1, 2 \ldots$), compute $\vec{w}^{(t+1)}$:
  - Choose (randomly) a minibatch $T \subseteq \{1, \ldots, p\}$
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$$w_{ji}^{(t+1)} = w_{ji}^{(t)} + \Delta w_{ji}^{(t)}$$

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    where

    $$\Delta w_{ji}^{(t)} = -\frac{\eta}{\sqrt{r_{ji}^{(t)} + \delta}} \cdot \sum_{k \in T} \frac{\partial E_k}{\partial w_{ji}}(\vec{w}^{(t)})$$

    and

    $$r_{ji}^{(t)} = r_{ji}^{(t-1)} + \left(\sum_{k \in T} \frac{\partial E_k}{\partial w_{ji}}(\vec{w}^{(t)}) \right)^2$$

- η is a constant expressing the influence of the learning rate, typically 0.01.
- $\delta > 0$ is a smoothing term (typically 1e-8) avoiding division by 0.

RMSProp

The main disadvantage of AdaGrad is the accumulation of the gradient throughout the whole learning process.

In case the learning needs to get over several "hills" before settling in a deep "valley", the weight updates get far too small before getting to it.

RMSProp uses an exponentially decaying average to discard history from the extreme past so that it can converge rapidly after finding a convex bowl, as if it were an instance of the AdaGrad algorithm initialized within that bowl.

SGD with RMSProp

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
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    and

    $$r_{ji}^{(t)} = \rho r_{ji}^{(t-1)} + (1-\rho)\left(\sum_{k \in T} \frac{\partial E_k}{\partial w_{ji}}(\vec{w}^{(t)})\right)^2$$

- η is a constant expressing the influence of the learning rate (Hinton suggests $\rho = 0.9$ and $\eta = 0.001$).
- $\delta > 0$ is a smoothing term (typically 1e-8) avoiding division by 0.

Other optimization methods

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Unfortunately, there is currently no consensus on this point.

According to a recent study, the family of algorithms with adaptive learning rates (represented by RMSProp and AdaDelta) performed fairly robustly, no single best algorithm has emerged.

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According to a recent study, the family of algorithms with adaptive learning rates (represented by RMSProp and AdaDelta) performed fairly robustly, no single best algorithm has emerged.

Currently, the most popular optimization algorithms actively in use include SGD, SGD with momentum, RMSProp, RMSProp with momentum, AdaDelta and Adam.

The choice of which algorithm to use, at this point, seems to depend largely on the user's familiarity with the algorithm.

Choice of (hidden) activations

Generic requirements imposed on activation functions:

1. differentiability

   (to do gradient descent)

2. non-linearity

   (linear multi-layer networks are equivalent to single-layer)

3. monotonicity

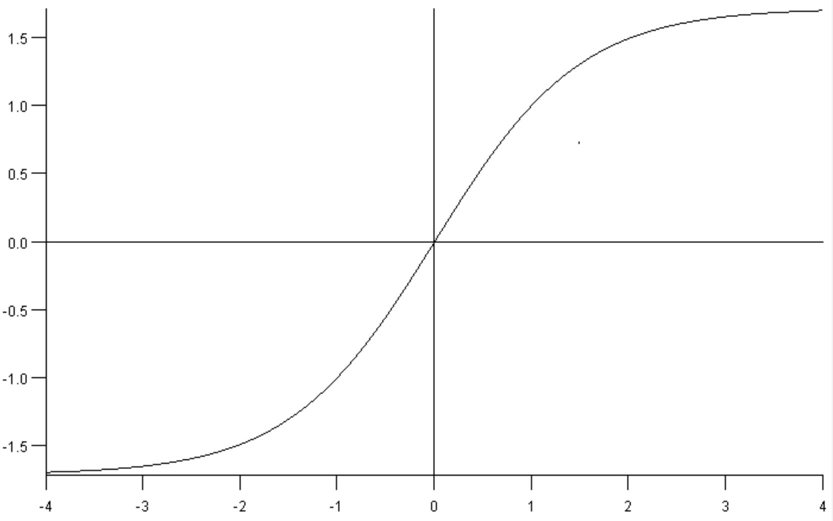
   (local extrema of activation functions induce local extrema of the error function)

4. "linearity"

   (i.e. preserve as much linearity as possible; linear models are easiest to fit; find the "minimum" non-linearity needed to solve a given task)

The choice of activation functions is closely related to input preprocessing and the initial choice of weights. I will illustrate the reasoning on sigmoidal functions; say few words about other activation functions later.

Activation functions – tanh



$\sigma(\xi) = 1.7159 \cdot \tanh(\frac{2}{3} \cdot \xi)$, we have $\lim_{\xi \to \infty} \sigma(\xi) = 1.7159$ and $\lim_{\xi \to -\infty} \sigma(\xi) = -1.7159$

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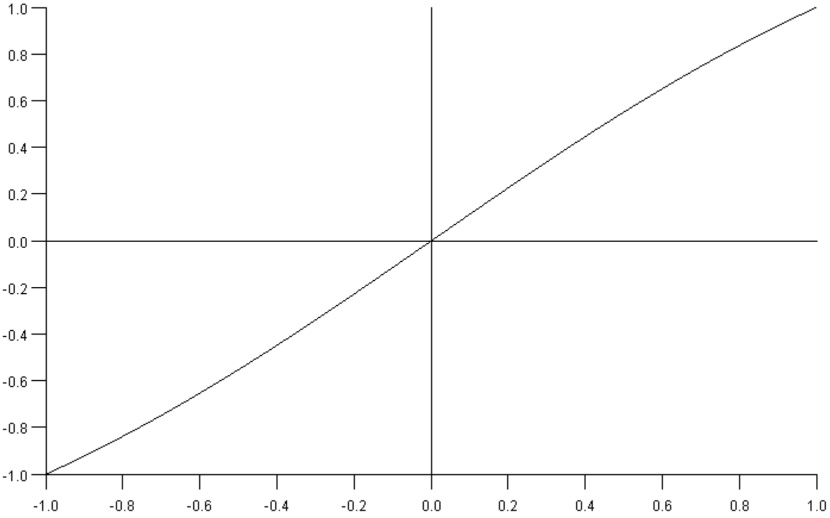

$\sigma(\xi) = 1.7159 \cdot \mathtt{tanh}(\frac{2}{3} \cdot \xi)$ is almost linear on $[-1, 1]$

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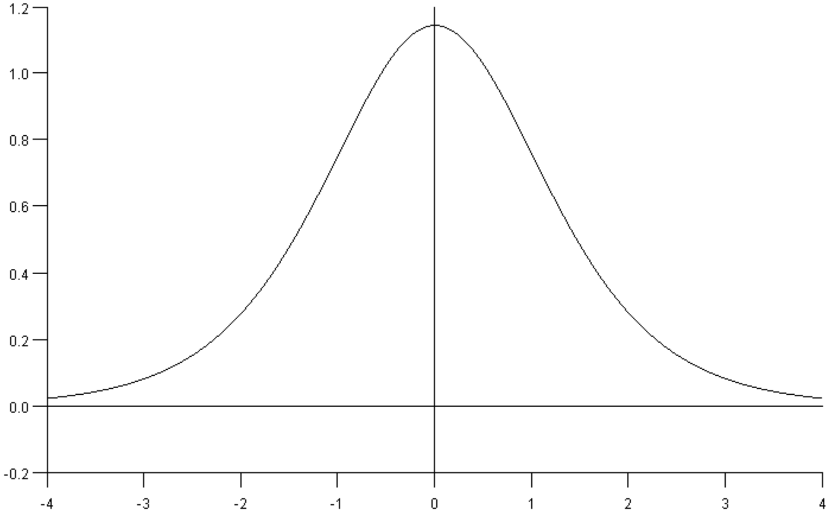

first derivative: $\sigma(\xi) = 1.7159 \cdot \mathtt{tanh}(\frac{2}{3} \cdot \xi)$

Input preprocessing

- Some inputs may be much larger than others.

  E.g..: Height vs weight of a person, maximum speed of a car (in km/h) vs its price (in CZK), etc.

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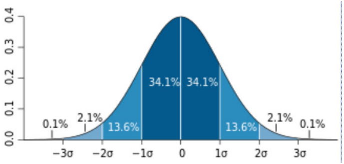
- Large inputs have greater influence on the training than the small ones. In addition, too large inputs may slow down learning (saturation of activation functions).
- Typical standardization:
  - average $= 0$ (subtract the mean)
  - variance $= 1$ (divide by the standard deviation)

  Here the mean and standard deviation may be estimated from data (the training set).



(illustration of standard deviation)

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  Thus
  - for too small w we may get (almost) linear model.
  - for too large w (i.e. much larger than 1) the activations may get saturated and the learning will be very slow.

  Hence, we want to choose w so that the inner potentials of neurons will be roughly in the interval $[-1, 1]$.

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- The same works for higher layers, n corresponds to the number of neurons in the layer one level lower.

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Glorot & Bengio (2010) presented a **normalized initialization** by choosing *w* uniformly from the interval:

$$\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right) = \left(-\sqrt{\frac{3}{(m+n)/2}}, \sqrt{\frac{3}{(m+n)/2}}\right)$$

Here n is the number of inputs to the layer, m is the number of outputs of the layer (i.e. the number of neurons in the layer).

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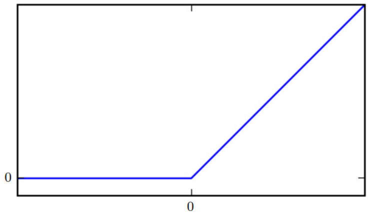
This is designed to compromise between the goal of initializing all layers to have the same activation variance and the goal of initializing all layers to have the same gradient variance.

The formula is derived using the assumption that the network consists only of a chain of matrix multiplications, with no non-linearities. Real neural networks obviously violate this assumption, but many strategies designed for the linear model perform reasonably well on its non-linear counterparts.

Modern activation functions

For hidden neurons sigmoidal functions are often substituted with piece-wise linear activations functions. Most prominent is ReLU:



$$\sigma(\xi) = \max\{0, \xi\}$$

- THE default activation function recommended for use with most feedforward neural networks.
- As close to linear function as possible; very simple; does not saturate for large potentials.
- Dead for negative potentials.

