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.)

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Evaluation:

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  - teams of two students
  - implementation of a selected model + analysis of given data
  - implementation either in C, C++, or in Java **without use of any specialized libraries for data analysis and machine learning**
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- Application of any deep learning toolset on given (difficult) data. We prefer TensorFlow but you may use another library (CNTK, Caffe, DeepLearning4j, ...) The goal is to get the best results on increasingly more difficult datasets.

  The team with the best result on the hardest dataset will automatically get $> F$ at the exam.

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Q: Why we cannot use specialized libraries in projects?

A: In order to "touch" the low level implementation details of the algorithms. You should not even use libraries for linear algebra and numerical methods, so that you will be confronted with rounding errors and numerical instabilities.

Machine learning in general

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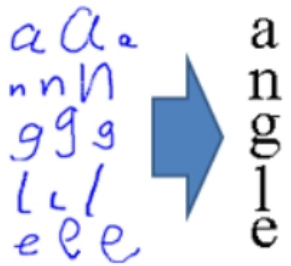

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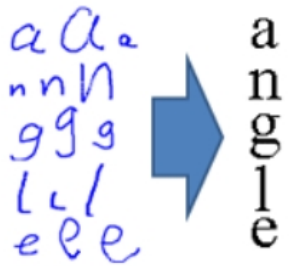

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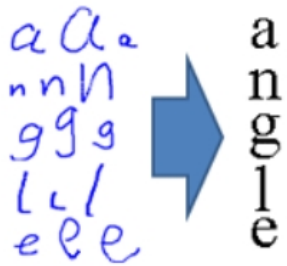

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- Basic attributes of learning algorithms:
  - **representation**: ability to capture the inner structure of training data
  - **generalization**: ability to work properly on new data

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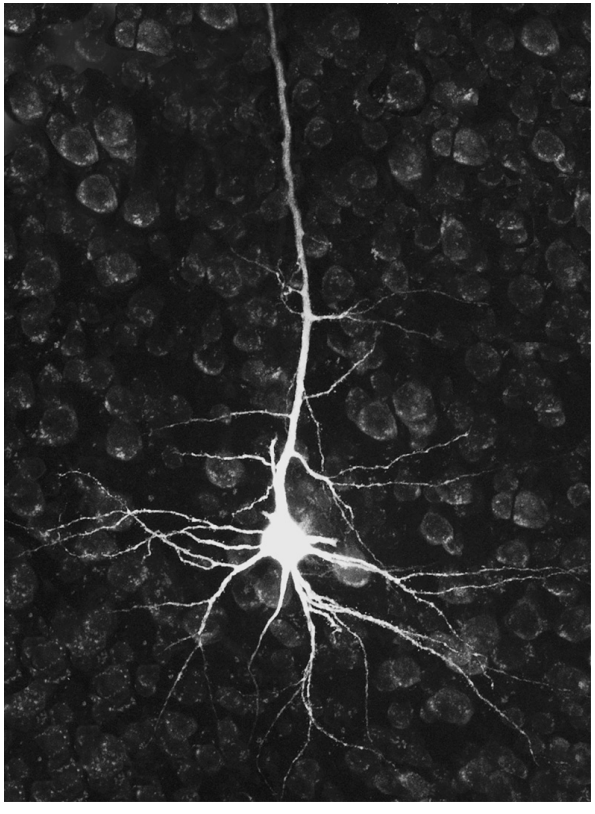
There are many types of models:

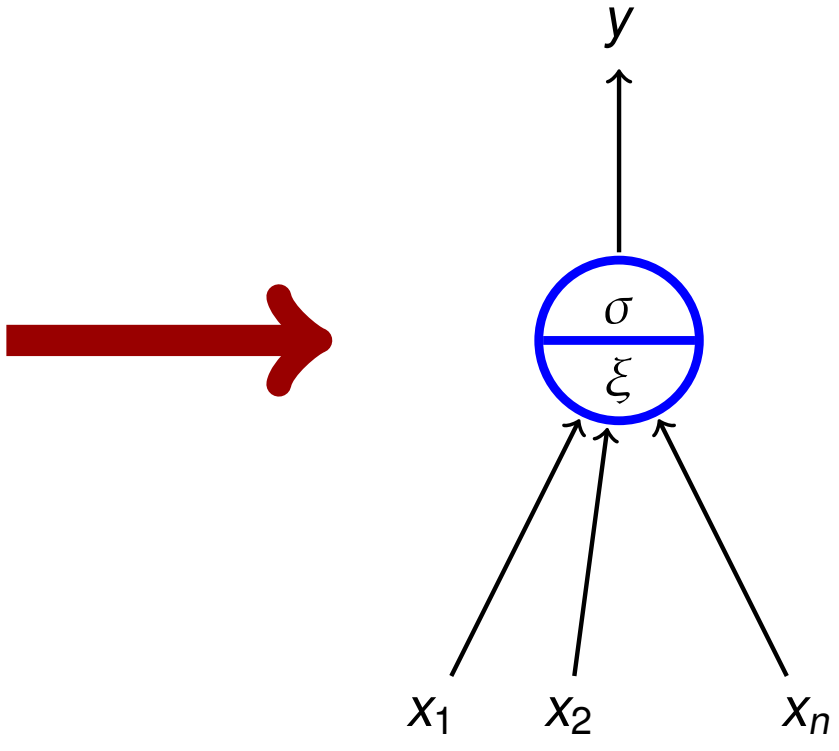
- decision trees
- support vector machines
- hidden Markov models
- Bayes networks and other graphical models
- **neural networks**
- ...

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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- 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
  - finance - stock prices, risk analysis
  - medicine - diagnosis, signal processing (EKG, EEG, ...), image processing (MRI, roentgen, ...)
  - 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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- 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.
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  - basic models

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  - Basic information about current implementations
    (TensorFlow, CNTK)

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.
- Each neuron is connected with approx. 10^4 neurons.
- Neurons themselves are very complex systems.

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- Afterwards, the output signal is transfered via PNS to *effectors* (e.g. muscle cells).

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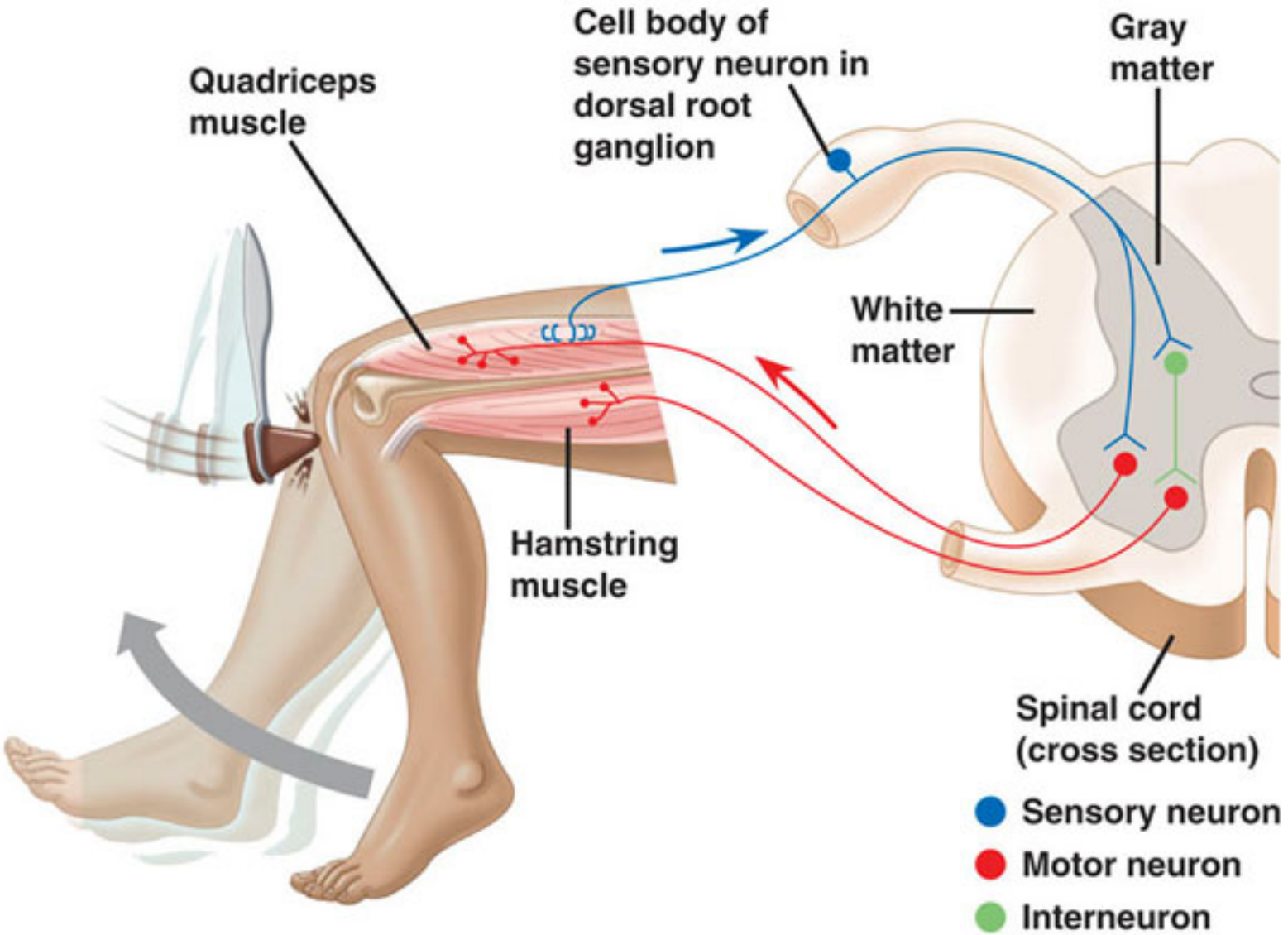

Zdroj: N. Campbell and J. Reece; Biology, 7th Edition; ISBN: 080537146X

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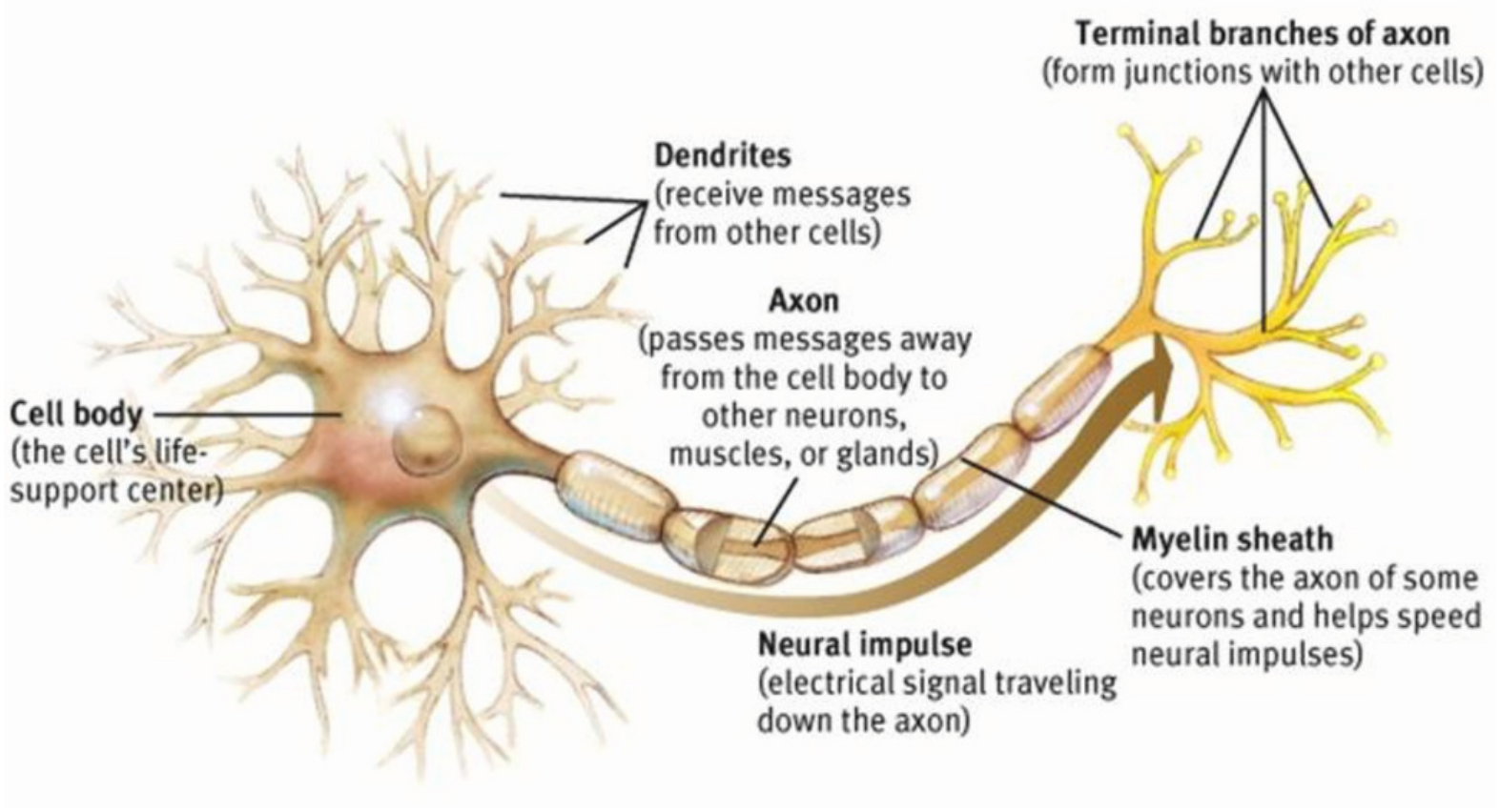
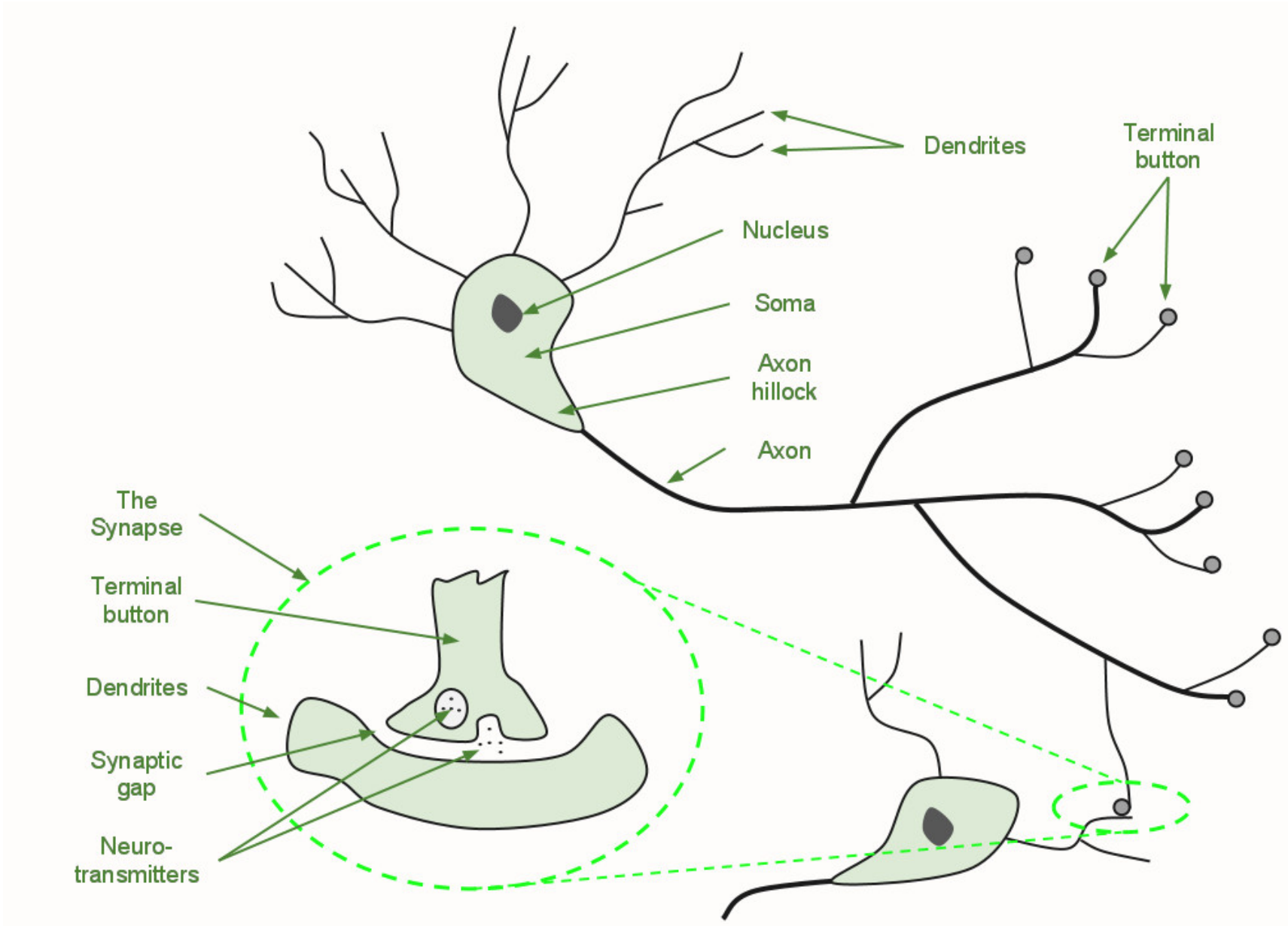
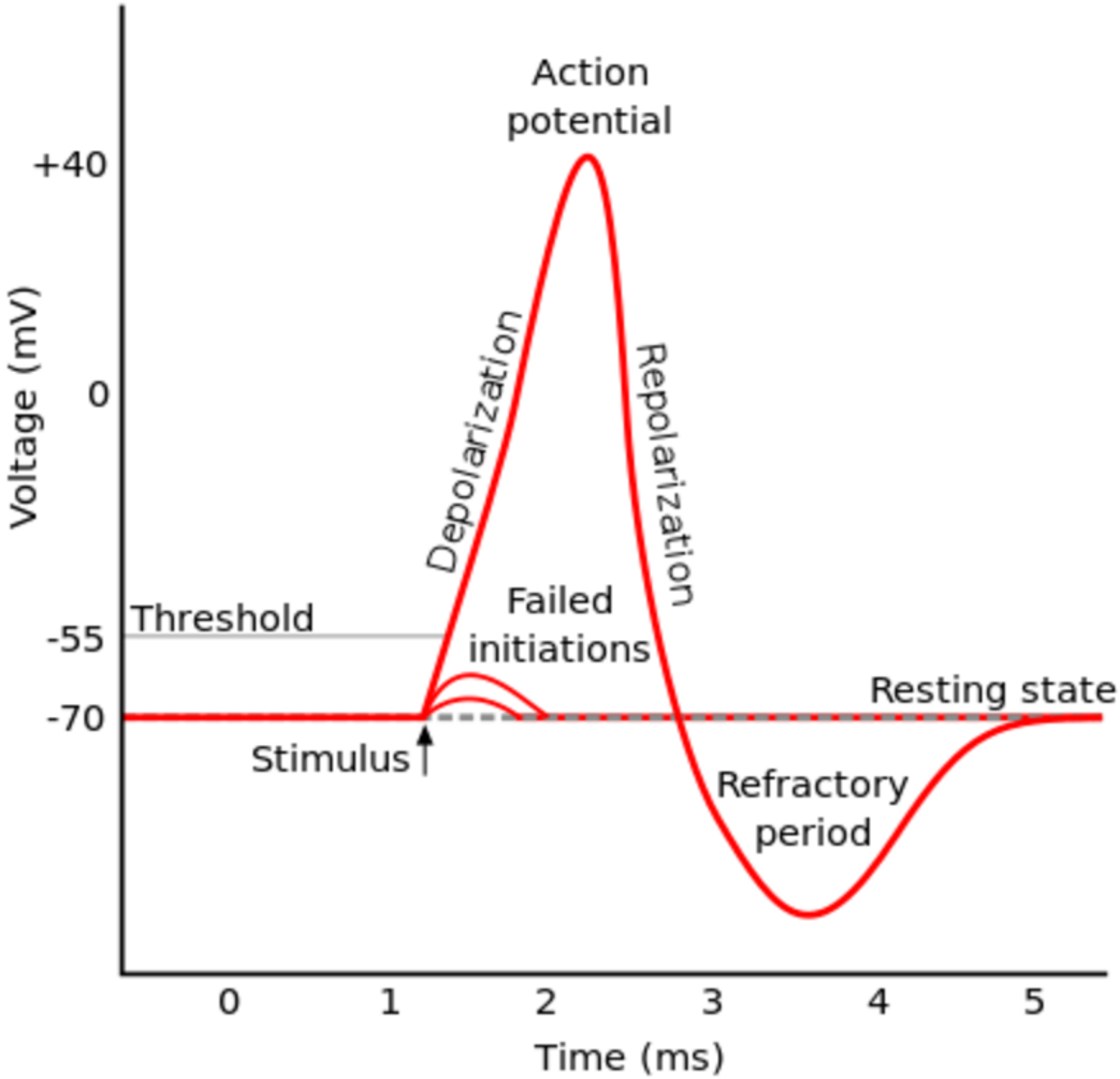