More modern activation functions

- Leaky ReLU (greenboard):
  - Generalizes ReLU, not dead for negative potentials.
  - Experimentally not much better than ReLU.

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- ELU: "Smoothed" ReLU:

$$\sigma(\xi) = \begin{cases} \alpha(\exp(\xi) - 1) & \text{for } \xi < 0 \\ \xi & \text{for } \xi \geq 0 \end{cases}$$

  Here α is a parameter, ELU converges to $-\alpha$ as $\xi \to -\infty$. As opposed to ReLU: Smooth, always non-zero gradient (but saturates), slower to compute.

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- SELU: Scaled variant of ELU: :

  $$\sigma(\xi) = \lambda \begin{cases} \alpha(\exp(\xi) - 1) & \text{for } \xi < 0 \\ \xi & \text{for } \xi \geq 0 \end{cases}$$

  Self-normalizing, i.e. output of each layer will tend to preserve a mean (close to) 0 and a standard deviation (close to) 1 for $\lambda \approx 1.050$ and $\alpha \approx 1.673$, properly initialized weights (see below) and normalized inputs (zero mean, standard deviation 1).

Initializing with Normal Distribution

Denote by n the number of inputs to the initialized layer, and m the number of neurons in the layer.

- Glorot & Bengio (2010): Choose weights randomly from the normal distribution with mean 0 and variance $2/(n+m)$

  Suitable for activation functions: None, tanh, logistic, softmax

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- He (2015): Choose weights randomly from the normal distribution with mean 0 and variance $2/n$
  Designed for ReLU, leaky ReLU
- LeCun (1990): Choose weights randomly from the normal distribution with mean 0 and variance $1/n$
  Suitable for SELU

How to choose activation of hidden neurons

- Default is ReLU.
- According to Aurélien Géron:

$$SELU > ELU > leakyReLU > ReLU > tanh > logistic$$

For discussion see: Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems, Aurélien Géron

Output neurons

The choice of activation functions for output units depends on the concrete applications.

For regression (function approximation) the output is typically linear.

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For classification, the current activation functions of choice are

- logistic sigmoid – binary classification
- softmax: Given an output neuron $j \in Y$

  $$y_j = \sigma_j(\xi_j) = \frac{e^{\xi_j}}{\sum_{i \in Y} e^{\xi_i}}$$

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The error function used with softmax (assuming that the target values d_{kj} are from $\{0, 1\}$) is typically **cross-entropy**:

$$-\frac{1}{p} \sum_{k=1}^{p} \sum_{j \in Y} d_{kj} \ln(y_j)$$

... which somewhat corresponds to the maximum likelihood principle.

Sigmoidal outputs with cross-entropy – in detail

Consider

- Binary classification, two classes $\{0, 1\}$
- One output neuron j, its activation logistic sigmoid

$$\sigma_j(\xi_j) = \frac{1}{1 + e^{-\xi_j}}$$

The output of the network is $y = \sigma_j(\xi_j)$.

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  The output of the network is $y = \sigma_j(\xi_j)$.
- For a training set

$$\mathcal{T} = \left\{ \left(\vec{x}_k, d_k\right) \;\middle|\; k = 1, \ldots, p \right\}$$

  (here $\vec{x}_k \in \mathbb{R}^{|X|}$ and $d_k \in \mathbb{R}$), the cross-entropy looks like this:

$$E^{cross} = -\frac{1}{p} \sum_{k=1}^{p} \left[d_k \ln(y_k) + (1 - d_k) \ln(1 - y_k) \right]$$

  where y_k is the output of the network for the k-th training input $\vec{x}_k$, and d_k is the k-th desired output.

Generalization

Intuition: Generalization = ability to cope with new unseen instances.

Data are mostly noisy, so it is not good idea to fit exactly.

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More formally: It is typically assumed that the training set has been generated as follows:

$$d_{kj} = g_j(\vec{x}_k) + \Theta_{kj}$$

where g_j is the "underlying" function corresponding to the output neuron $j \in Y$ and Θ_{kj} is random noise.

The network should fit g_j not the noise.

Methods improving generalization are called **regularization methods**.

Regularization

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von Neumann: **"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."**

... and I ask you prof. Neumann:

What can you fit with 40GB of parameters??

Early stopping

Early stopping means that we stop learning before it reaches a minimum of the error E.

When to stop?

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When to stop?

In many applications the error function is not the main thing we want to optimize.

E.g. in the case of a trading system, we typically want to maximize our profit not to minimize (strange) error functions designed to be easily differentiable.

Also, as noted before, minimizing E completely is not good for generalization.

For start: We may employ standard approach of training on one set and stopping on another one.

Early stopping

Divide your dataset into several subsets:

- **training set** (e.g. 60%) – train the network here
- **validation set** (e.g. 20%) – use to stop the training
- (possibly) **test set** (e.g. 20%) – use to compare trained models

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What to use as a stopping rule?

You may observe E (or any other function of interest) on the validation set, if it does not improve for last k steps, stop.

Alternatively, you may observe the gradient, if it is small for some time, stop.

(recent studies shown that this traditional rule is not too good: it may happen that the gradient is larger close to minimum values; on the other hand, E does not have to be evaluated which saves time.

To compare models you may use ML techniques such as various types of cross-validation etc.

Size of the network

Similar problem as in the case of the training duration:

- Too small network is not able to capture intrinsic properties of the training set.
- Large networks overfit faster.

Solution: Optimal number of neurons :-)

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- Too small network is not able to capture intrinsic properties of the training set.
- Large networks overfit faster.

Solution: Optimal number of neurons :-)

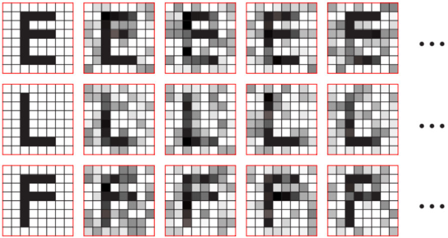
- there are some (useless) theoretical bounds
- there are algorithms dynamically adding/removing neurons (not much use nowadays)
- In practice:
  - start with a model solving similar problem (transfer learning).
  - experiment, experiment, experiment.

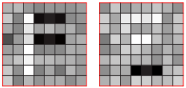
Feature extraction

Consider a two layer network. Hidden neurons are supposed to represent "patterns" in the inputs.

Example: Network 64-2-3 for letter classification:

sample training patterns





learned input-to-hidden weights

Ensemble methods

Techniques for reducing generalization error by combining several models.

The reason that ensemble methods work is that different models will usually not make all the same errors on the test set.

Idea: Train several different models separately, then have all of the models vote on the output for test examples.

Ensemble methods

Techniques for reducing generalization error by combining several models.

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Idea: Train several different models separately, then have all of the models vote on the output for test examples.

Bagging:

- Generate k training sets $T_1, ..., T_k$ by *sampling from* $\mathcal{T}$ *uniformly with replacement*.

  If the number of samples is $|\mathcal{T}|$, then on average $|T_i| = (1 - 1/e)|\mathcal{T}|$.
- For each i, train a model M_i on T_i.
- Combine outputs of the models: for regression by averaging, for classification by (majority) voting.

Dropout

The algorithm: In every step of the gradient descent

- choose randomly a set N of neurons, each neuron is included in N independently with probability $1/2$,

  (in practice, different probabilities are used as well).

- do forward and backward propagations only using the selected neurons

  (i.e. leave weights of the other neurons unchanged)

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Dropout resembles bagging: Large ensemble of neural networks is trained "at once" on parts of the data.

Dropout is not exactly the same as bagging: The models share parameters, with each model inheriting a different subset of parameters from the parent neural network. This parameter sharing makes it possible to represent an exponential number of models with a tractable amount of memory.
In the case of bagging, each model is trained to convergence on its respective training set. This would be infeasible for large networks/training sets.

Weight decay and L2 regularization

Generalization can be improved by removing "unimportant" weights.

Penalising large weights gives stronger indication about their importance.

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In every step we decrease weights (multiplicatively) as follows:

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

Intuition: Unimportant weights will be pushed to 0, important weights will survive the decay.

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Weight decay is equivalent to the gradient descent with a constant learning rate ε and the following error function:

$$E'(\vec{w}) = E(\vec{w}) + \frac{\zeta}{2\varepsilon}(\vec{w} \cdot \vec{w})$$

Here $\frac{\zeta}{2\varepsilon}(\vec{w} \cdot \vec{w})$ is the L2 regularization that penalizes large weights.

More optimization, regularization ...

There are many more practical tips, optimization methods, regularization methods, etc.

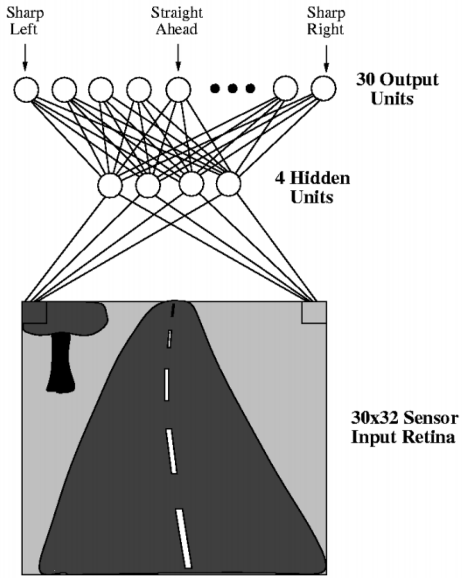
For a very nice survey see

`http://www.deeplearningbook.org/`

... and also all other infinitely many urls concerned with deep learning.

Some applications

ALVINN (history)



ALVINN

Architecture:

- MLP, 960 – 4 – 30 (also 960 – 5 – 30)
- inputs correspond to pixels

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- MLP, 960 – 4 – 30 (also 960 – 5 – 30)
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Activity:

- activation functions: logistic sigmoid
- Steering wheel position determined by "center of mass" of neuron values.

ALVINN

Learning: Trained during (live) drive.

- Front window view captured by a camera, 25 images per second.
- Training samples of the form $(\vec{x}_k, \vec{d}_k)$ where
  - $\vec{x}_k$ = image of the road
  - $\vec{d}_k$ = corresponding position of the steering wheel
- position of the steering wheel "blurred" by Gaussian distribution:

$$d_{ki} = e^{-D_i^2/10}$$

where D_i is the distance of the i-th output from the one which corresponds to the correct position of the wheel.

(The authors claim that this was better than the binary output.)

ALVINN – Selection of training samples

Naive approach: take images directly from the camera and adapt accordingly.

ALVINN – Selection of training samples

Naive approach: take images directly from the camera and adapt accordingly.

Problems:

- If the driver is gentle enough, the car never learns how to get out of dangerous situations. A solution may be
  - turn off learning for a moment, then suddenly switch on, and let the net catch on,
  - let the driver drive as if being insane (dangerous, possibly expensive).
- The real view out of the front window is repetitive and boring, the net would overfit on few examples.

ALVINN – Selection of training examples

Problem with a "good" driver is solved as follows:

ALVINN – Selection of training examples

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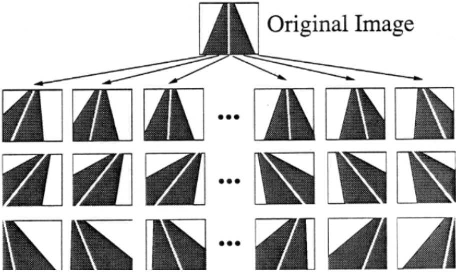
- 15 distorted copies of each image:



- desired output generated for each copy

ALVINN – Selection of training examples

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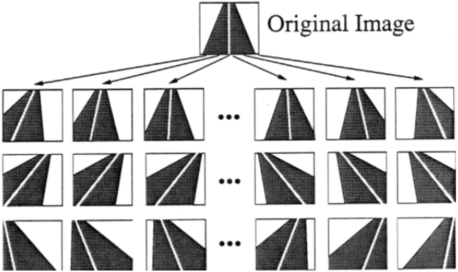


- desired output generated for each copy

"Boring" images solved as follows:

- a buffer of 200 images (including 15 copies of the original), in every step the system trains on the buffer
- after several updates a new image is captured, 15 copies are made and they will substitute 15 images in the buffer (5 chosen randomly, 10 with the **smallest** error).

ALVINN - learning

- pure backpropagation
- constant learning rate
- momentum, slowly increasing.

Results:

- Trained for 5 minutes, speed 4 miles per hour.
- ALVINN was able to drive well on a new road it has never seen (in different weather conditions).

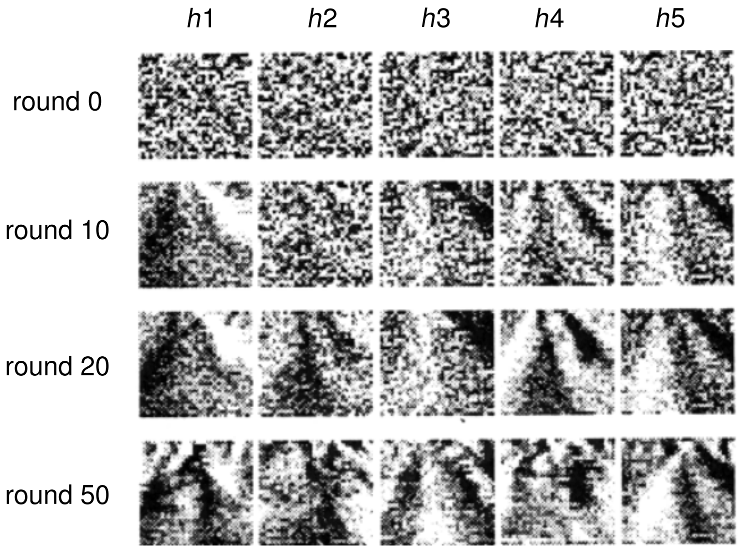
ALVINN - learning

- pure backpropagation
- constant learning rate
- momentum, slowly increasing.

Results:

- Trained for 5 minutes, speed 4 miles per hour.
- ALVINN was able to drive well on a new road it has never seen (in different weather conditions).
- The maximum speed was limited by the hydraulic controller of the steering wheel, not the learning algorithm.

ALVINN - weight development



Here $h1, \ldots, h5$ are hidden neurons.

MNIST – handwritten digits recognition

- Database of labelled images of handwritten digits: 60 000 training examples, 10 000 testing.
- Dimensions: 28 x 28, digits are centered to the "center of gravity" of pixel values and normalized to fixed size.
- More at `http://yann.lecun.com/exdb/mnist/`

Fig. 4. Size-normalized examples from the MNIST database.

The database is used as a standard benchmark in lots of publications.

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Fig. 4. Size-normalized examples from the MNIST database.

The database is used as a standard benchmark in lots of publications.

Allows comparison of various methods.

MNIST

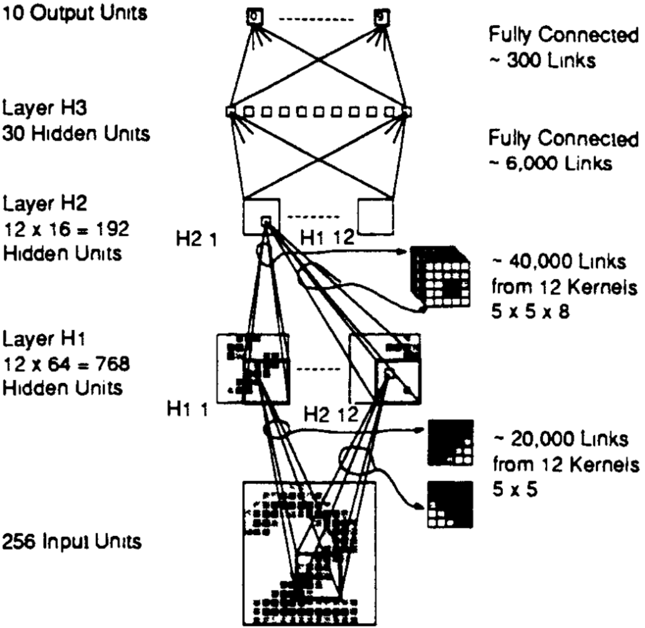
One of the best "old" results is the following:

6-layer NN 784-2500-2000-1500-1000-500-10 (on GPU)
(Ciresan et al. 2010)

Abstract: Good old on-line back-propagation for plain multi-layer perceptrons yields a very low 0.35 error rate on the famous MNIST handwritten digits benchmark. All we need to achieve this best result so far are many hidden layers, many neurons per layer, numerous deformed training images, and graphics cards to greatly speed up learning.

A famous application of a learning convolutional network LeNet-1 in 1998.

MNIST – LeNet1



MNIST – LeNet1

Interpretation of output:

- the output neuron with the highest value identifies the digit.
- the same, but if the two largest neuron values are too close together, the input is rejected (i.e. no answer).

Learning:
Inputs:

- training on 7291 samples, tested on 2007 samples

Results:

- error on test set without rejection: 5%
- error on test set with rejection: 1% (12% rejected)

- compare with dense MLP with 40 hidden neurons: error 1% (19.4% rejected)

Modern convolutional networks

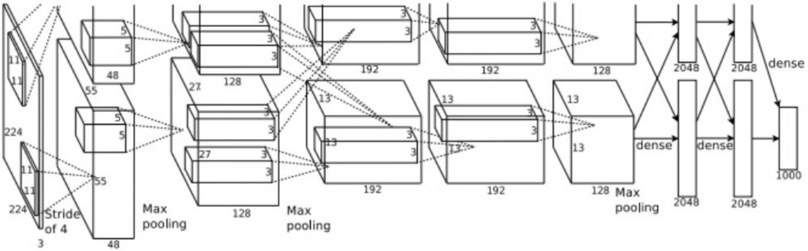
The rest of the lecture is based on the online book Neural Networks and Deep Learning by Michael Nielsen.
`http://neuralnetworksanddeeplearning.com/index.html`

- Convolutional networks are currently the best networks for image classification.
- Their common ancestor is LeNet-5 (and other LeNets) from nineties.

  Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. Proceedings of the IEEE, 1998

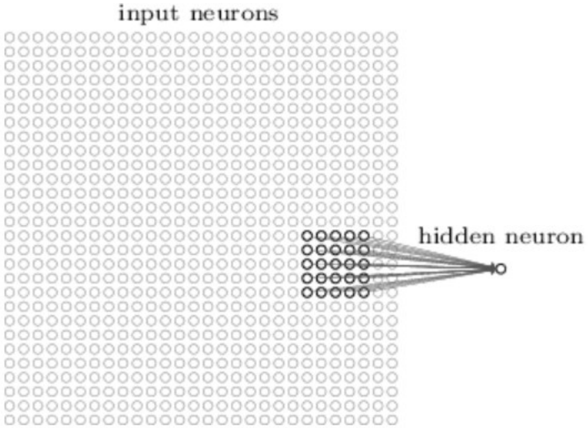
AlexNet

In 2012 this network made a breakthrough in ILVSCR competition, taking the classification error from around 28% to 16%:



A convolutional network, trained on two GPUs.

Convolutional networks - local receptive fields

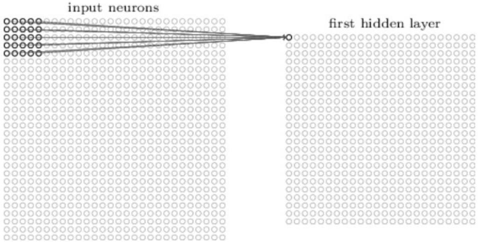


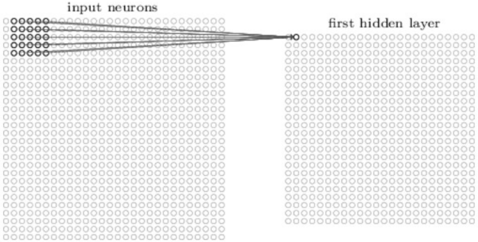
Every neuron is connected with a field of $k \times k$ (in this case 5×5) neurons in the lower layer (this filed is *receptive field*).

Neuron is "standard": Computes a weighted sum of its inputs, applies an activation function.