Zdroj: http://www.web-books.com/eLibrary/Medicine/Physiology/Nervous/Nervous.htm

Synaptic connections



Action potential



Summation

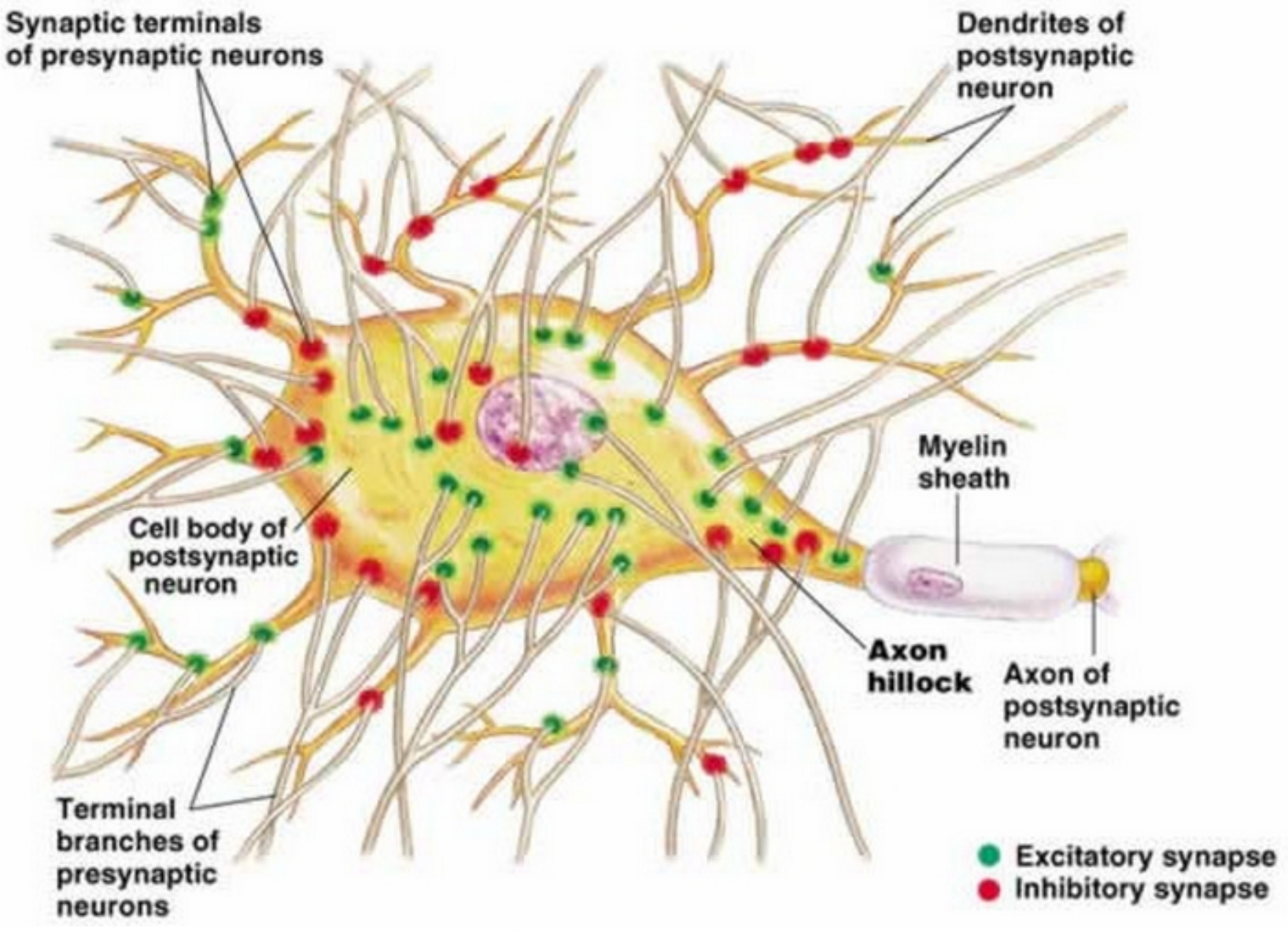
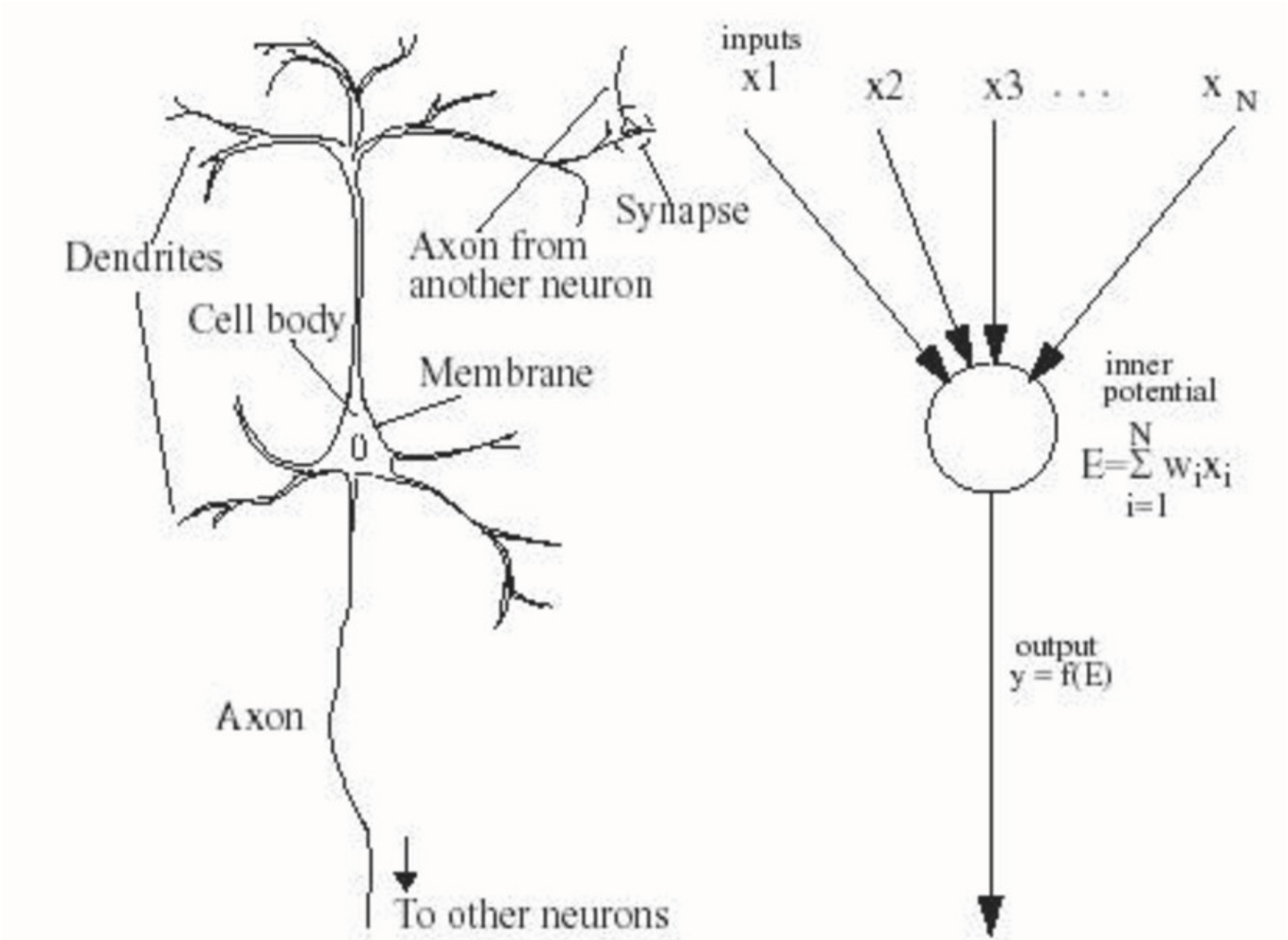
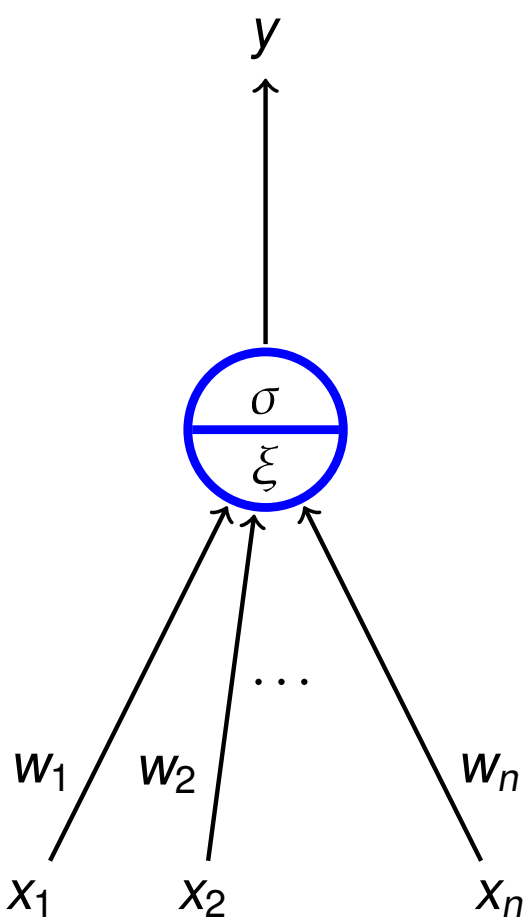


Figure 48.11(a), page 972, Campbell's *Biology, 5th Edition*

Biological and Mathematical neurons



Formal neuron (without bias)



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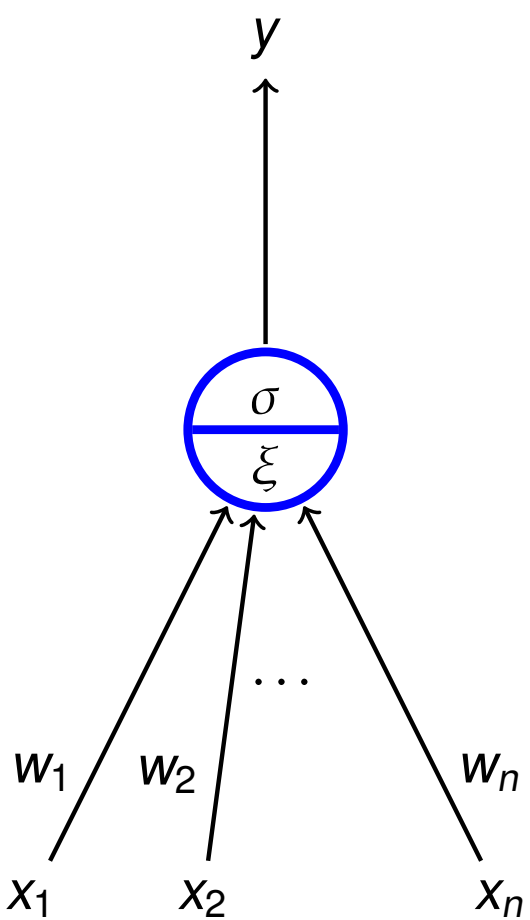

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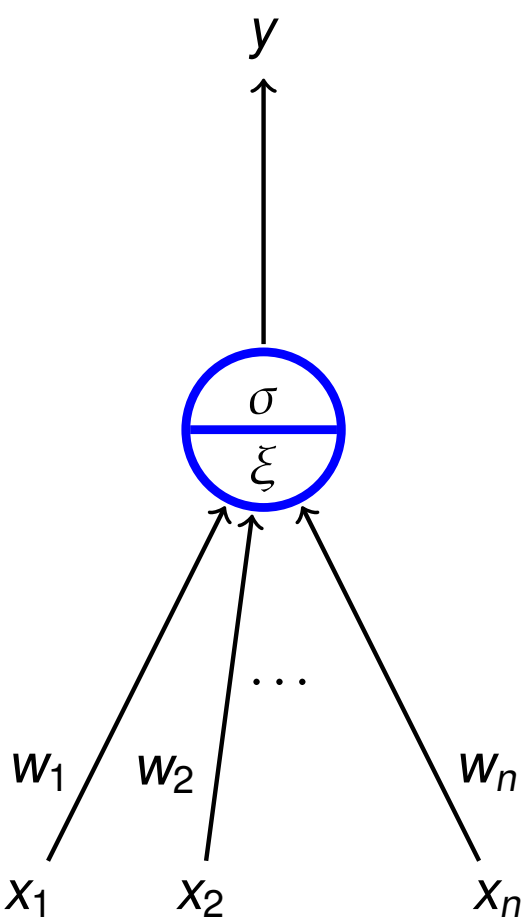

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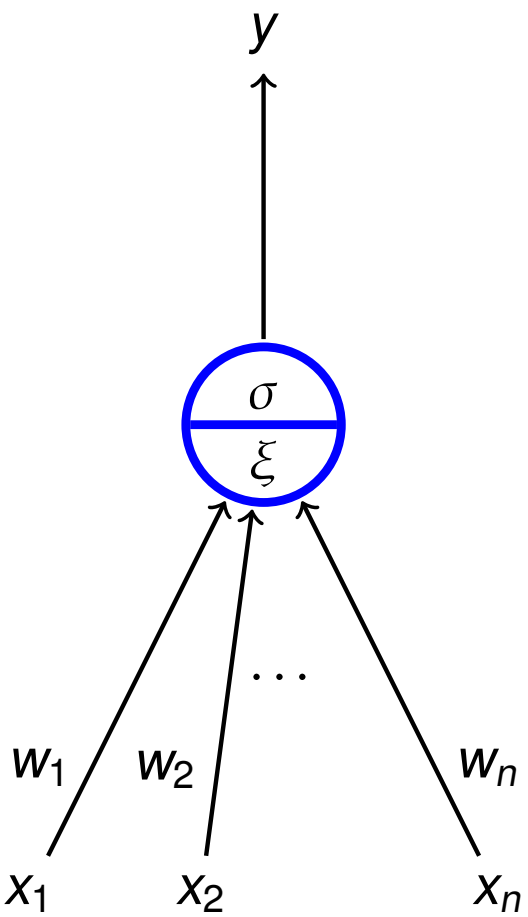