Convolutional networks - stride length

Then we slide the local receptive field over by one pixel to the right (i.e., by one neuron), to connect to a second hidden neuron:

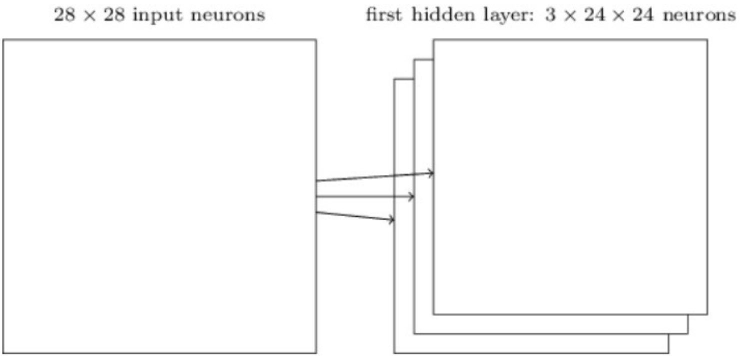




The "size" of the slide is called *stride length*.

The group of all such neurons is *feature map*. all these neurons *share weights and biases*!

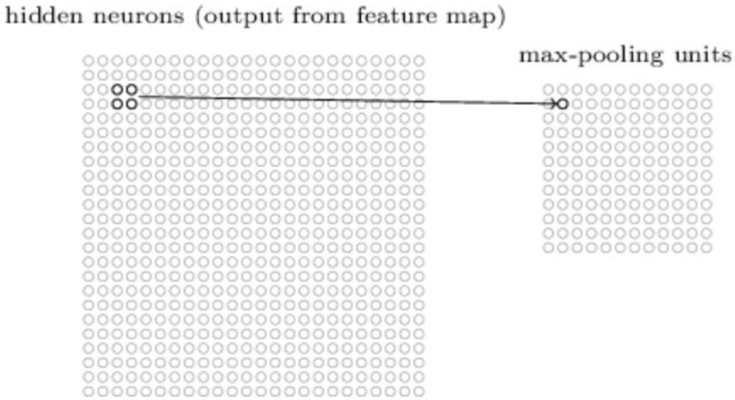
Feature maps



Each feature map represents a property of the input that is supposed to be spatially invariant.

Typically, we consider several feature maps in a single layer.

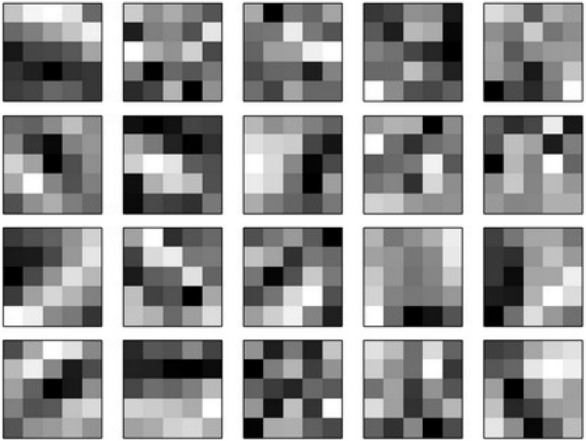
Pooling



Neurons in the pooling layer compute functions of their receptive fields:

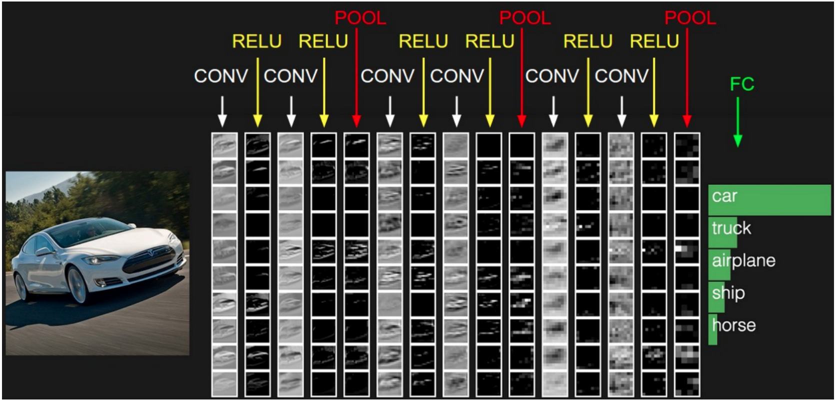
- **Max-pooling** : maximum of inputs
- **L2-pooling** : square root of the sum of squres
- **Average-pooling** : mean
- . . .

Trained feature maps

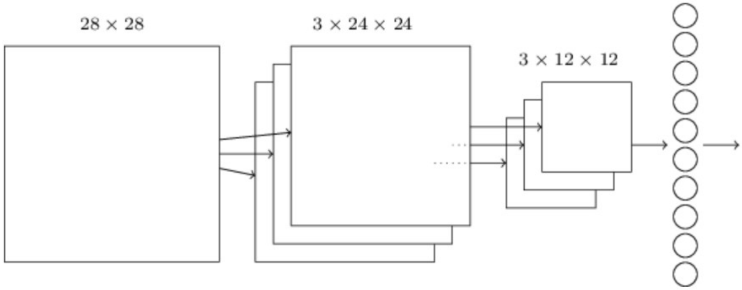


(20 feature maps, receptive fields 5×5)

Trained feature maps



Simple convolutional network

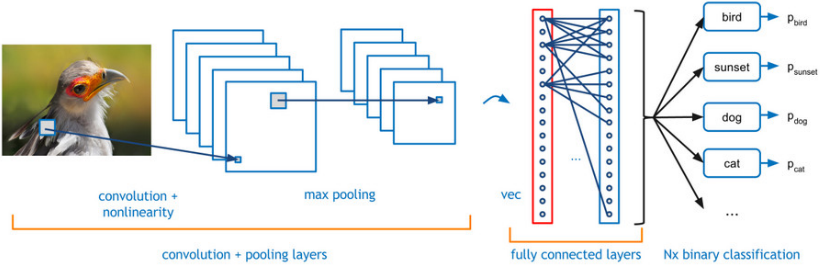


28×28 input image, 3 feature maps, each feature map has its own max-pooling (field 5×5, stride = 1), 10 output neurons.

Each neuron in the output layer gets input from each neuron in the pooling layer.

Trained using the gradient descent with the backprop, which can be easily adapted to convolutional networks.

Convolutional network



Simple convolutional network vs MNIST

two convolutional-pooling layers, one 20, second 40 feature maps, two dense (MLP) layers (1000-1000), outputs (10)

- Activation functions of the feature maps and dense layers: ReLU
- max-pooling
- output layer: soft-max

- Error function: negative log-likelihood (= cross-entropy)

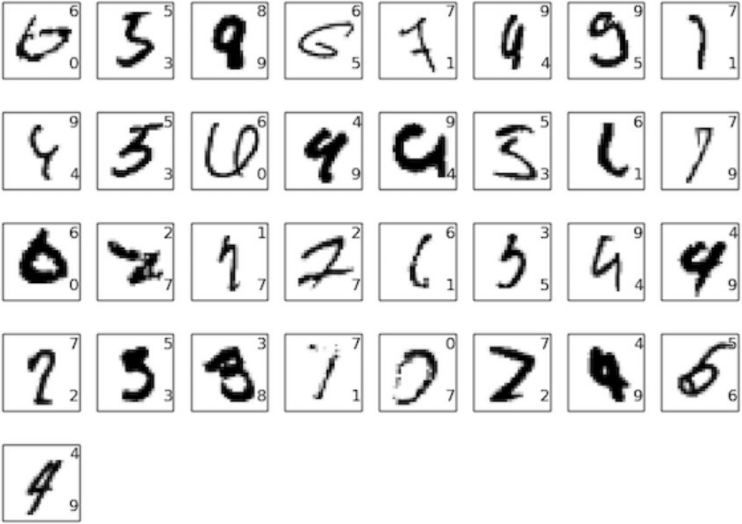
- Training: SGD, mini-batch size 10
- learning rate 0.03
- L2 regularization with "weight" $\lambda = 0.1$ + dropout with prob. $1/2$
- training for 40 epochs (i.e. every training example is considered 40 times)

- Expanded dataset: displacement by one pixel to an arbitrary direction.

- Committee voting of 5 networks.

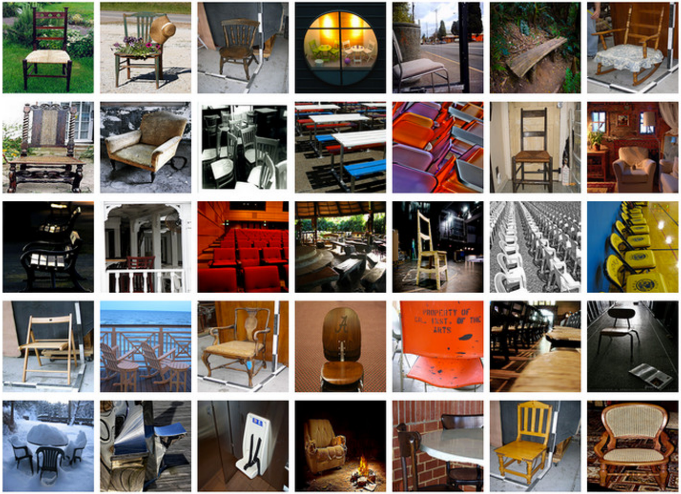
MNIST

Out of 10 000 images in the test set, only these 33 have been incorrectly classified:



More complex convolutional networks

Convolutional networks have been used for classification of images from the ImageNet database (16 million color images, 20 thousand classes)



ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

Competition in classification over a subset of images from ImageNet.

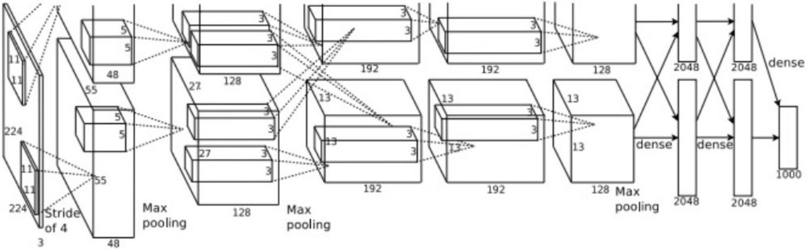
Started in 2010, assisted in breakthrough in image recognition.

Training set 1.2 million images, 1000 classes. Validation set: 50 000, test set: 150 000.

Many images contain more than one object ⇒ model is allowed to choose five classes, the correct label must be among the five. (top-5 criterion).

AlexNet

ImageNet classification with deep convolutional neural networks, by Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton (2012).



Trained on two GPUs (NVIDIA GeForce GTX 580)

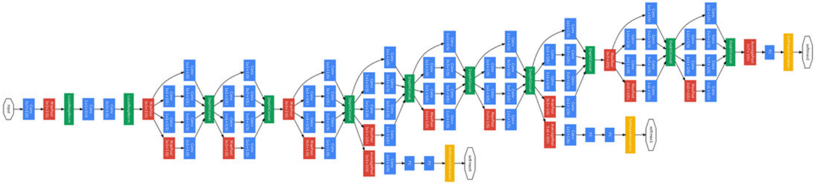
Výsledky:

- accuracy 84.7% in top-5 (second best algorithm at the time 73.8%)
- 63.3% "perfect" (top-1) classification

ILSVRC 2014

The same set as in 2012, top-5 criterion.

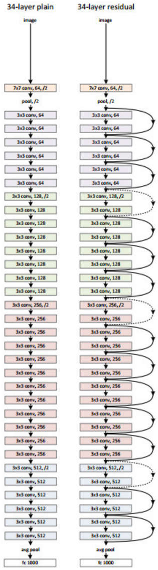
GoogLeNet: deep convolutional network, 22 layers



Results:

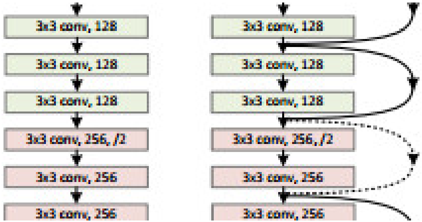
- Accuracy 93.33% top-5

ILSVRC 2015



- Deep convolutional network
- Various numbers of layers, the winner has 152 layers
- Skip connections implementing residual learning

- Error **3.57%** in top-5.



ILSVRC 2016

Trimps-Soushen (The Third Research Institute of Ministry of Public Security)

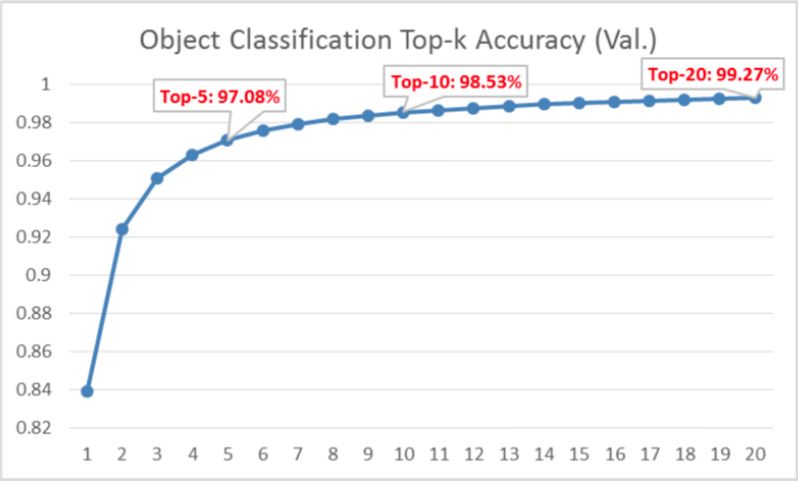
There is no new innovative technology or novelty by Trimps-Soushen.

Ensemble of the pretrained models from Inception-v3, Inception-v4, Inception-ResNet-v2, Pre-Activation ResNet-200, and Wide ResNet (WRN-68–2).

Each of the models are strong at classifying some categories, but also weak at classifying some categories.

Test error: 2.99%

Top-k accuracy analyzed



https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Top-20 typical errors

Out of 1458 misclassified images in Top-20:

Error Categories	Numbers	Percentages(%)
Label May Wrong	221	15.16
Multiple Objects (>5)	118	8.09
Non-Obvious Main Object	355	24.35
Confusing Label	206	14.13
Fine-grained Label	258	17.70
Obvious Wrong	234	16.05
Partial Object	66	4.53

https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Top-k accuracy analyzed

Predict:
1 *pencil box*
2 *diaper*
3 *bib*
4 *purse*
5 *running shoe*

Ground Truth:
sleeping bag

https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Top-k accuracy analyzed

Predict:

1 *dock*

2 *submarine*

3 *boathouse*

4 *breakwater*

5 *lifeboat*

Ground Truth:

paper towel

https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Top-k accuracy analyzed

Predict:

1 *bolete*

2 *earthstar*

3 *gyromitra*

4 *hen of the woods*

5 *mushroom*

Ground Truth:

stinkhorn

https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Top-k accuracy analyzed

Predict:
1 *apron*
2 *plastic bag*
3 *sleeping bag*
4 *umbrella*
5 *bulletproof vest*

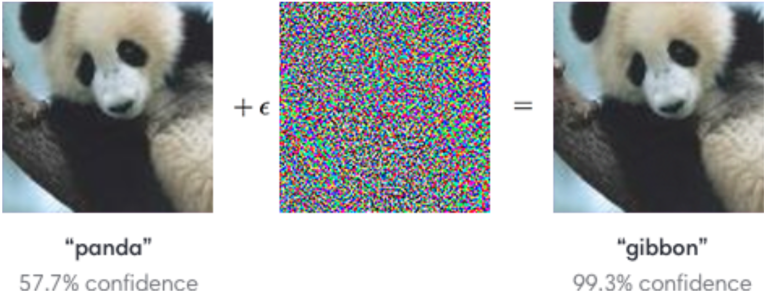
Ground Truth:
poncho

https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classification-dfbc423111dd

Superhuman convolutional nets?!

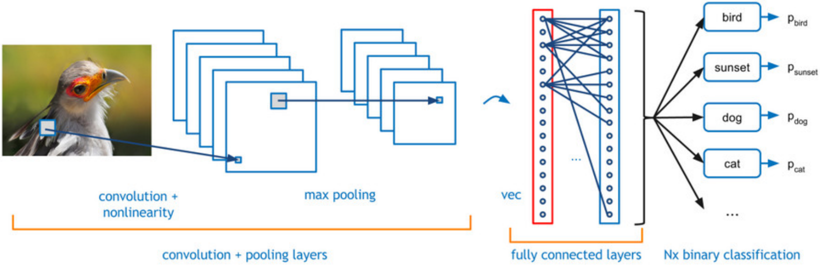
Andrej Karpathy: ...the task of labeling images with 5 out of 1000 categories quickly turned out to be extremely challenging, even for some friends in the lab who have been working on ILSVRC and its classes for a while. First we thought we would put it up on [Amazon Mechanical Turk]. Then we thought we could recruit paid undergrads. Then I organized a labeling party of intense labeling effort only among the (expert labelers) in our lab. Then I developed a modified interface that used GoogLeNet predictions to prune the number of categories from 1000 to only about 100. It was still too hard - people kept missing categories and getting up to ranges of 13-15% error rates. In the end I realized that to get anywhere competitively close to GoogLeNet, it was most efficient if I sat down and went through the painfully long training process and the subsequent careful annotation process myself... The labeling happened at a rate of about 1 per minute, but this decreased over time... Some images are easily recognized, while some images (such as those of fine-grained breeds of dogs, birds, or monkeys) can require multiple minutes of concentrated effort. I became very good at identifying breeds of dogs... Based on the sample of images I worked on, the GoogLeNet classification error turned out to be 6.8%... My own error in the end turned out to be 5.1%, approximately 1.7% better.

Does it really work?

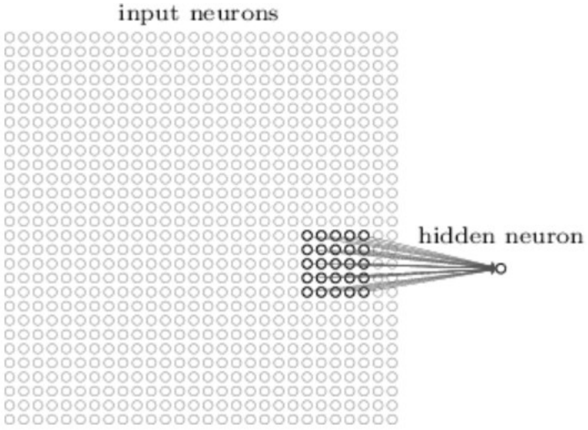


Convolutional networks – theory

Convolutional network



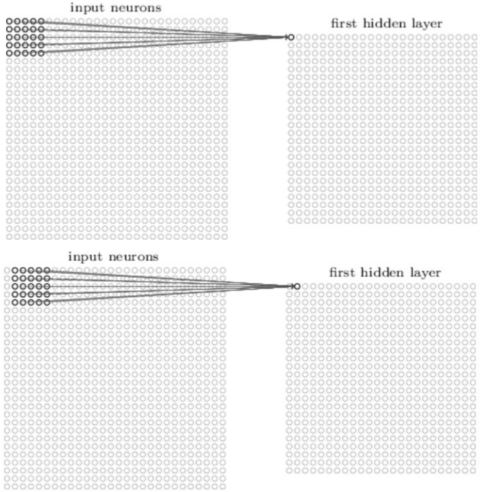
Convolutional layers



Every neuron is connected with a (typically small) *receptive field* of neurons in the lower layer.

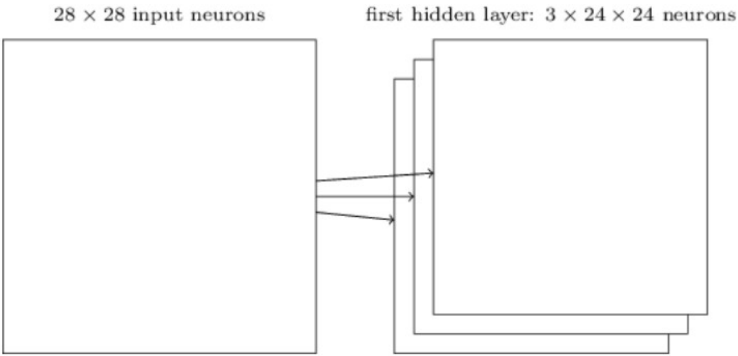
Neuron is "standard": Computes a weighted sum of its inputs, applies an activation function.