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- y is an **output** given by $y = \sigma(\xi)$ where σ is an **activation function**; e.g. a *unit step function*

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

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

Formal neuron (with bias)

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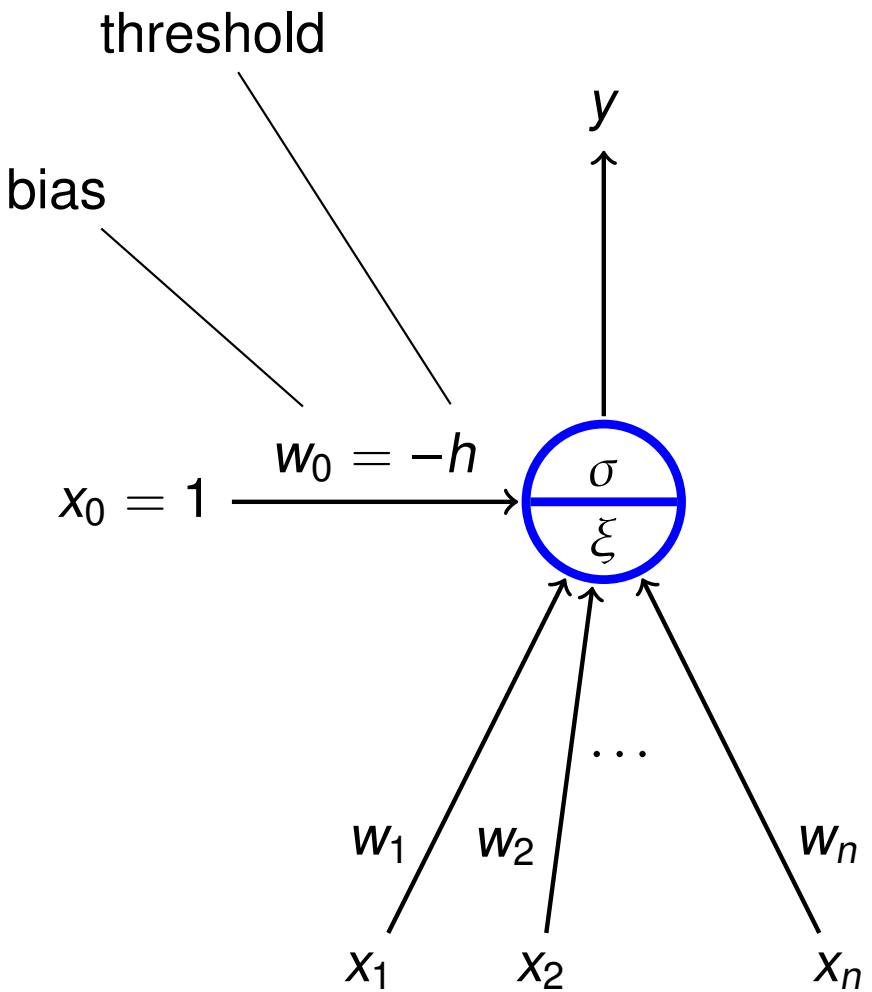

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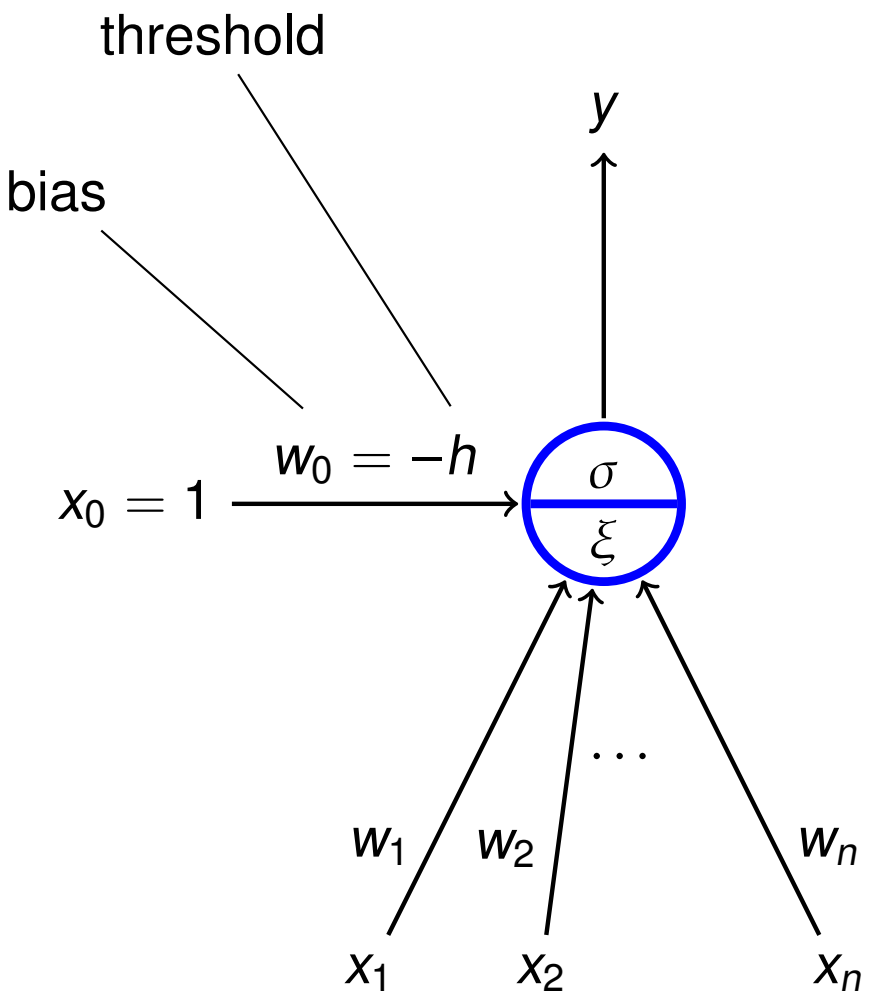

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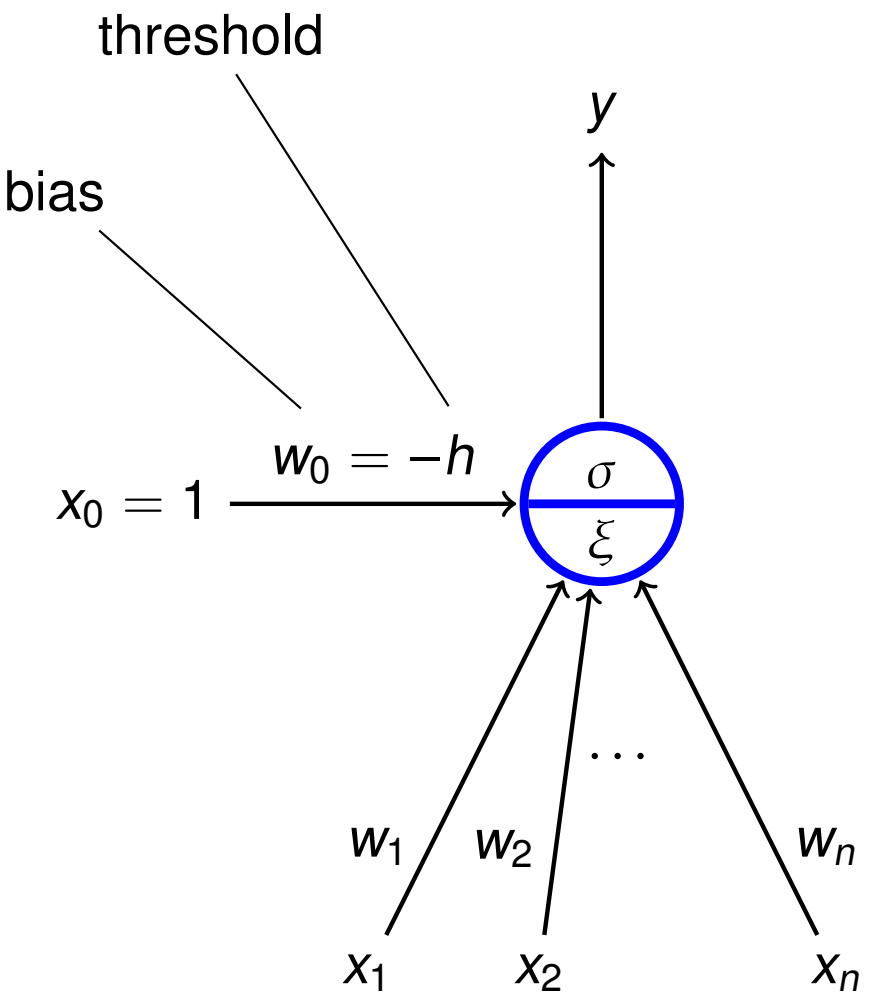

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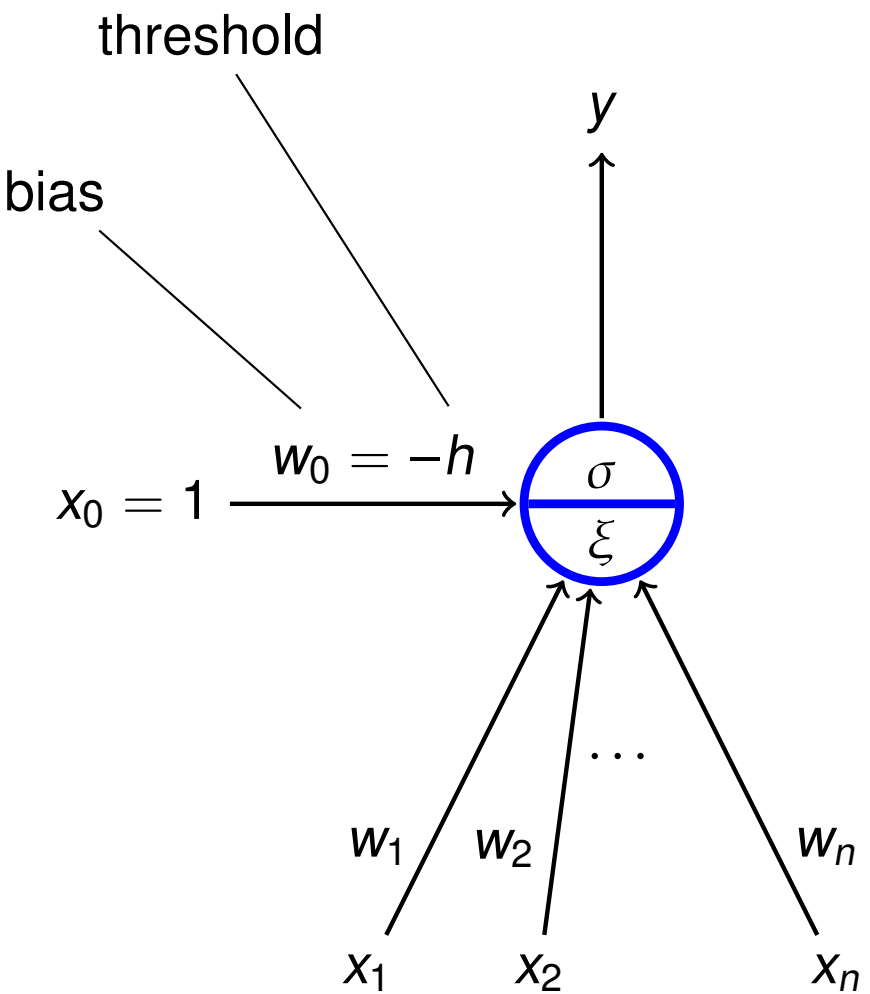

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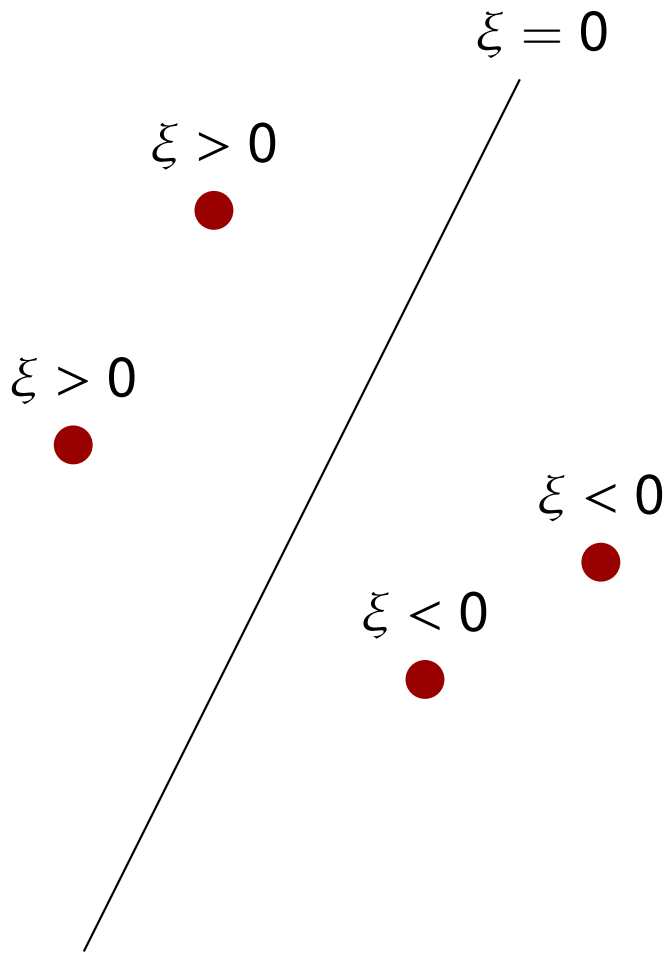
$$\sigma(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

(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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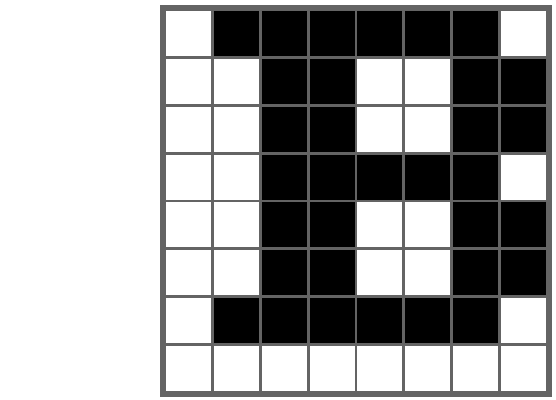
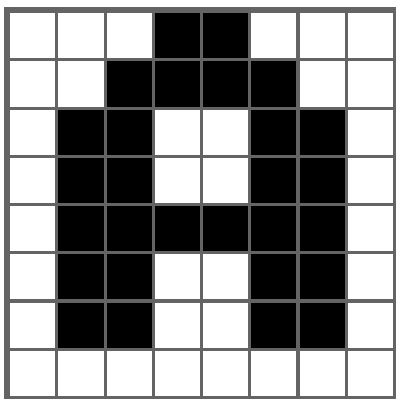
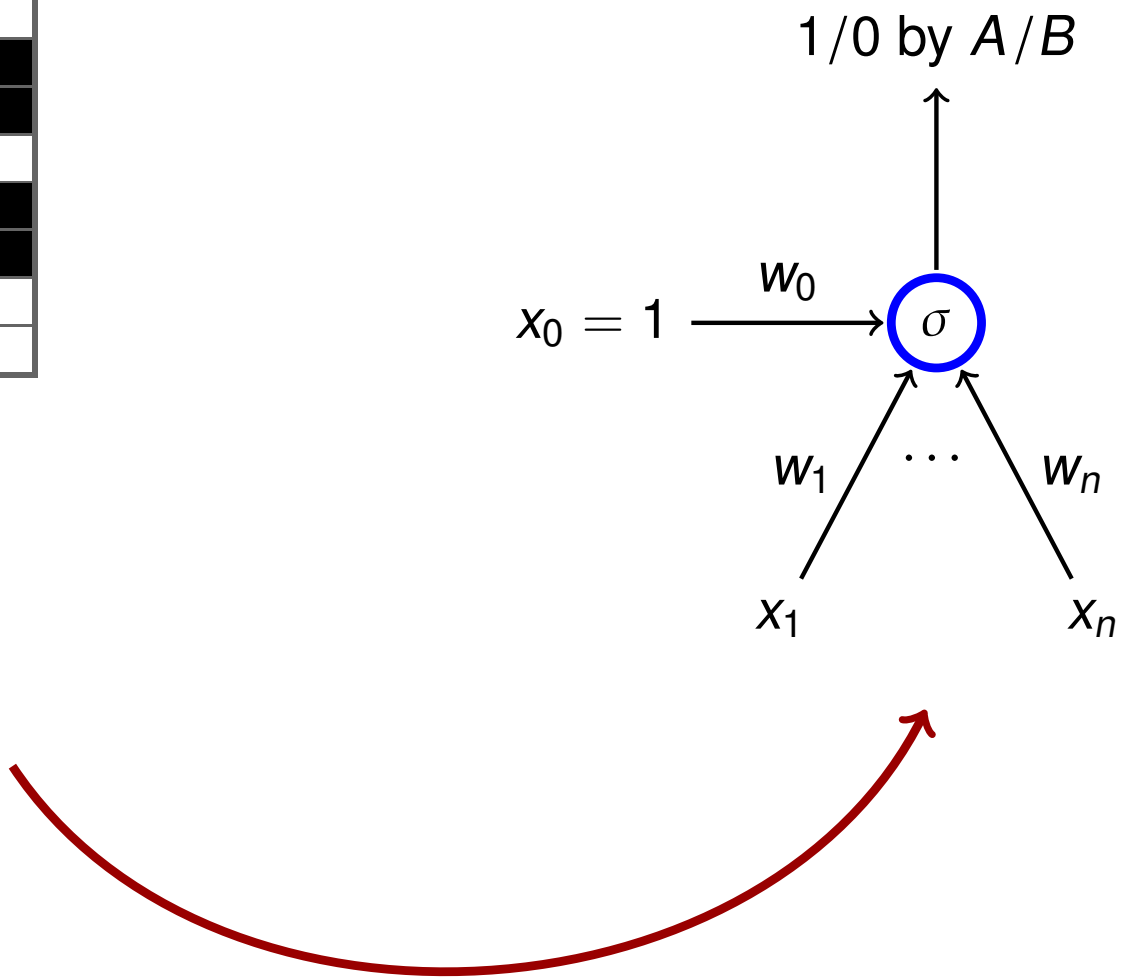
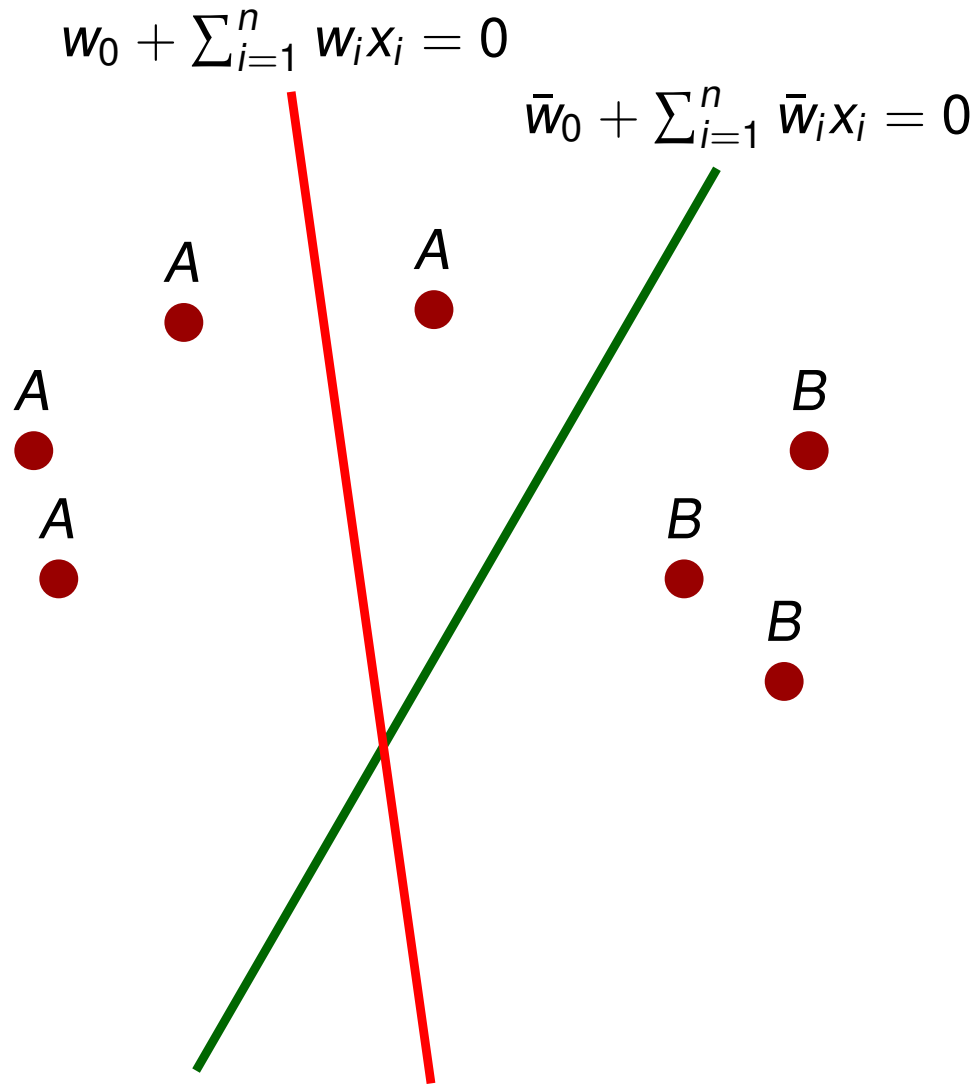






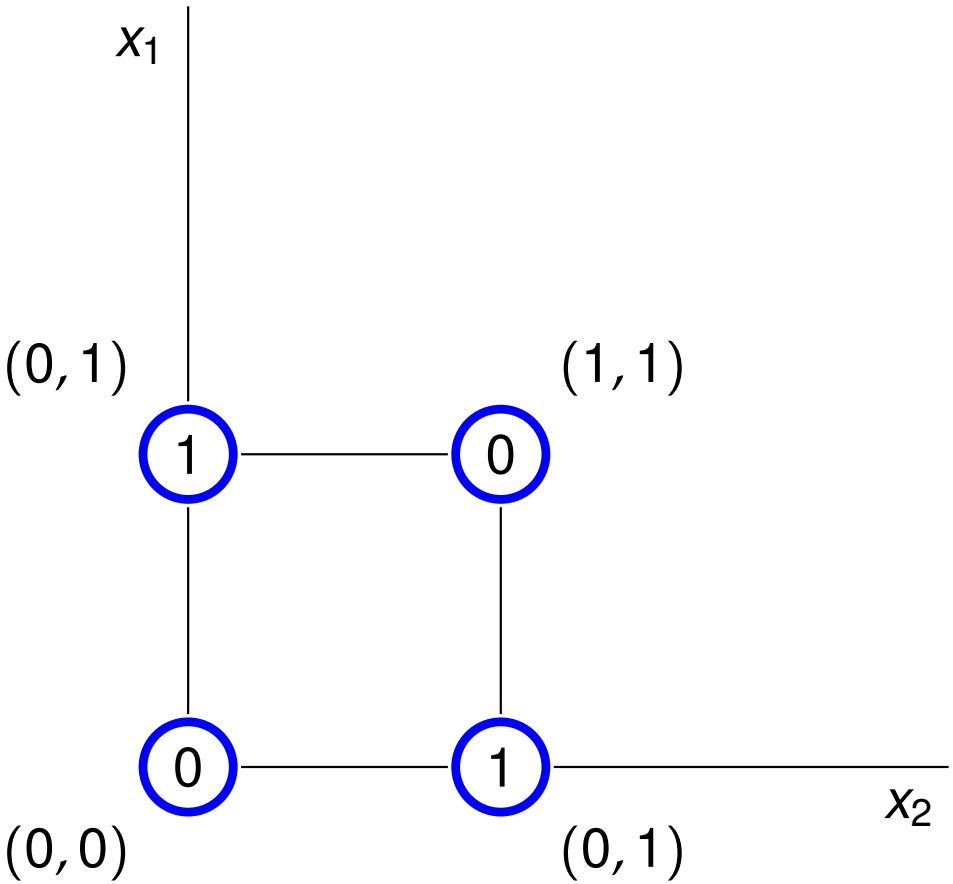
$n = 8 \cdot 8$, i.e. the number of pixels in the images. Inputs are binary vectors of dimension n (black pixel ≈ 1, white pixel ≈ 0).

Neuron and linear separation



- 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.

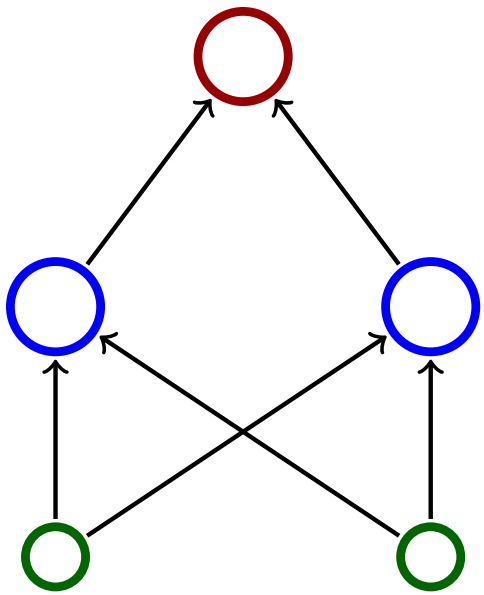
Architecture

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

We distinguish several categories of neurons:

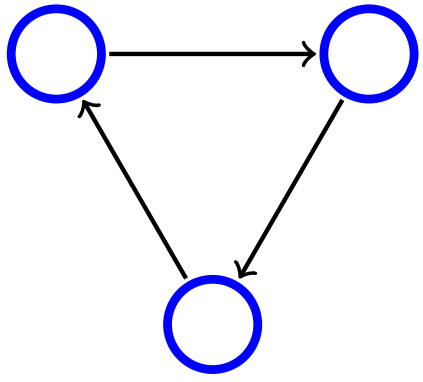
- Output neurons
- Hidden neurons
- Input neurons

(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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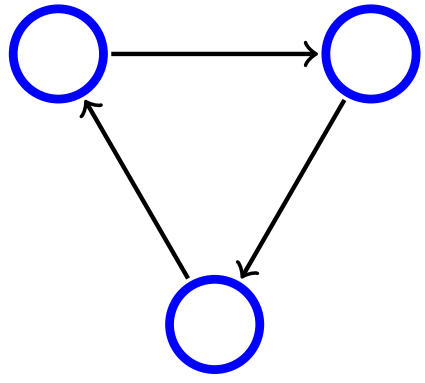
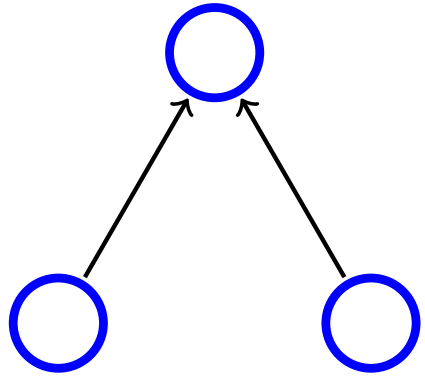
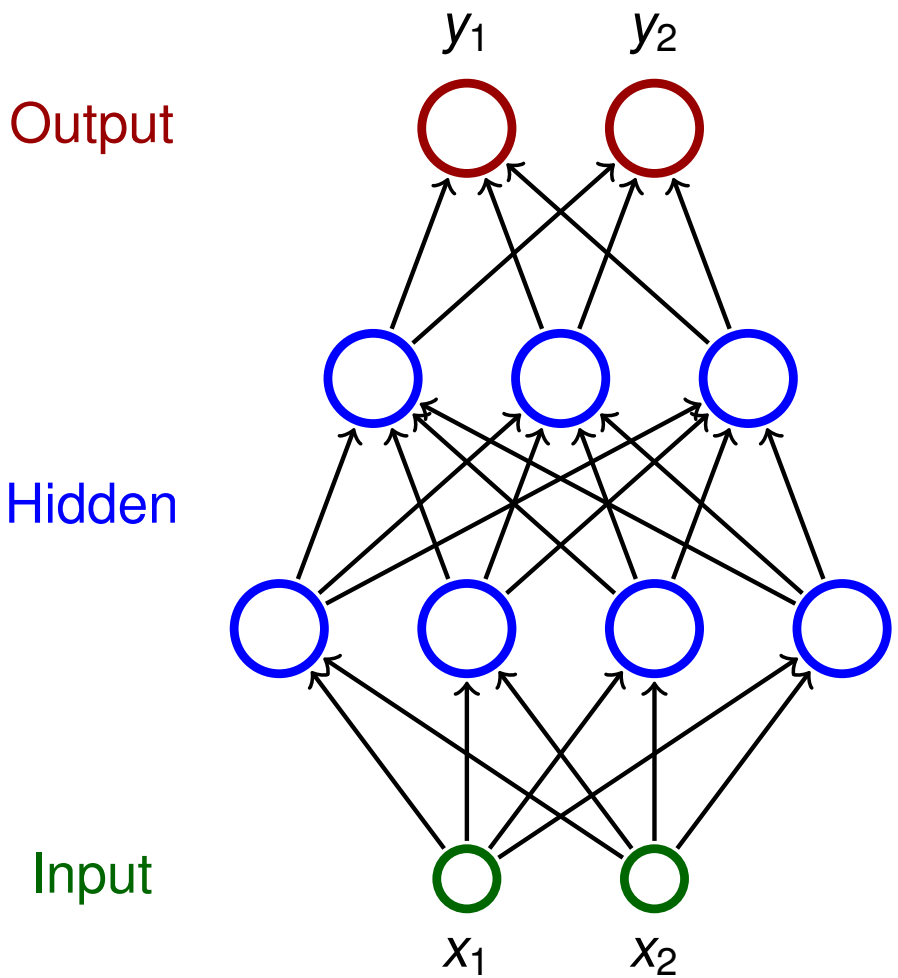


- Otherwise it is **acyclic** (feed-forward)



Architecture – Multilayer Perceptron (MLP)



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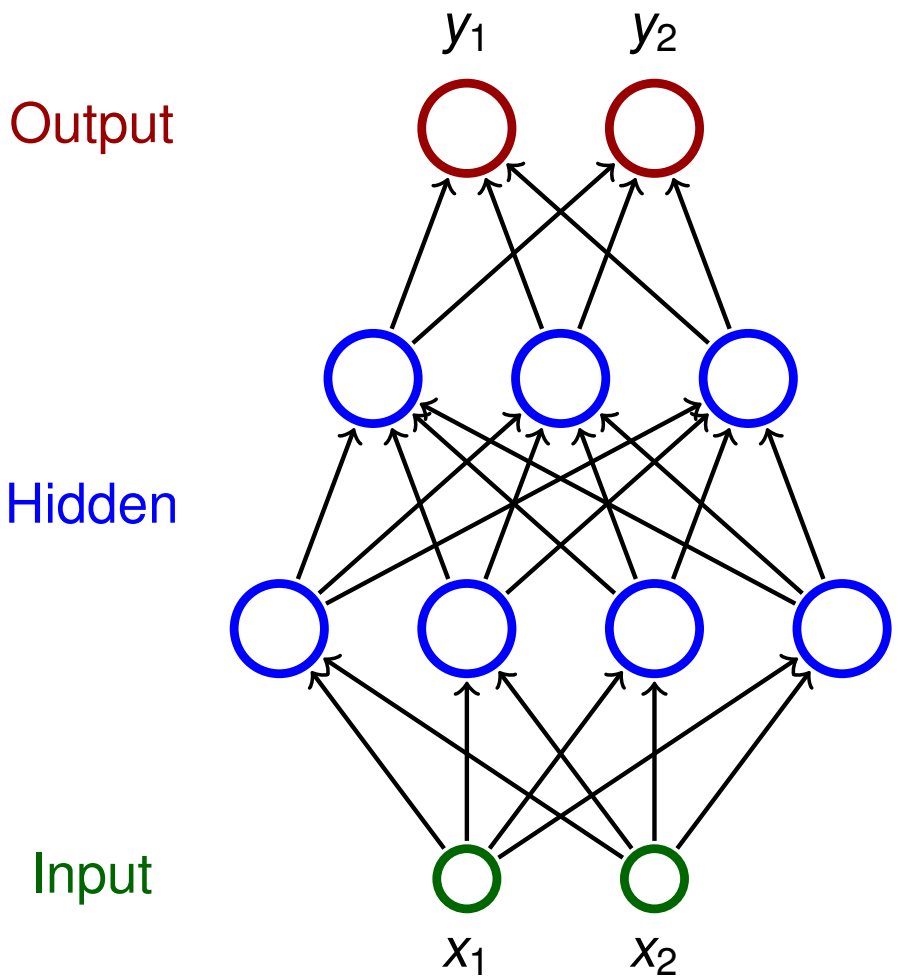