Convolutional layers



Neurons grouped into *feature maps* sharing weights.

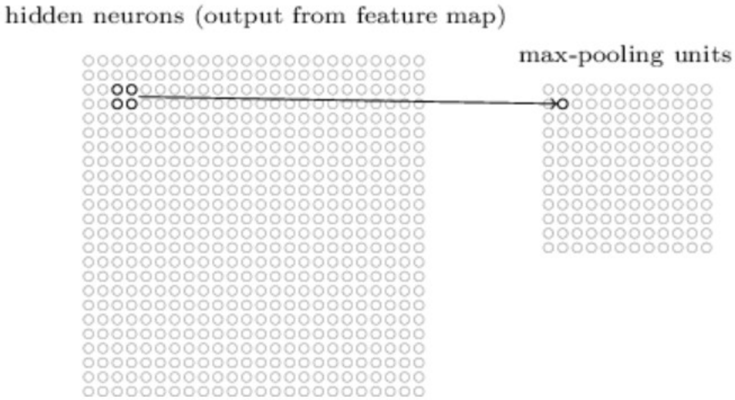
Convolutional layers



Each feature map represents a property of the input that is supposed to be spatially invariant.

Typically, we consider several feature maps in a single layer.

Pooling layers



Neurons in the pooling layer compute simple functions of their receptive fields (the fields are typically disjoint):

- **Max-pooling** : maximum of inputs
- **L2-pooling** : square root of the sum of squres
- **Average-pooling** : mean
- . . .

Convolutional networks – architecture

Neurons organized in layers, $L_0, L_1, \ldots, L_n$, connections (typically) only from L_m to L_{m+1}.

Convolutional networks – architecture

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Several types of layers:

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Convolutional networks – architecture

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Several types of layers:

- **input** layer L_0
- **dense** layer L_m: Each neuron of L_m connected with each neuron of L_{m-1}.
- **convolutional & pooling** layer L_m: Contains two sub-layers:
  - **convolutional layer**: Neurons organized into disjoint **feature maps**, all neurons of a given feature map *share weights* (but have different inputs)
  - **pooling layer**: Each (convolutional) feature map F has a corresponding **pooling map** P. Neurons of P
    - have inputs only from F (typically few of them),
    - compute a simple aggregate function (such as max),
    - have *disjoint inputs*.

Convolutional networks – architecture

- Denote
  - X a set of *input* neurons
  - Y a set of *output* neurons
  - Z a set of *all* neurons ($X, Y \subseteq Z$)
- individual neurons denoted by indices i, j etc.
  - ξ_j is the inner potential of the neuron j *after the computation stops*
  - y_j is the output of the neuron j *after the computation stops*

  (define $y_0 = 1$ is the value of the formal unit input)
- w_{ji} is the weight of the connection **from** i **to** j

  (in particular, w_{j0} is the weight of the connection from the formal unit input, i.e. $w_{j0} = -b_j$ where b_j is the bias of the neuron j)
- $j_{\leftarrow}$ is a set of all i such that j is adjacent from i
  (i.e. there is an arc **to** j from i)
- $j^{\rightarrow}$ is a set of all i such that j is adjacent to i
  (i.e. there is an arc **from** j to i)
- $[ji]$ is a set of all connections (i.e. pairs of neurons) sharing the weight w_{ji}.

Convolutional networks – activity

- neurons of dense and convolutional layers:
  - inner potential of neuron j:

$$\xi_j = \sum_{i \in j_{\leftarrow}} w_{ji} y_i$$

  - activation function σ_j for neuron j (arbitrary differentiable):

$$y_j = \sigma_j(\xi_j)$$

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- Neurons of pooling layers: Apply the "pooling" function:
  - max-pooling:

$$y_j = \max_{i \in j_\leftarrow} y_i$$

  - avg-pooling:

$$y_j = \frac{\sum_{i \in j_\leftarrow} y_i}{|j_\leftarrow|}$$

A convolutional network is evaluated layer-wise (as MLP), for each $j \in Y$ we have that $y_j(\vec{w}, \vec{x})$ is the value of the output neuron j after evaluating the network with weights $\vec{w}$ and input $\vec{x}$.

Convolutional networks – learning

Learning:

- Given a **training set** $\mathcal{T}$ of the form

$$\left\{ \left(\vec{x}_k, \vec{d}_k \right) \quad \middle| \quad k = 1, \ldots, p \right\}$$

  Here, every $\vec{x}_k \in \mathbb{R}^{|X|}$ is an *input vector* end every $\vec{d}_k \in \mathbb{R}^{|Y|}$ is the desired network output. For every $j \in Y$, denote by d_{kj} the desired output of the neuron j for a given network input $\vec{x}_k$ (the vector $\vec{d}_k$ can be written as $\left(d_{kj}\right)_{j \in Y}$).

- **Error function – mean squared error (for example):**

$$E(\vec{w}) = \frac{1}{p} \sum_{k=1}^{p} E_k(\vec{w})$$

  where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} \left(y_j(\vec{w}, \vec{x}_k) - d_{kj} \right)^2$$

Convolutional networks – SGD

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:
  - Choose (randomly) a set of training examples $T \subseteq \{1, \ldots, p\}$
  - Compute

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

where

$$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \frac{1}{|T|} \sum_{k \in T} \nabla E_k(\vec{w}^{(t)})$$

Here T is a *minibatch* (of a fixed size),

- $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$
- $\nabla E_k(\vec{w}^{(t)})$ is the gradient of the error of the example k

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially. **Epoch** consists of one round through all data.

Backprop

Recall that $\nabla E_k(\vec{w}^{(t)})$ is a vector of all partial derivatives of the form $\frac{\partial E_k}{\partial w_{ji}}$.

How to compute $\frac{\partial E_k}{\partial w_{ji}}$?

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First, switch from derivatives w.r.t. w_{ji} to derivatives w.r.t. y_j:

- Recall that for every w_{ji} where j is in a dense layer, i.e. does not share weights:

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- Now for every w_{ji} where j is in a convolutional layer:

$$\frac{\partial E_k}{\partial w_{ji}} = \sum_{r\ell \in [ji]} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot y_\ell$$

- Neurons of pooling layers do not have weights.

Backprop

Now compute derivatives w.r.t. y_j:

- for every $j \in Y$:

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj}$$

  This holds for the squared error, for other error functions the derivative w.r.t. outputs will be different.

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- for every $j \in Z \smallsetminus Y$ such that $j^{\rightarrow}$ is either a dense layer, or a convolutional layer:

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj}$$

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- for every $j \in Z \smallsetminus Y$ such that $j^{\rightarrow}$ is max-pooling: Then $j^{\rightarrow} = \{i\}$ for a single "max" neuron and we have

$$\frac{\partial E_k}{\partial y_j} = \begin{cases} \frac{\partial E_k}{\partial y_i} & \text{if } j = arg\ max_{r \in i_{\leftarrow}} y_r \\ 0 & \text{otherwise} \end{cases}$$

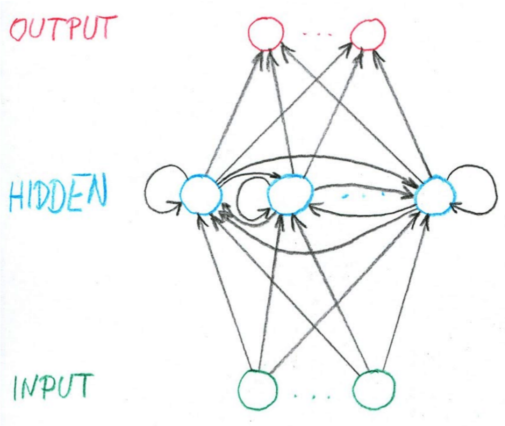
I.e. gradient can be propagated from the output layer downwards as in MLP.

Convolutional networks – summary

- Conv. nets. are nowadays the most used networks in image processing (and also in other areas where input has some local, "spatially" invariant properties)
- Typically trained using the gradient descent with the backpropagation.
- Due to the weight sharing allow (very) deep architectures.
- Typically extended with more adjustments and tricks in their topologies.

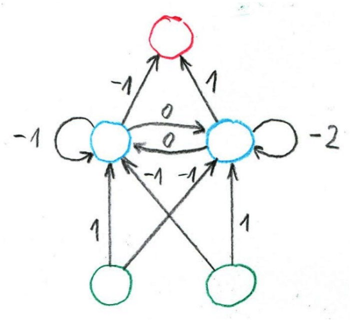
Recurrent Neural Networks - LSTM

RNN



- Input:
  $\vec{x} = (x_1, \ldots, x_M)$
- Hidden:
  $\vec{h} = (h_1, \ldots, h_H)$
- Output:
  $\vec{y} = (y_1, \ldots, y_N)$

RNN example

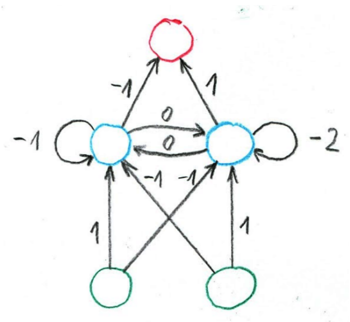


Activation function:

$$\sigma(\xi) = \begin{cases} 1 & \xi \geq 0 \\ 0 & \xi < 0 \end{cases}$$

y		1	0	1	
h	(0, 0)	(1, 1)	(1, 0)	(0, 1)	$\cdots$
x		(0, 0)	(1, 0)	(1, 1)	