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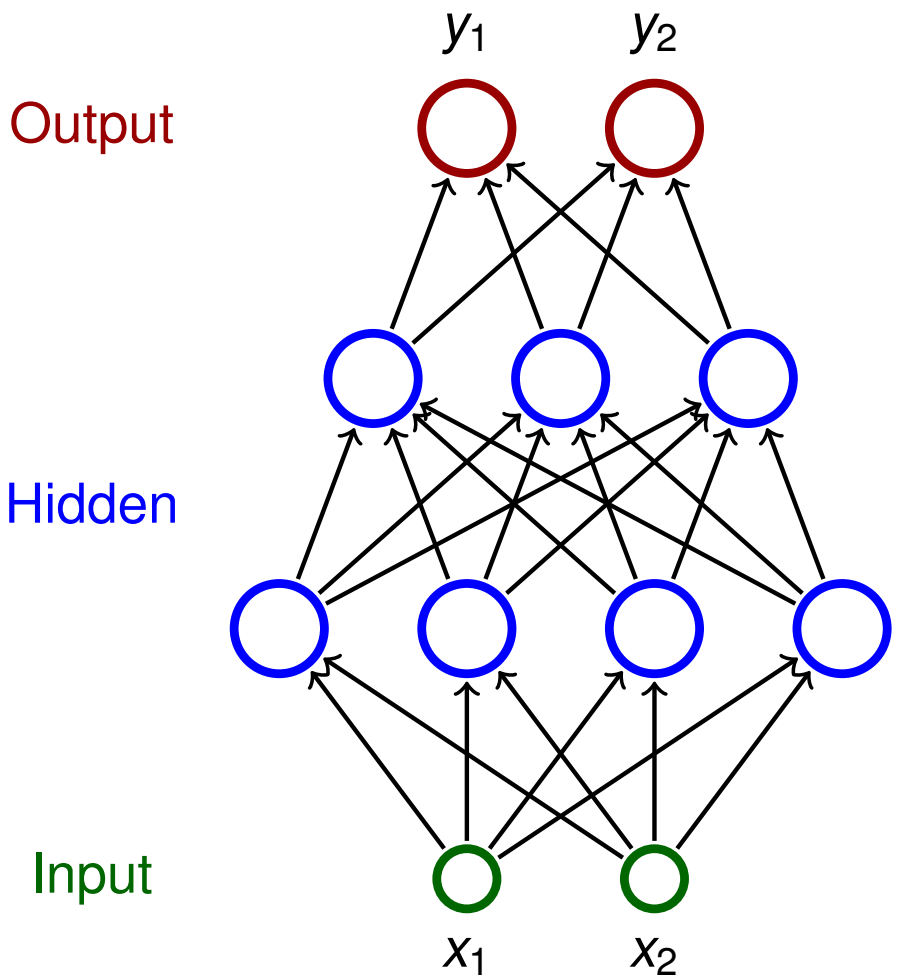

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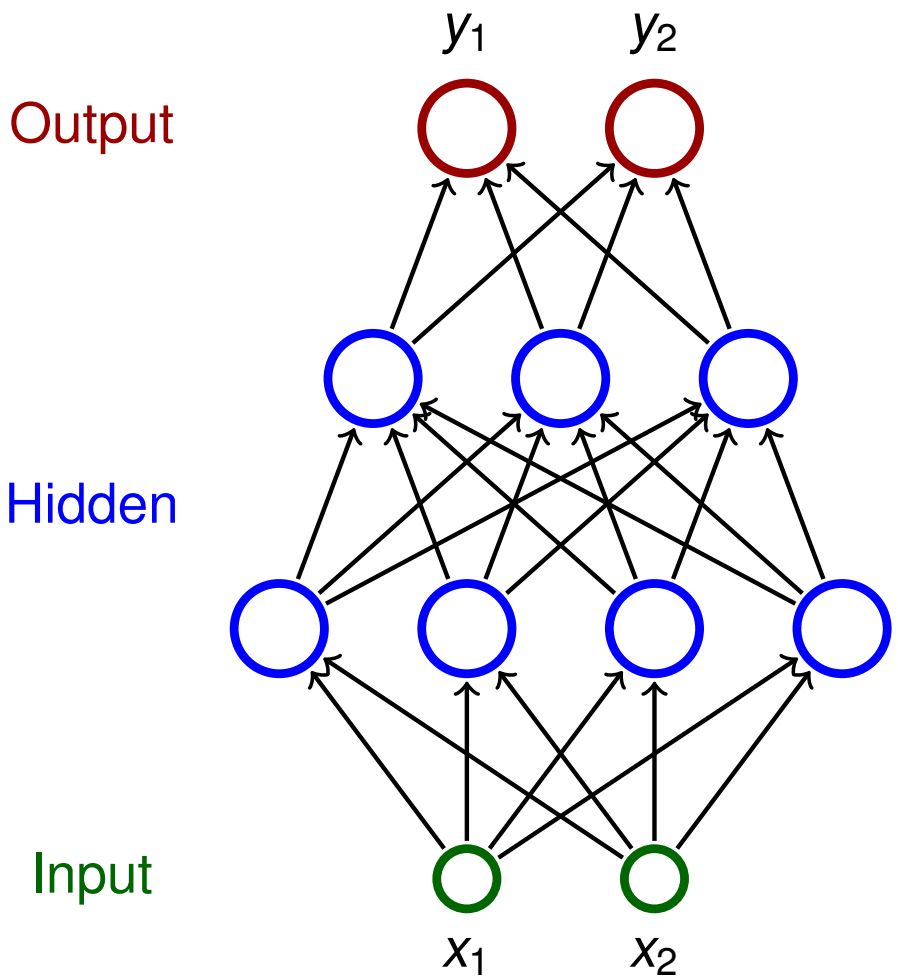

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- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

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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 *$F : A \to B$ 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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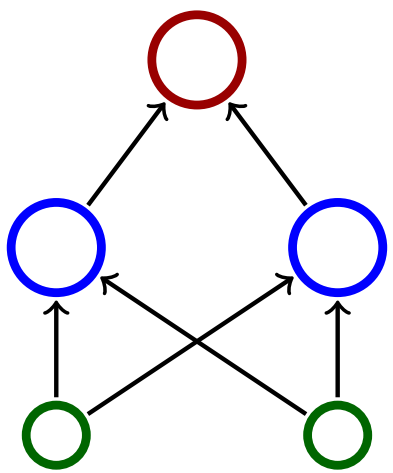
Example 1

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



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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.

Activity – inner potential and activation functions

There are many activation functions, typical examples:

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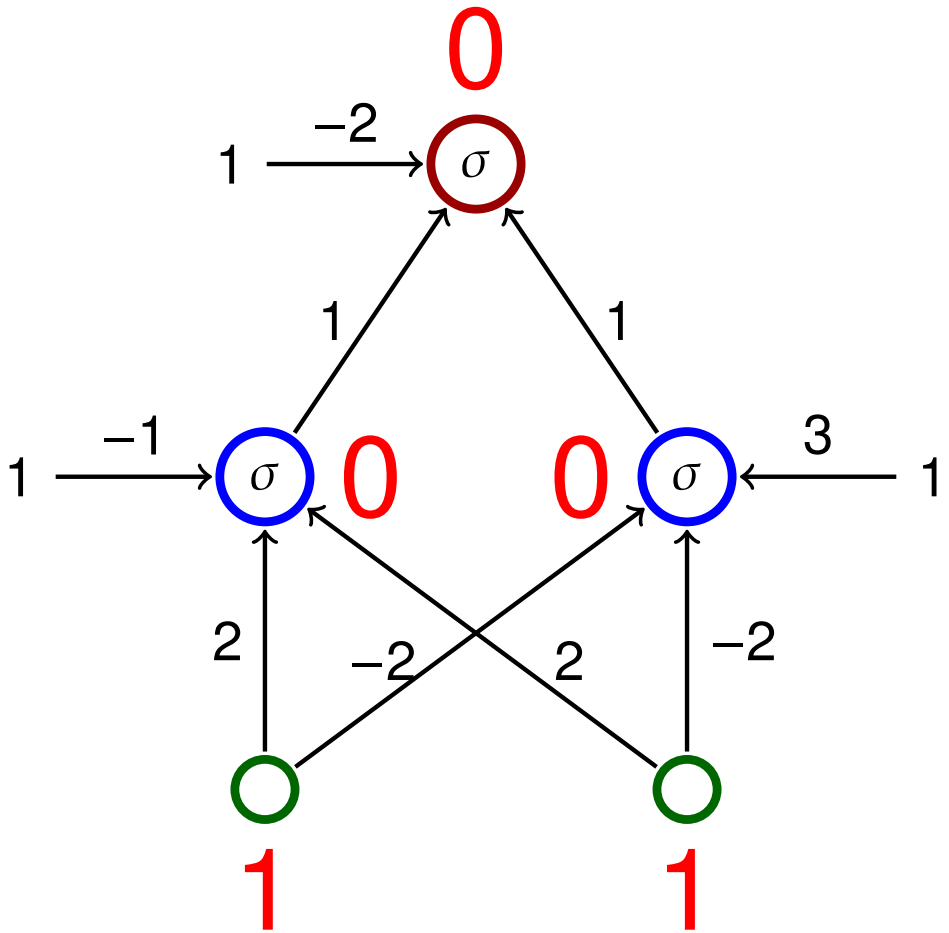
- (Logistic) sigmoid

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

- Hyperbolic tangens

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

Activity – XOR



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

x_1	x_2	y
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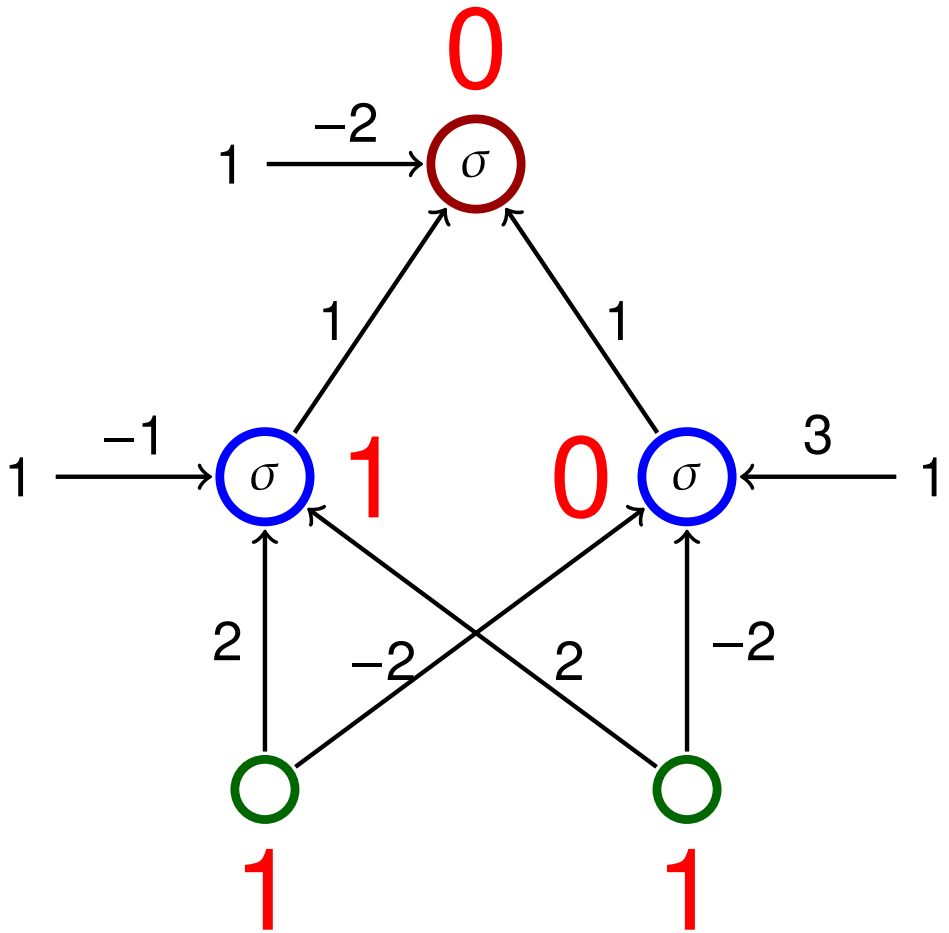

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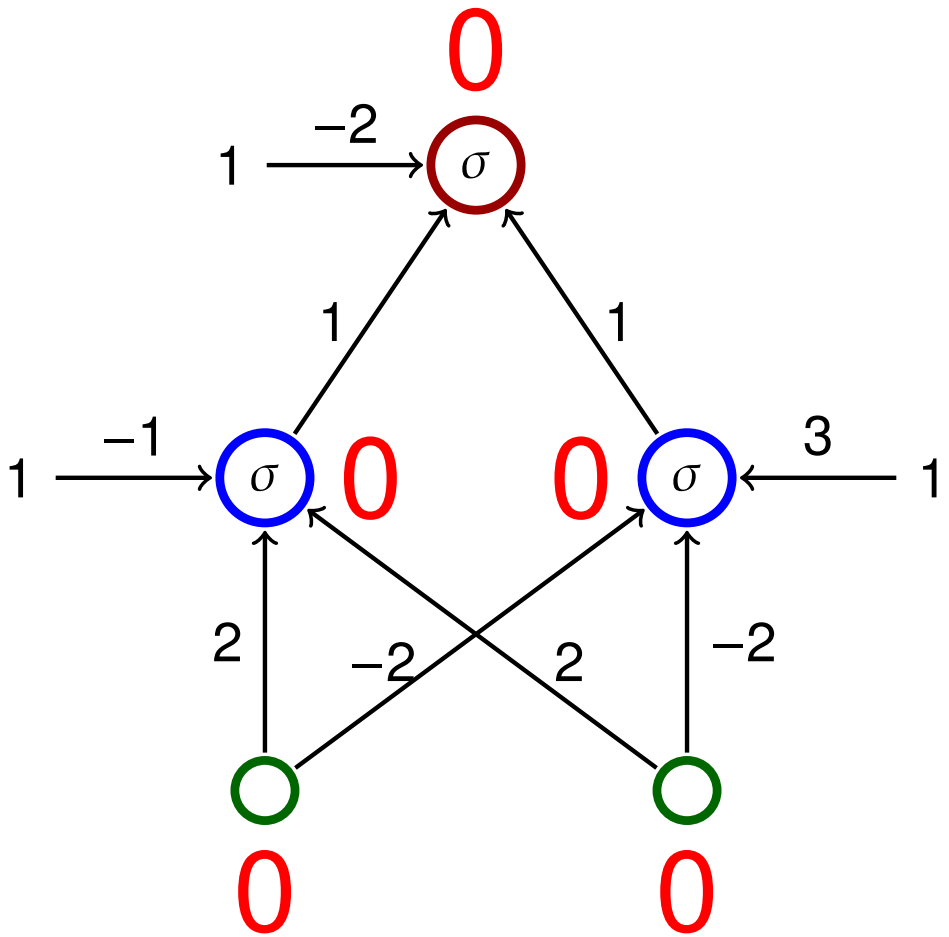

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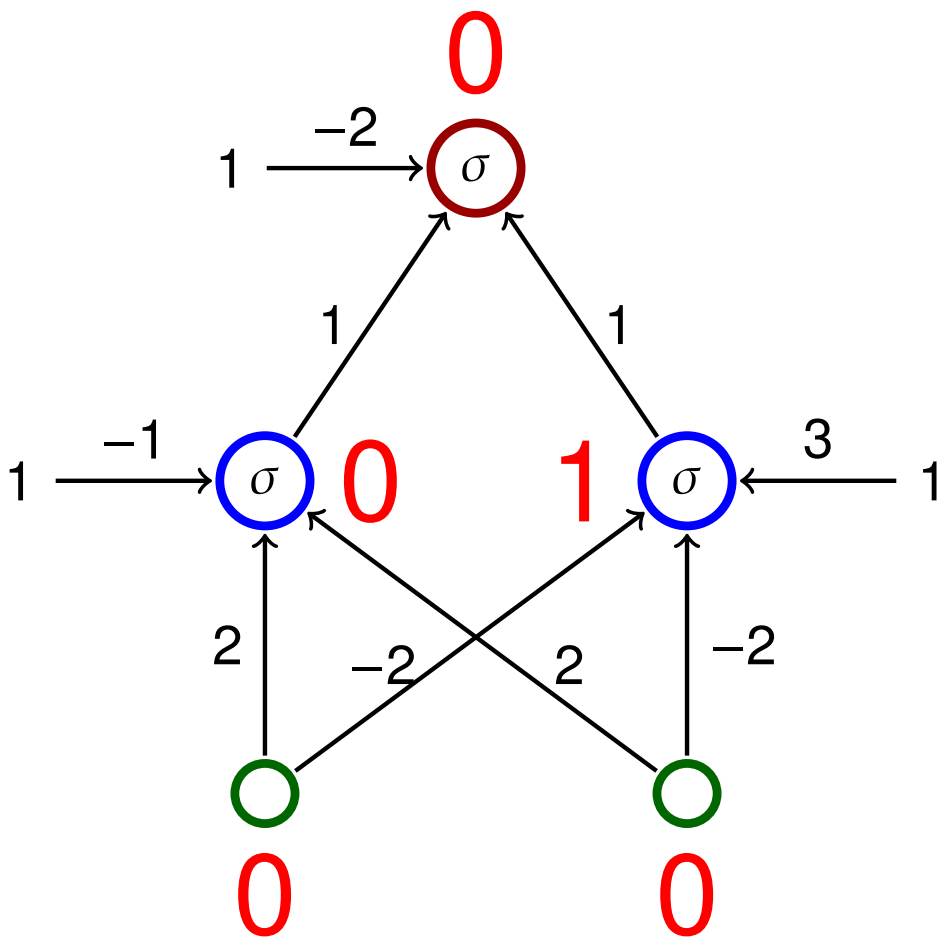

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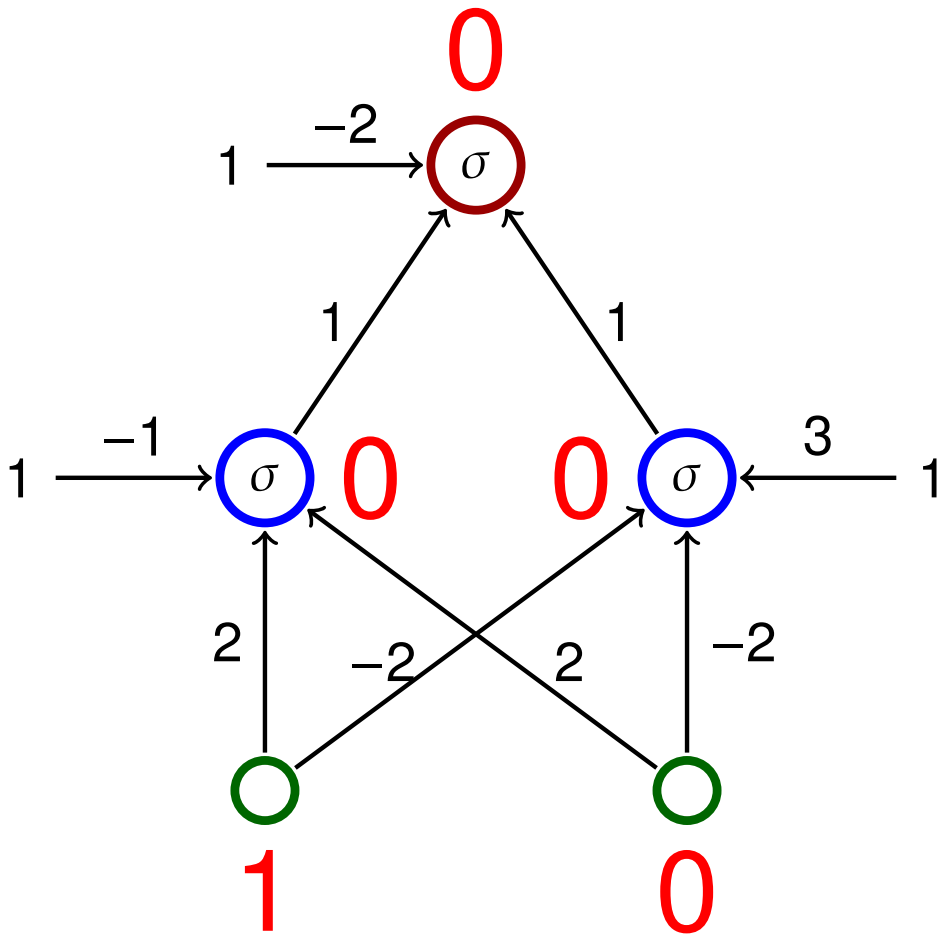

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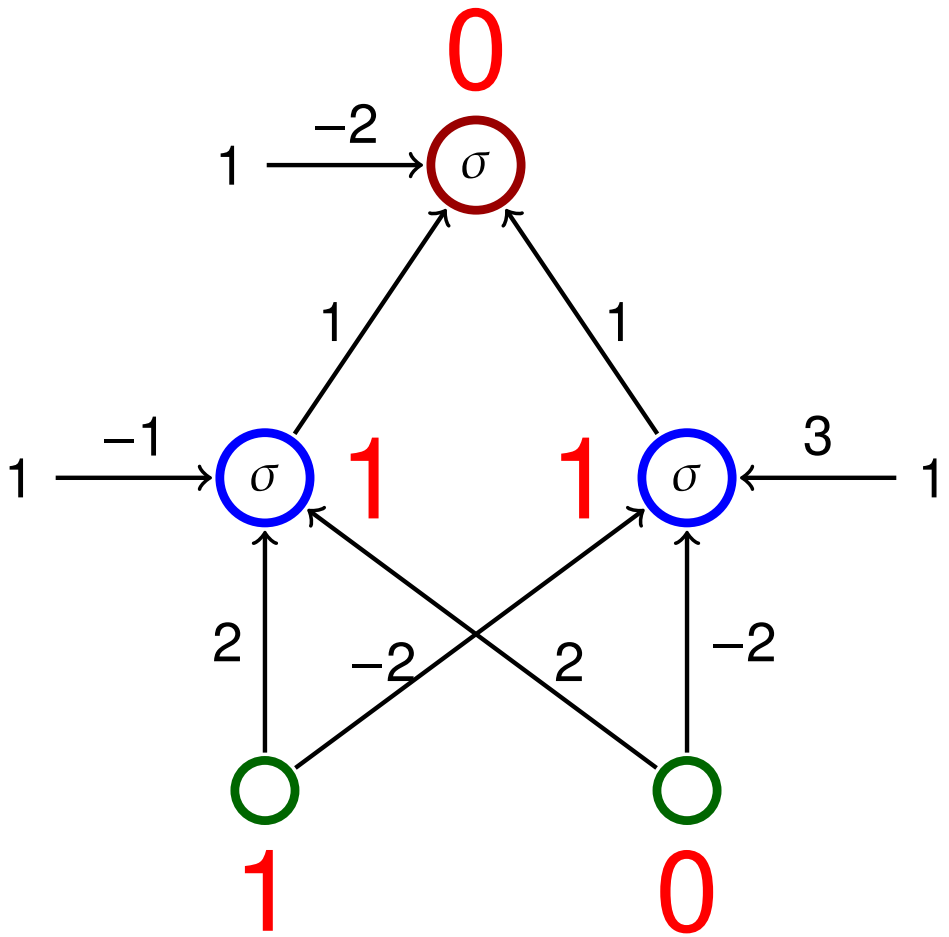

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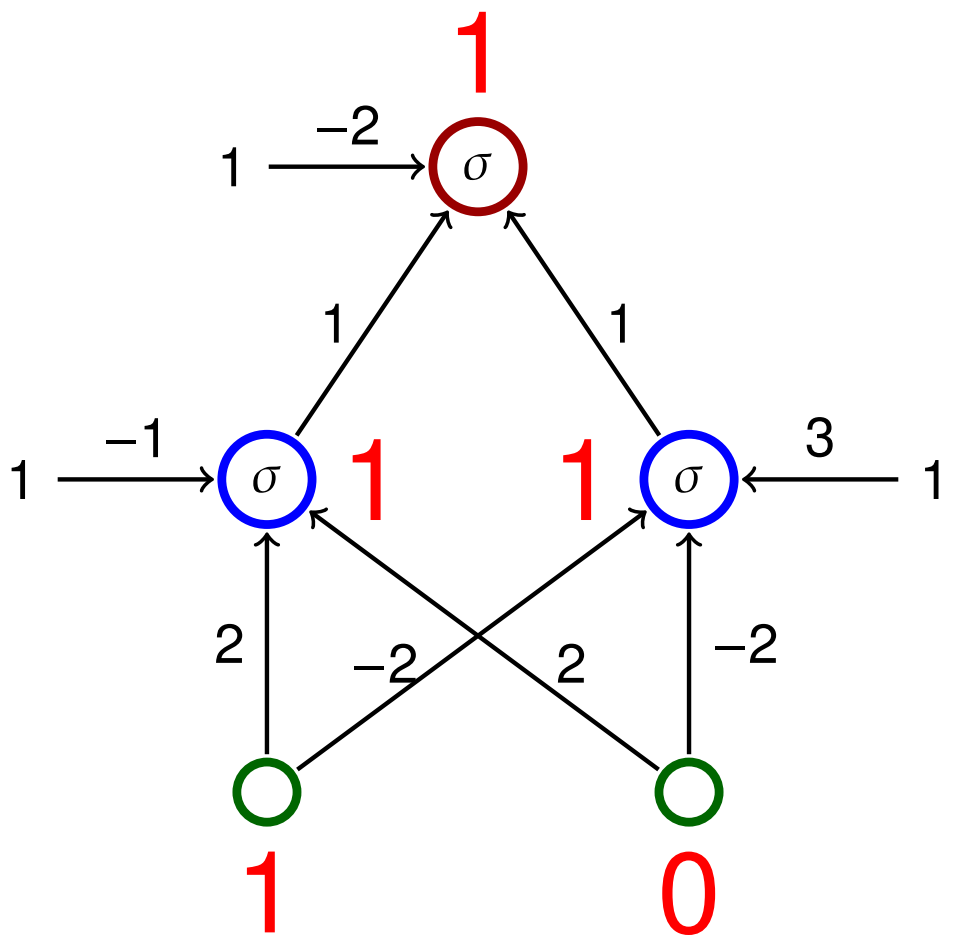

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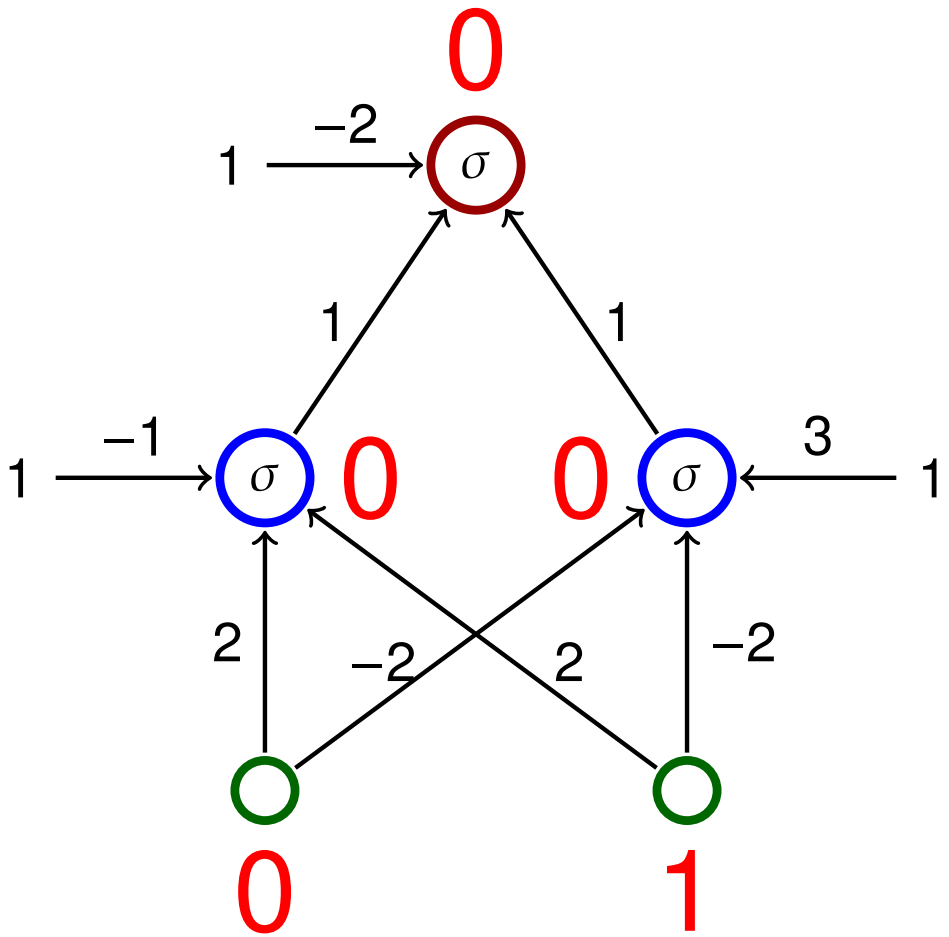

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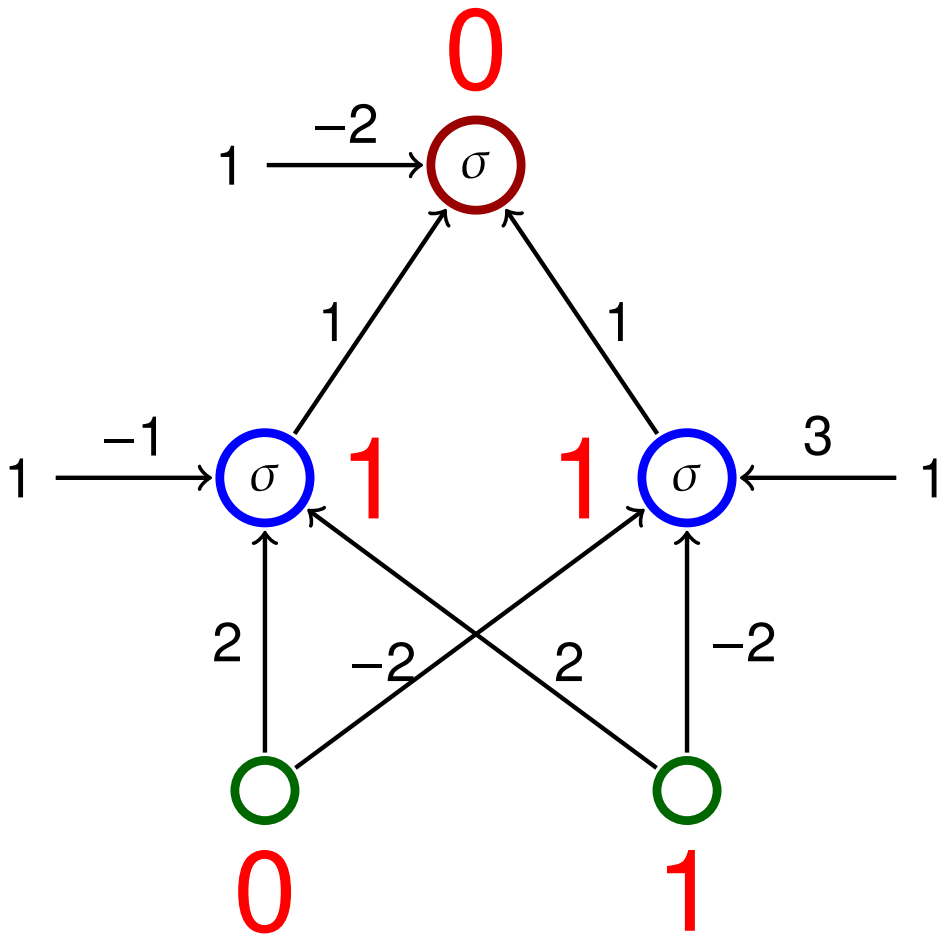

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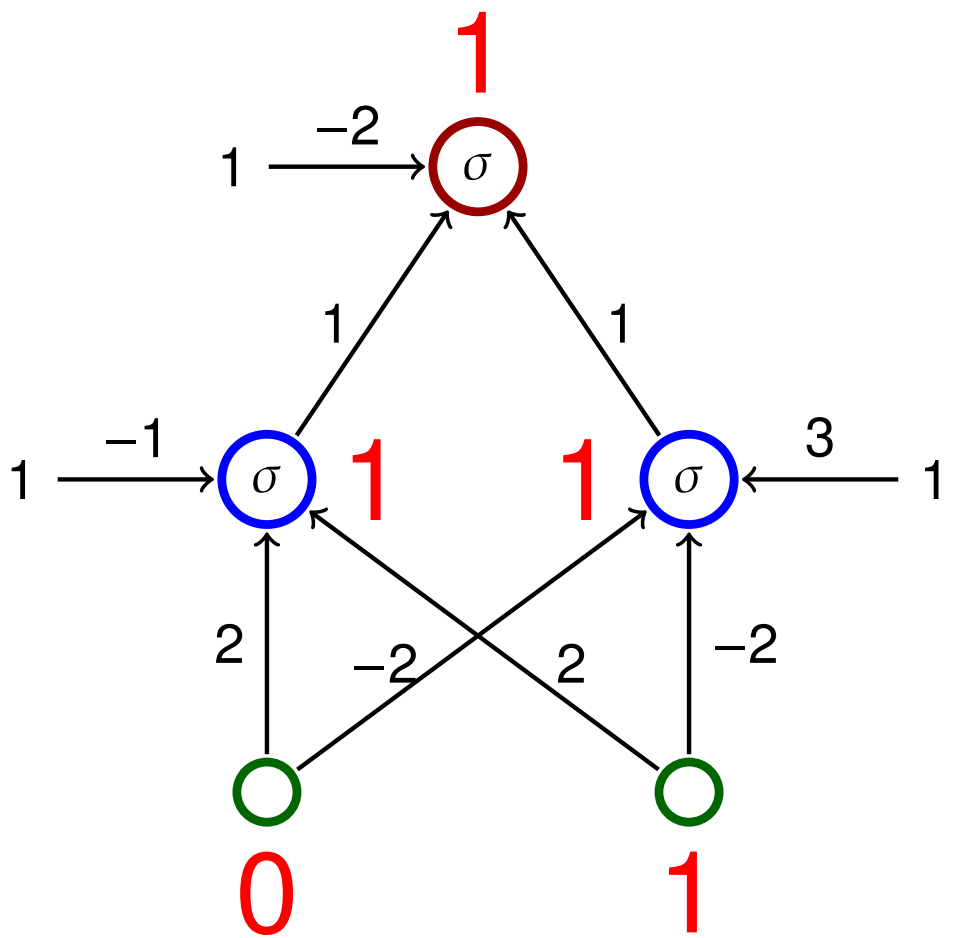