RNN example



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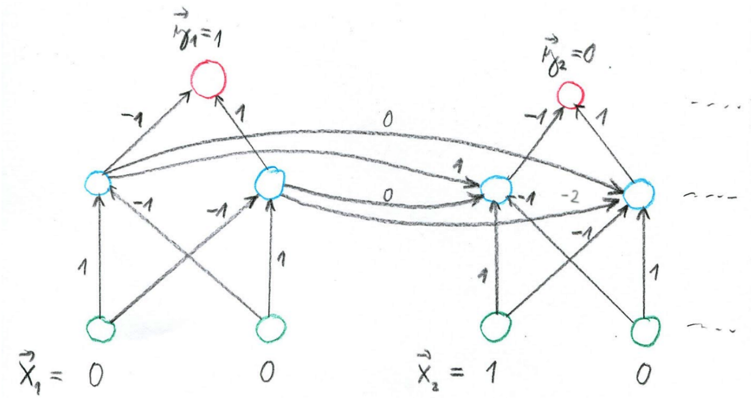
y		$\vec{y}_1 = 1$	$\vec{y}_2 = 0$	$\vec{y}_3 = 1$	
h	$\vec{h}_0 = (0,0)$	$\vec{h}_1 = (1,1)$	$\vec{h}_2 = (1,0)$	$\vec{h}_3 = (0,1)$	$\cdots$
x		$\vec{x}_1 = (0,0)$	$\vec{x}_2 = (1,0)$	$\vec{x}_3 = (1,1)$	

RNN example



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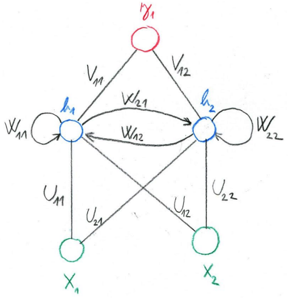
x		$\vec{x}_1 = (0,0)$	$\vec{x}_2 = (1,0)$	$\vec{x}_3 = (1,1)$	

RNN – formally

- M inputs: $\vec{x} = (x_1, \ldots, x_M)$
- H hidden neurons: $\vec{h} = (h_1, \ldots, h_H)$
- N output neurons: $\vec{y} = (y_1, \ldots, y_N)$
- Weights:
  - $U_{kk'}$ from input $x_{k'}$ to hidden h_k
  - $W_{kk'}$ from hidden $h_{k'}$ to hidden h_k
  - $V_{kk'}$ from hidden $h_{k'}$ to output y_k



RNN – formally

- Input sequence: $\mathbf{x} = \vec{x}_1, \ldots, \vec{x}_T$

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$$\vec{h}_t = (h_{t1}, \dots, h_{tH})$$

We have $\vec{h}_0 = (0, \dots, 0)$ and

$$\vec{h}_{tk} = \sigma\left(\sum_{k'=1}^{M} U_{kk'} x_{tk'} + \sum_{k'=1}^{H} W_{kk'} h_{(t-1)k'}\right)$$

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  where $y_{tk} = \sigma\left(\sum_{k'=1}^{H} V_{kk'} h_{tk'}\right)$.

RNN – in matrix form

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$$y_t = \sigma(Vh_t)$$

RNN – Comments

- $\vec{h}_t$ is the memory of the network, captures what happened in all previous steps (with decaying quality).
- RNN **shares weights** U, V, W along the sequence.
  Note the similarity to convolutional networks where the weights were shared spatially over images, here they are shared temporally over sequences.
- RNN can deal with **sequences of variable length.**
  Compare with MLP which accepts only fixed-dimension vectors on input.

RNN – training

Training set

$$\mathcal{T} = \left\{(\mathbf{x}_1, \mathbf{d}_1), \ldots, (\mathbf{x}_p, \mathbf{y}_p)\right\}$$

here

- each $\mathbf{x}_\ell = \vec{x}_{\ell 1}, \ldots, \vec{x}_{\ell T_\ell}$ is an input sequence,
- each $\mathbf{d}_\ell = \vec{d}_{\ell 1}, \ldots, \vec{d}_{\ell T_\ell}$ is an expected output sequence.

Here each $\vec{x}_{\ell t} = (x_{\ell t 1}, \ldots, x_{\ell t M})$ is an input vector and each $\vec{d}_{\ell t} = (d_{\ell t 1}, \ldots, d_{\ell t N})$ is an expected output vector.

Error function

In what follows I will consider a training set with a **single element** $(\mathbf{x}, \mathbf{d})$. I.e. drop the index ℓ and have

- $\mathbf{x} = \vec{x}_1, \ldots, \vec{x}_T$ where $\vec{x}_t = (x_{t1}, \ldots, x_{tM})$
- $\mathbf{d} = \vec{d}_1, \ldots, \vec{d}_T$ where $\vec{d}_t = (d_{t1}, \ldots, d_{tN})$

The squared error of $(\mathbf{x}, \mathbf{d})$ is defined by

$$E_{(\mathbf{x},\mathbf{d})} = \sum_{t=1}^{T} \sum_{k=1}^{N} \frac{1}{2}(y_{tk} - d_{tk})^2$$

Recall that we have a sequence of network outputs $\mathbf{y} = \vec{y}_1, \ldots, \vec{y}_T$ and thus y_{tk} is the k-th component of $\vec{y}_t$

Gradient descent (single training example)

Consider a single training example $(\mathbf{x}, \mathbf{d})$.

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$$U_{kk'}^{(\ell+1)} = U_{kk'}^{(\ell)} - \varepsilon(\ell) \cdot \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta U_{kk'}}$$

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The above is THE learning algorithm that modifies weights!

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Computes the derivatives of E, no weights are modified!

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$$\frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta U_{kk'}} = \sum_{t=1}^{T} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta h_{tk}} \cdot \sigma' \cdot x_{tk'} \qquad k' = 1, \ldots, M$$

$$\frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta V_{kk'}} = \sum_{t=1}^{T} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta y_{tk}} \cdot \sigma' \cdot h_{tk'} \qquad k' = 1, \ldots, H$$

$$\frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta W_{kk'}} = \sum_{t=1}^{T} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta h_{tk}} \cdot \sigma' \cdot h_{(t-1)k'} \qquad k' = 1, \ldots, H$$

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Backpropagation:

$$\frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta y_{tk}} = y_{tk} - d_{tk} \qquad \text{(assuming squared error)}$$

$$\frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta h_{tk}} = \sum_{k'=1}^{N} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta y_{tk'}} \cdot \sigma' \cdot V_{k'k} + \sum_{k'=1}^{H} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta h_{(t+1)k'}} \cdot \sigma' \cdot W_{k'k}$$

Long-term dependencies

$$\frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta h_{tk}} = \sum_{k'=1}^{N} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta y_{tk'}} \cdot \sigma' \cdot V_{k'k} + \sum_{k'=1}^{H} \frac{\delta E_{(\mathbf{x},\mathbf{d})}}{\delta h_{(t+1)k'}} \cdot \sigma' \cdot W_{k'k}$$

- Unless $\sum_{k'=1}^{H} \sigma' \cdot W_{k'k} \approx 1$, the gradient either vanishes, or explodes.
- For a large T (long-term dependency), the gradient "deeper" in the past tends to be too small (large).
- A solution: LSTM

LSTM

$$\vec{h}_t = \vec{o}_t \circ \sigma_h(\vec{C}_t) \qquad \text{output}$$

$$\vec{C}_t = \vec{f}_t \circ \vec{C}_{t-1} + \vec{i}_t \circ \tilde{C}_t \qquad \text{memory}$$

$$\tilde{C}_t = \sigma_h(W_C \cdot \vec{h}_{t-1} + U_C \cdot \vec{x}_t) \qquad \text{new memory contents}$$

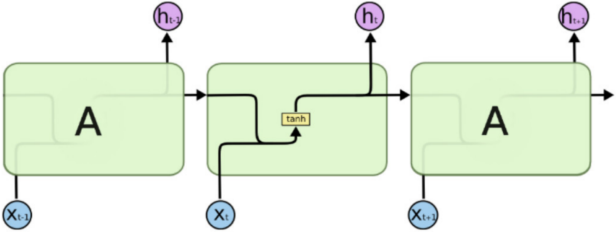
$$\vec{o}_t = \sigma_g(W_o \cdot \vec{h}_{t-1} + U_o \cdot \vec{x}_t) \qquad \text{output gate}$$

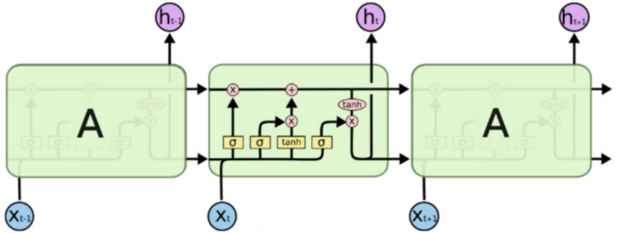
$$\vec{f}_t = \sigma_g(W_f \cdot \vec{h}_{t-1} + U_f \cdot \vec{x}_t) \qquad \text{forget gate}$$

$$\vec{i}_t = \sigma_g(W_i \cdot \vec{h}_{t-1} + U_i \cdot \vec{x}_t) \qquad \text{input gate}$$

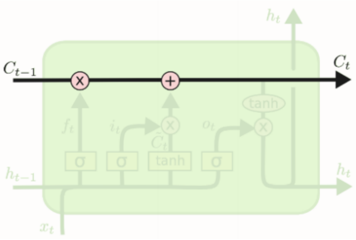
- $\circ$ is the component-wise product of vectors
- $\cdot$ is the matrix-vector product
- σ_h hyperbolic tangents (applied component-wise)
- σ_g logistic sigmoid (aplied component-wise)

RNN vs LSTM





Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/



$$\vec{h}_t = \vec{o}_t \circ \sigma_h(\vec{C}_t)$$

$$\Rightarrow \vec{C}_t = \vec{f}_t \circ \vec{C}_{t-1} + \vec{i}_t \circ \tilde{C}_t$$

$$\tilde{C}_t = \sigma_h(W_C \cdot \vec{h}_{t-1} + U_C \cdot \vec{x}_t)$$

$$\vec{o}_t = \sigma_g(W_o \cdot \vec{h}_{t-1} + U_o \cdot \vec{x}_t)$$

$$\vec{f}_t = \sigma_g(W_f \cdot \vec{h}_{t-1} + U_f \cdot \vec{x}_t)$$

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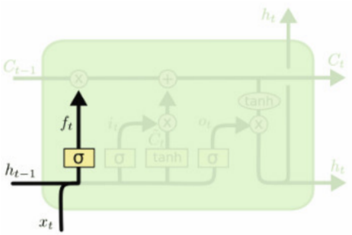
LSTM



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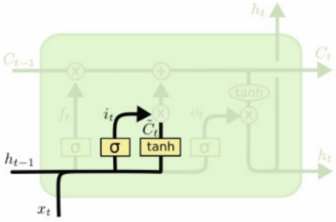
$$\vec{o}_t = \sigma_g(W_o \cdot \vec{h}_{t-1} + U_o \cdot \vec{x}_t)$$

$$\Rightarrow \vec{f}_t = \sigma_g(W_f \cdot \vec{h}_{t-1} + U_f \cdot \vec{x}_t)$$

$$\vec{i}_t = \sigma_g(W_i \cdot \vec{h}_{t-1} + U_i \cdot \vec{x}_t)$$

Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

LSTM



$$\vec{h}_t = \vec{o}_t \circ \sigma_h(\vec{C}_t)$$

$$\vec{C}_t = \vec{f}_t \circ \vec{C}_{t-1} + \vec{i}_t \circ \tilde{C}_t$$

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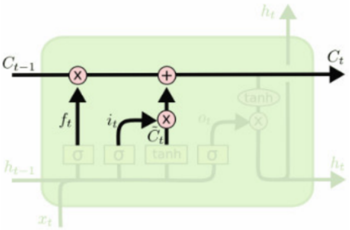

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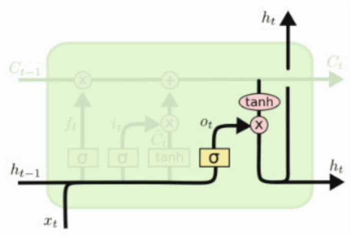

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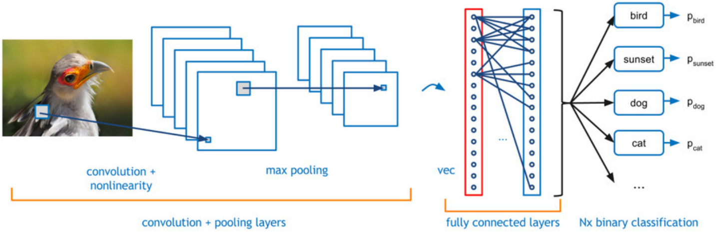
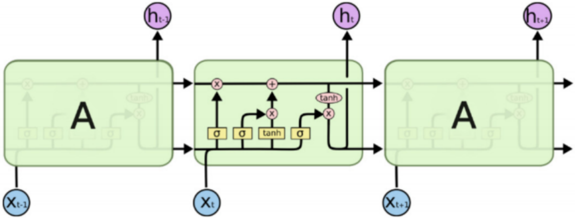
LSTM – summary

- LSTM (almost) solves the vanishing gradient problem w.r.t. the "internal" state of the network.
- Learns to control its own memory (via forget gate).
- Revolution in machine translation and text processing.

Convolutions & LSTM in action – cancer research





Colorectal cancer outcome prediction

The problem: Predict 5-year survival probability from an image of a small region of tumour tissue (1 mm diameter).

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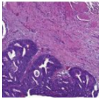
Input: Digitized haematoxylin-eosin-stained tumour tissue microarray samples.
Output: Estimated survival probability.



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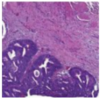

Data:

- Training set: 420 patients of Helsinki University Centre Hospital, diagnosed with colorectal cancer, underwent primary surgery.
- Test set: 182 patients
- Follow-up time and outcome known for each patient.

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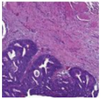

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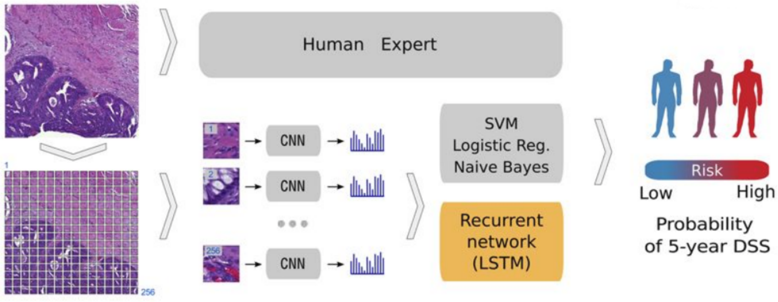
Human expert comparison:

- Histological grade assessed at the time of diagnosis.
- Visual Risk Score: Three pathologists classified to high/low-risk categories (by majority vote).

Source: D. Bychkov et al. Deep learning based tissue analysis predicts outcome in colorectal cancer. Scientific Reports, Nature, 2018.

Colorectal cancer outcome prediction



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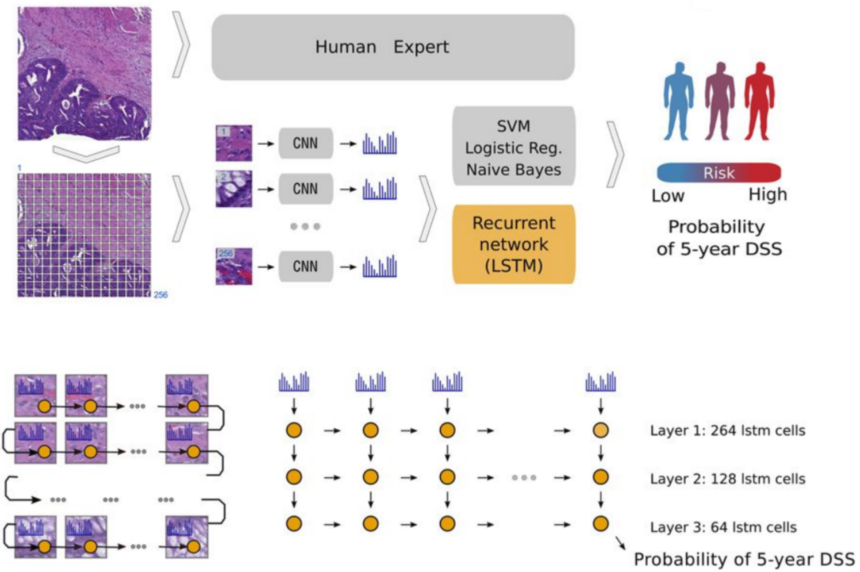

Data & workflow

- Input images: 3500 px $\times$ 3500 px
  - Cut into tiles: 224 px $\times$ 224 px $\Rightarrow$ 256 tiles
- Each tile pased to a convolutional network (CNN)
  - Ouptut of CNN: 4096 dimensional vector.
- A "string" of 256 vectors (each of the dimension 4096) pased into a LSTM.
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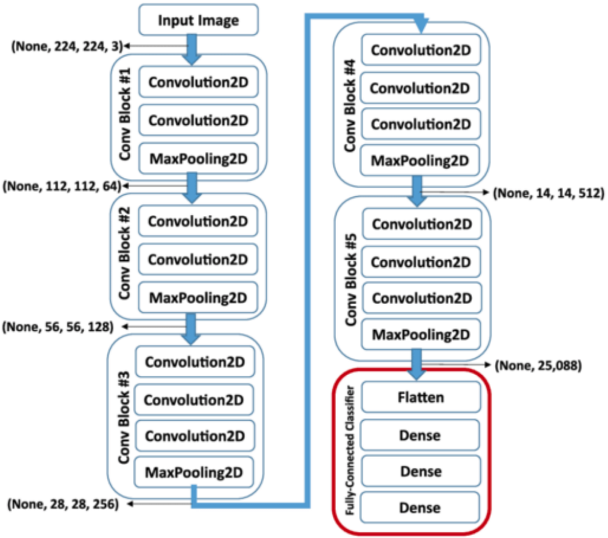
The authors also tried to substitute the LSTM on top of CNN with

- logistic regression
- naive Bayes
- support vector machines

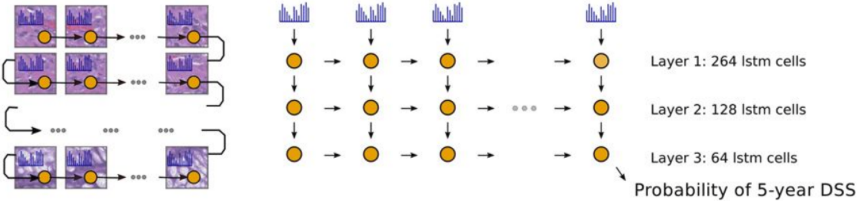
CNN architecture – VGG-16



(Pre)trained on ImageNet (cats, dogs, chairs, etc.)

LSTM architecture

- LSTM has three layers (264, 128, 64 cells)

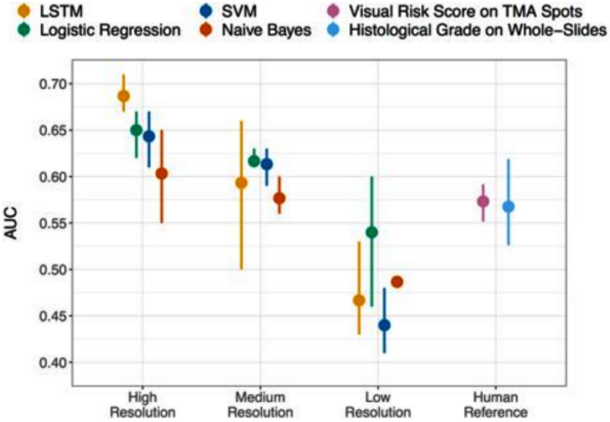


LSTM – training

- L1 regularization (0.005) at each hidden layer of LSTM
  i.e. 0.005 times the sum of absolute values of weights added to the error
- L2 regularization (0.005) at each hidden layer of LSTM
  i.e. 0.005 times the sum of squared values of weights added to the error
- Dropout 5% at the input and the last hidden layers of LSTM

- Datasets:
  - Training: 220 samples,
  - Validation 60 samples,
  - Test 140 samples.

Colorectal cancer outcome prediction



Source: D. Bychkov et al. Deep learning based tissue analysis predicts outcome in colorectal cancer. Scientific Reports, Nature, 2018.

Feed-forward networks summary

Architectures:

- Multi-layer perceptron (MLP):
  - dense connections between layers
- Convolutional networks (CNN):
  - local receptors, feature maps
  - pooling
- Recurrent networks (RNN, LSTM):
  - self-loops but still feed-forward through time

Training:

- gradient descent algorithm + heuristics