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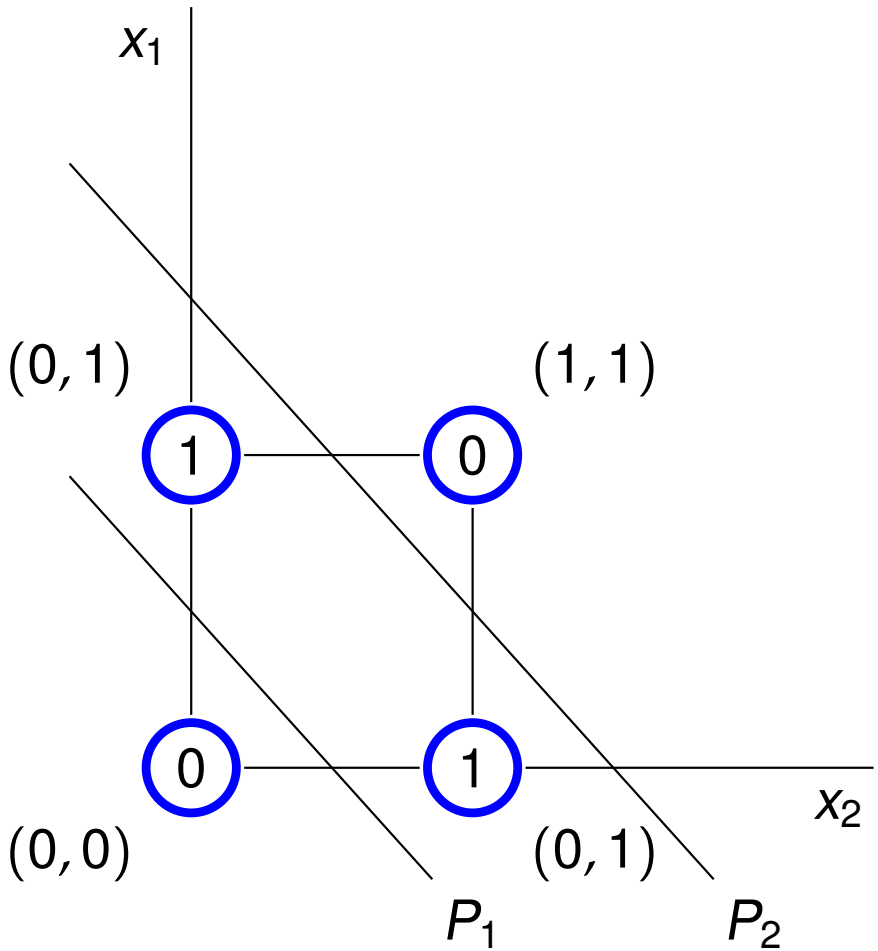
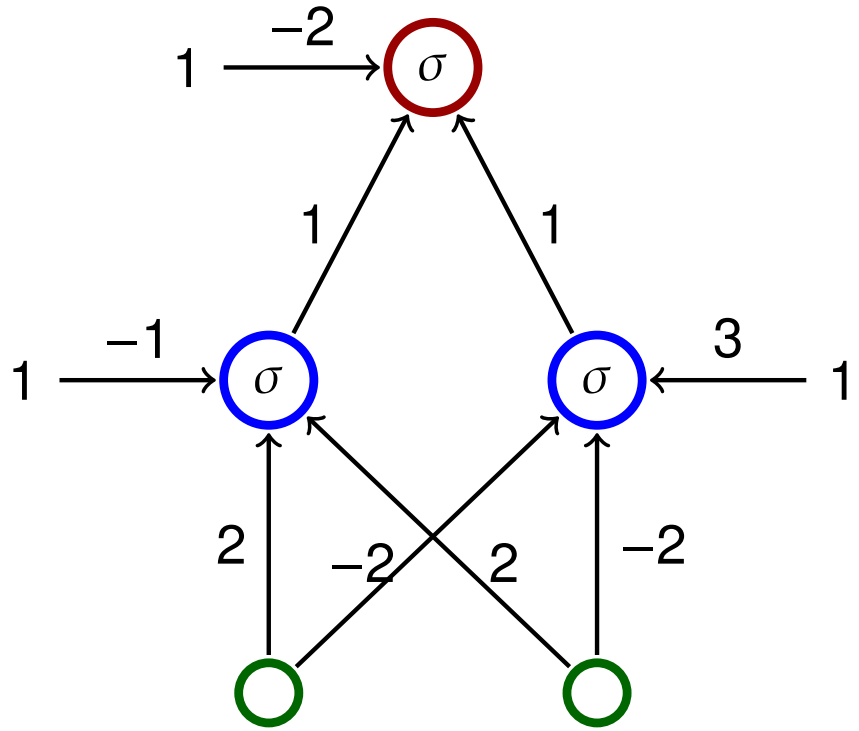
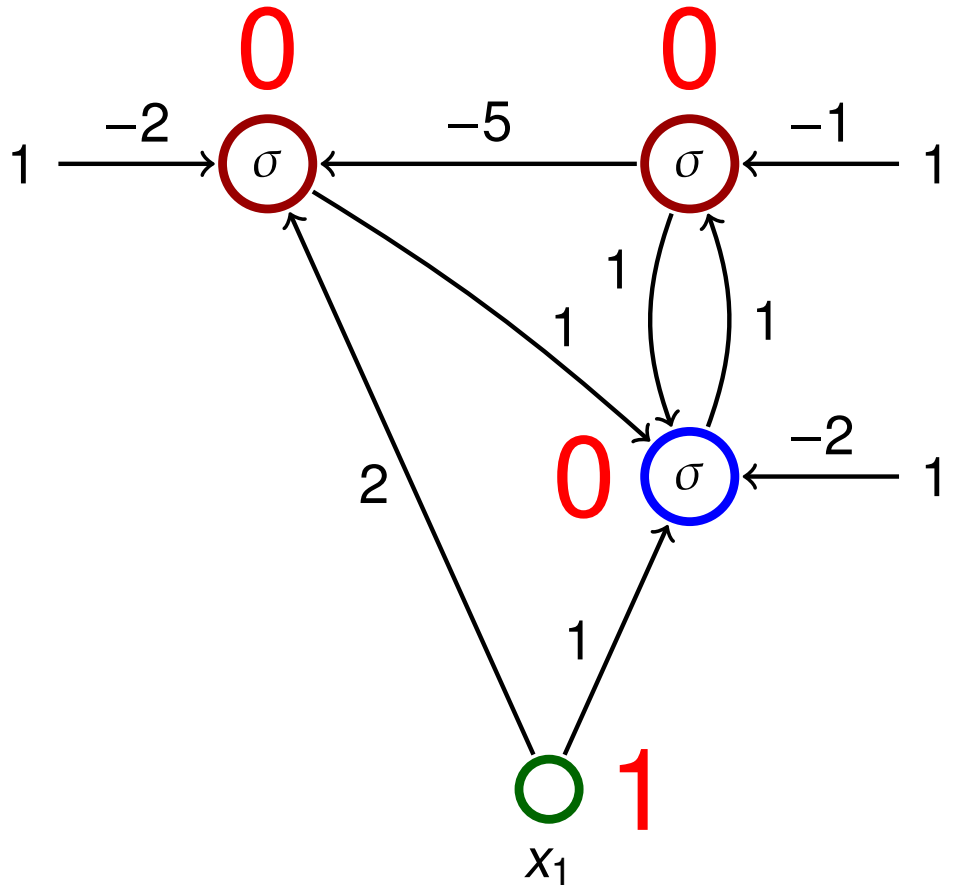
Activity – MLP and linear separation





- 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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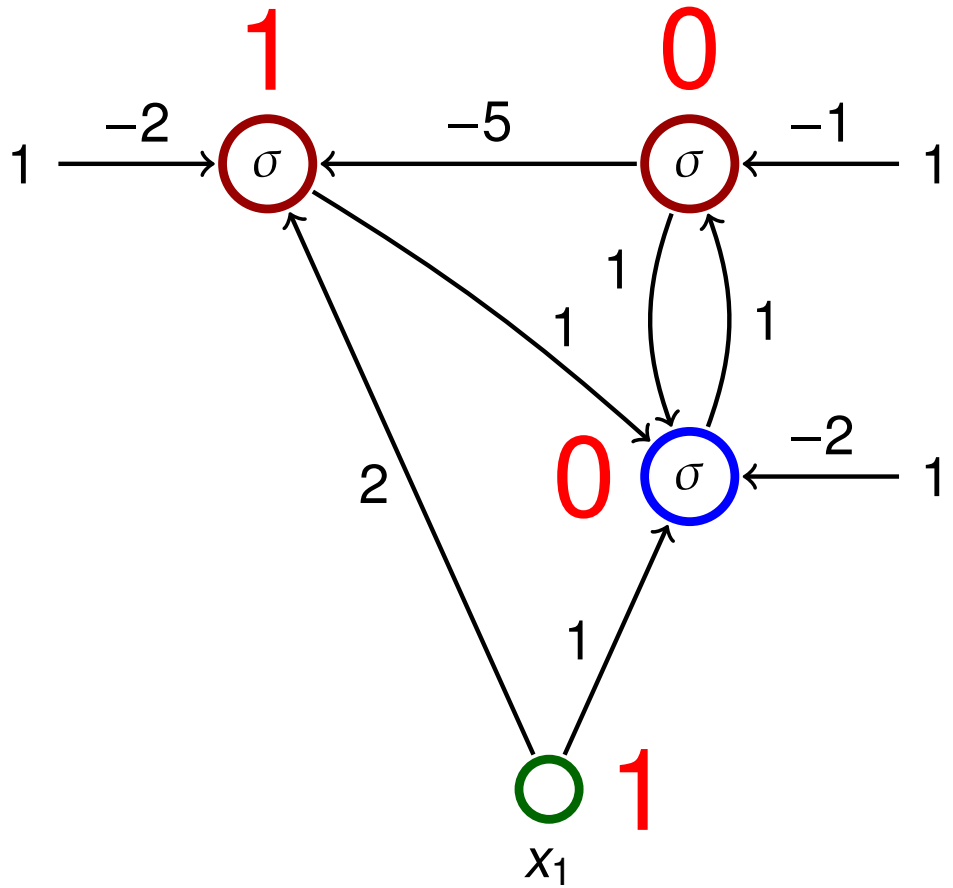

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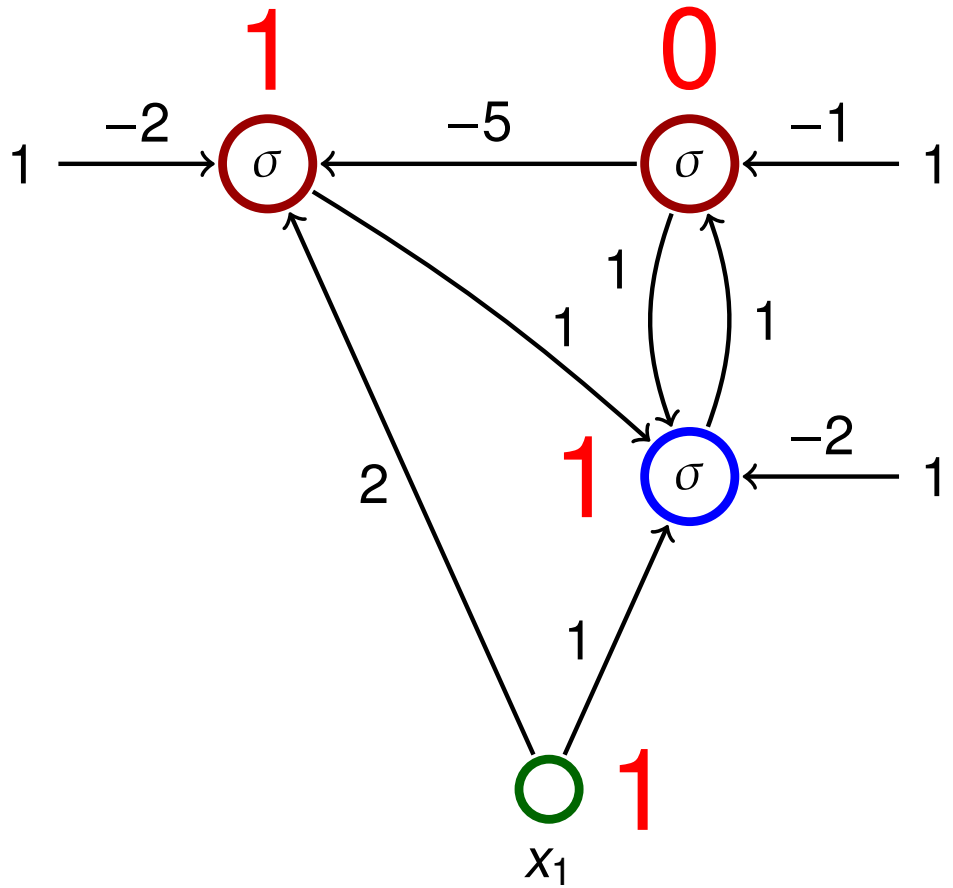

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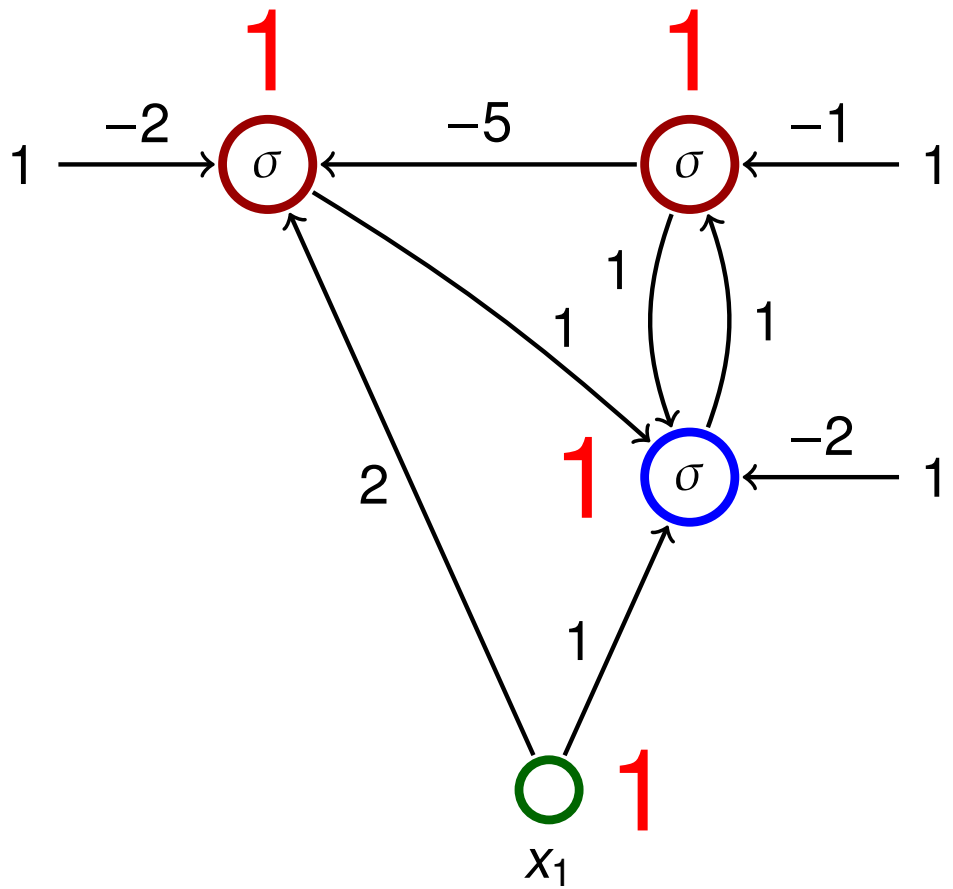

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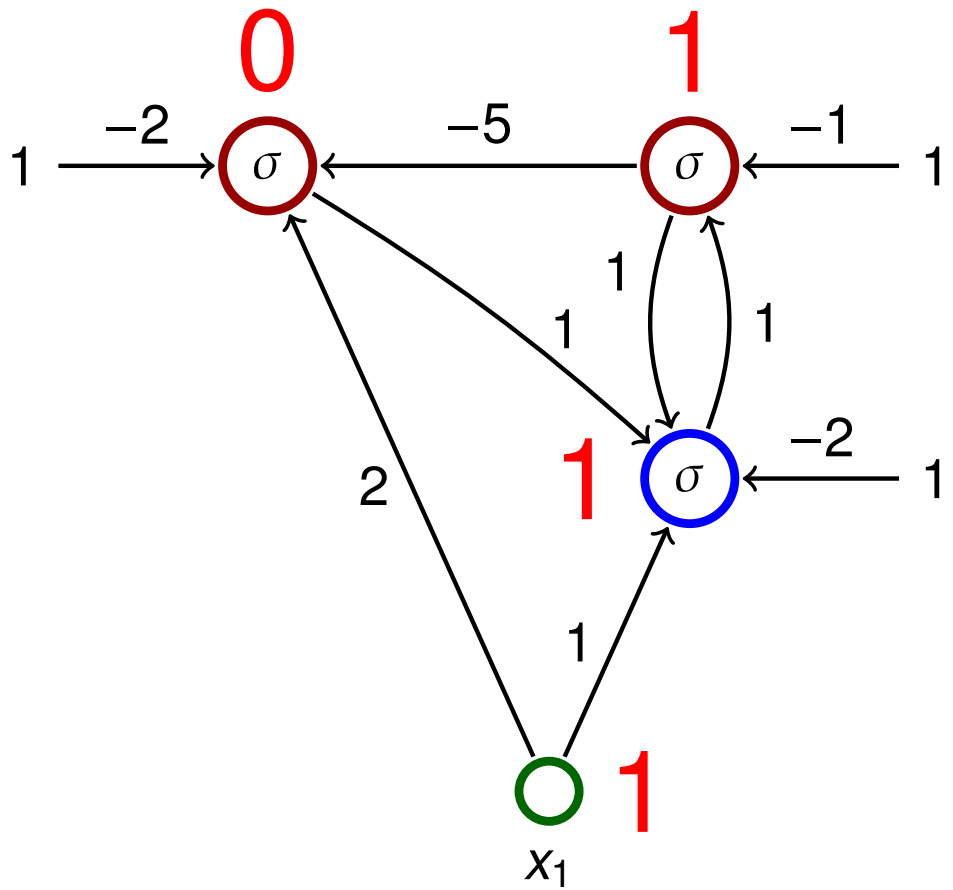

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- **Weight-space** of a network is a set of all configurations.
- **initial configuration**
  weights can be initialized randomly or using some sophisticated algorithm

Learning algorithms

Learning rule for weight adaptation.
(the goal is to find a configuration in which the network computes a desired function)

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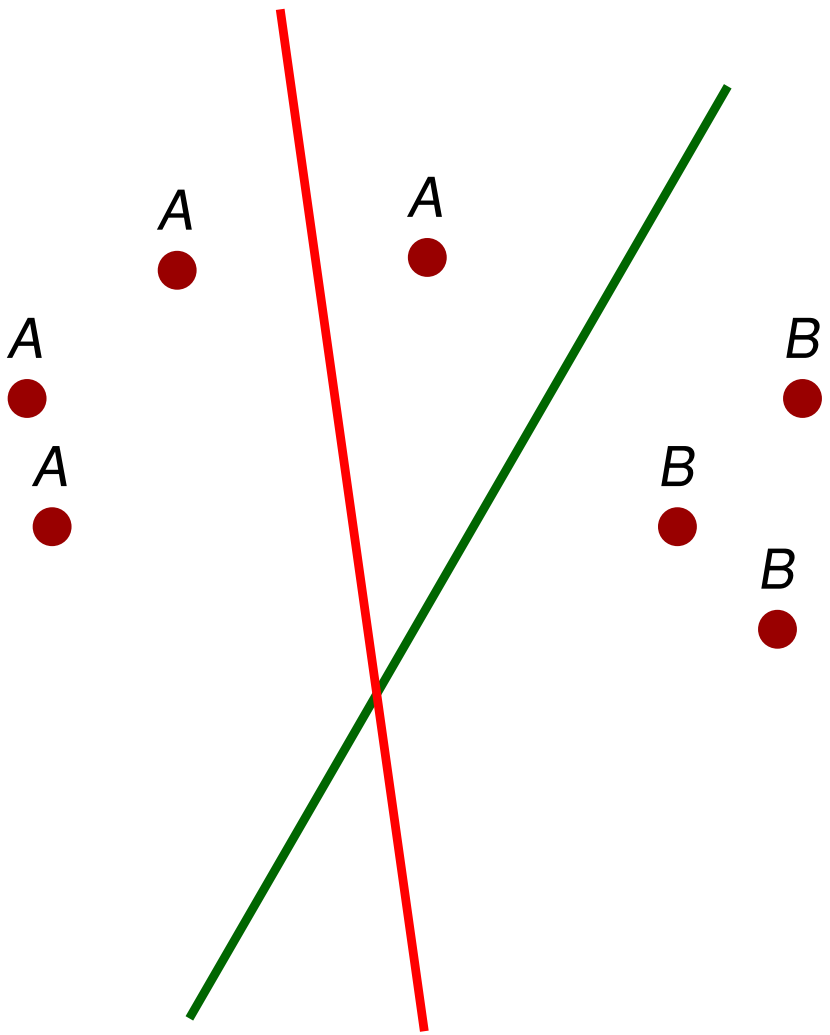
- Unsupervised learning
  - The training set contains only inputs.
  - The goal is to determine distribution of the inputs (clustering, deep belief networks, etc.)

Supervised learning – illustration



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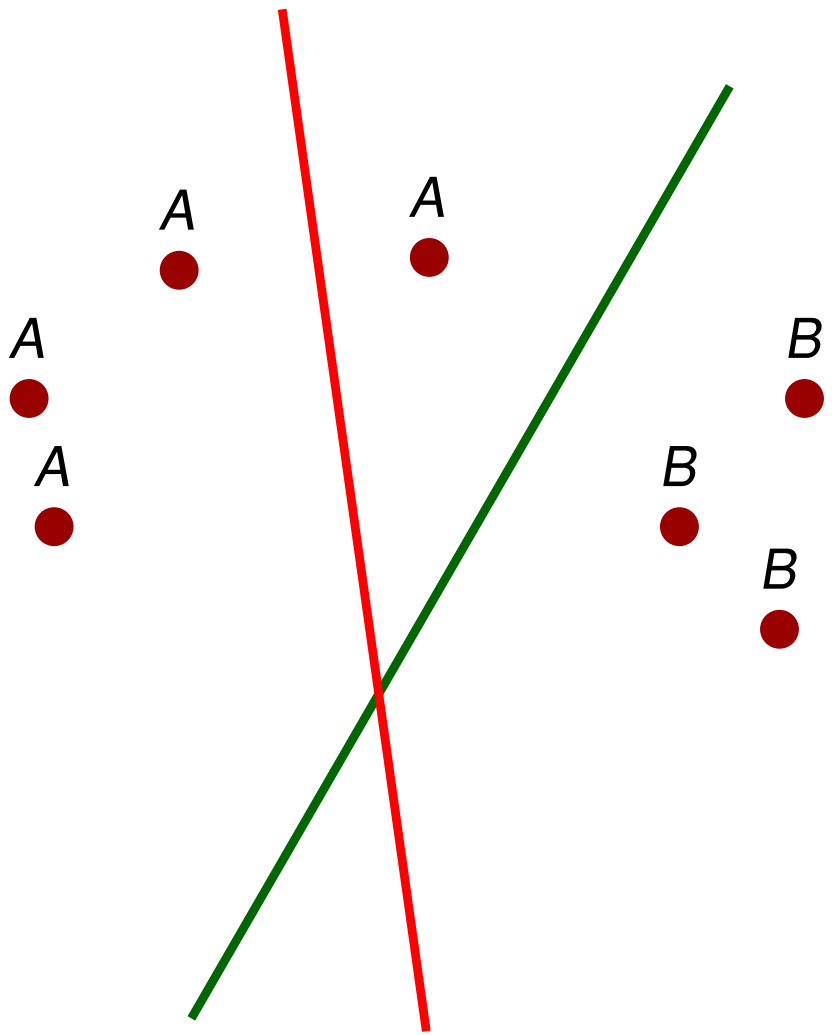

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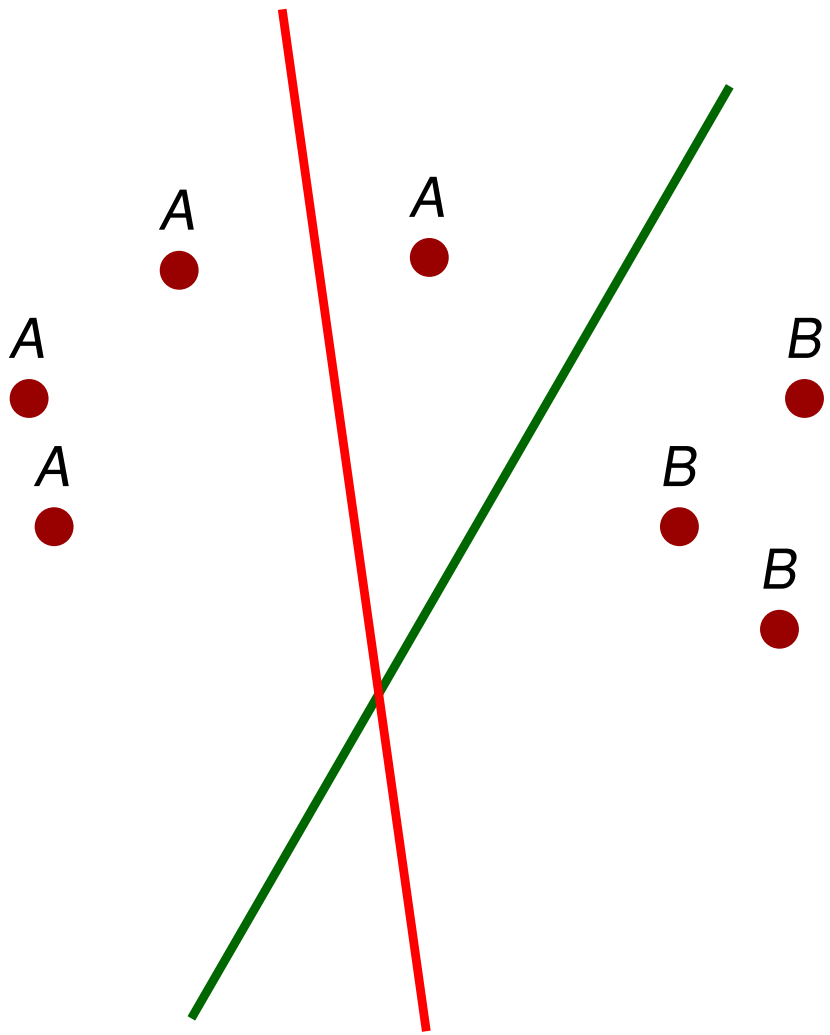

- classification in the plane using a single neuron
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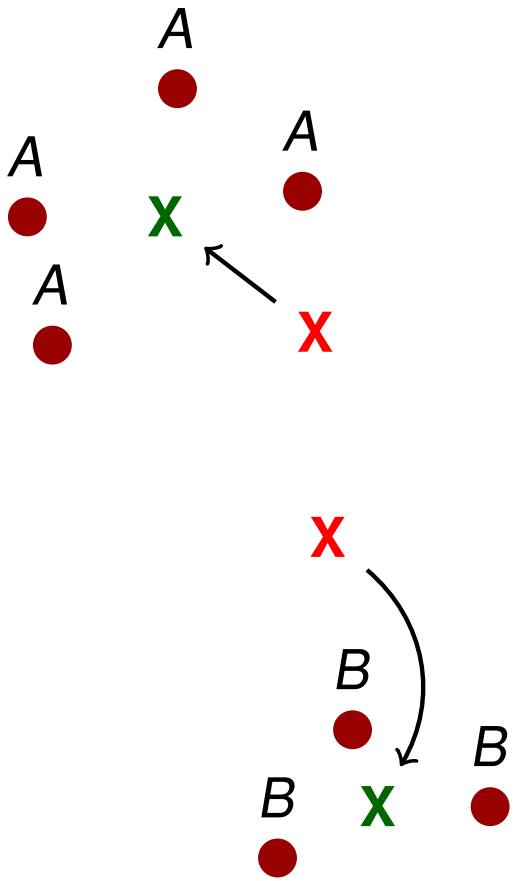
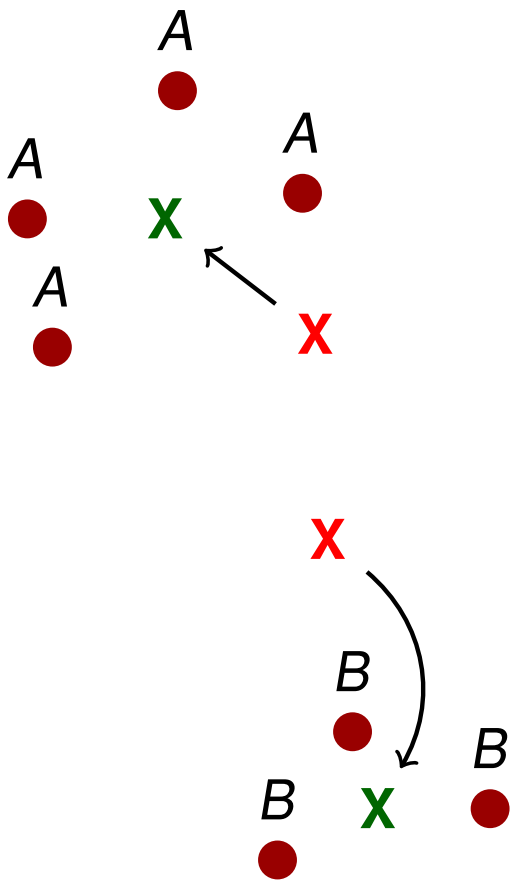
- the algorithm considers examples one after another
- whenever an incorrectly classified point is considered, the learning algorithm turns the line in the direction of the point

Unsupervised learning – illustration



- we search for two *centres* of clusters

Unsupervised learning – illustration



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- red crosses correspond to potential centres before application of the learning algorithm, green ones after the application

Summary – Advantages of neural networks

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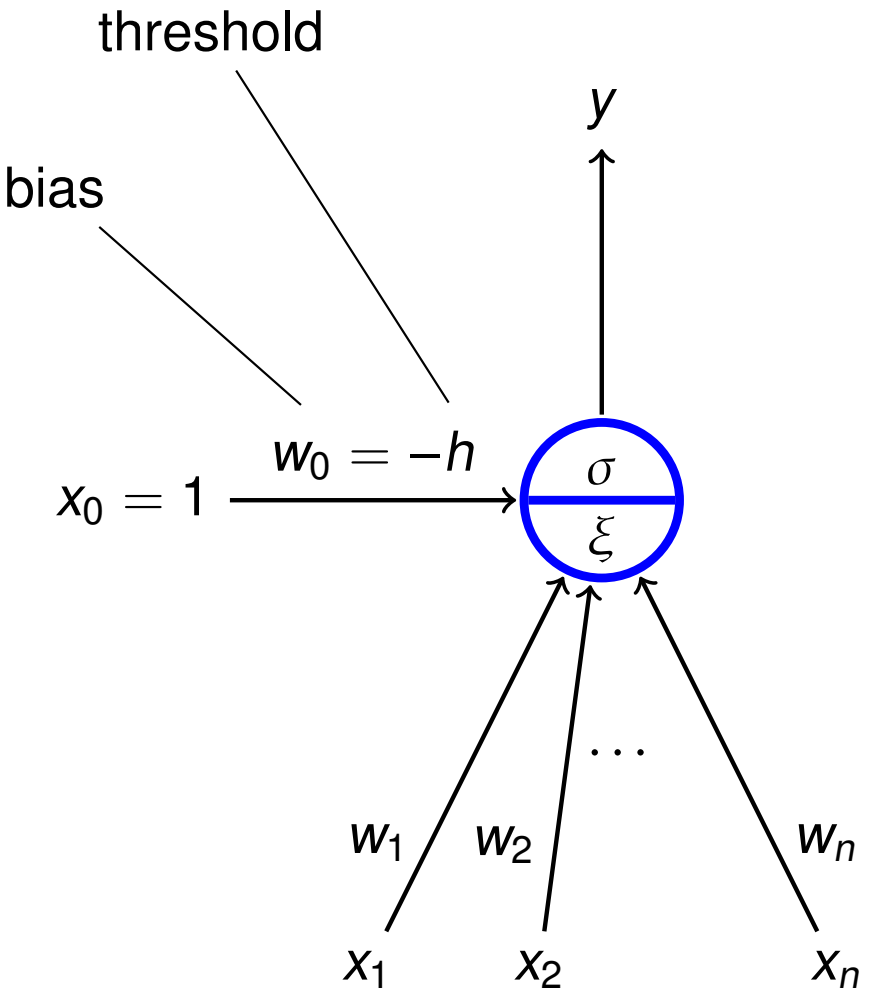
  - "close" inputs typicaly get similar values
- Graceful degradation
  - damage typically causes only a decrease in precision of results

Formal neuron (with bias)



- $x_0 = 1, x_1, \dots, x_n \in \mathbb{R}$ are **inputs**
- $w_0, w_1, \dots, w_n \in \mathbb{R}$ 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

Activation function: *unit step function* $\sigma(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$

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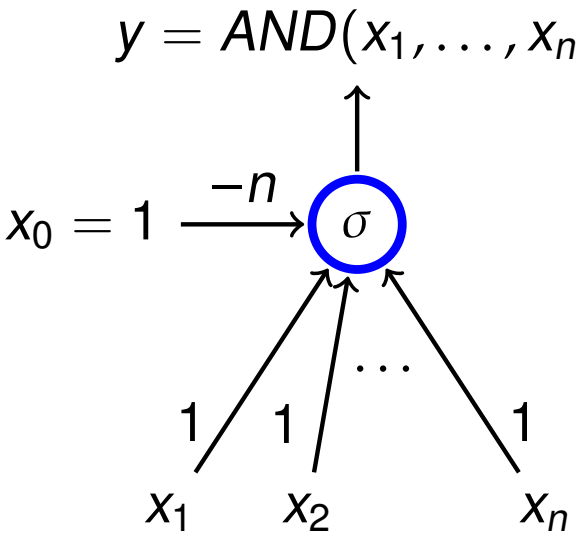

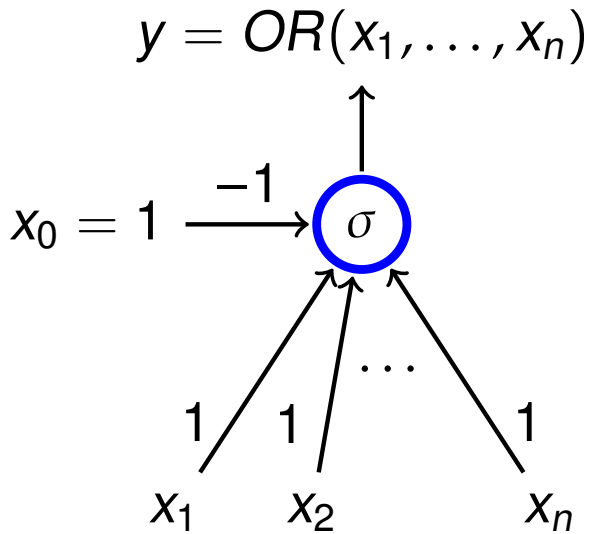

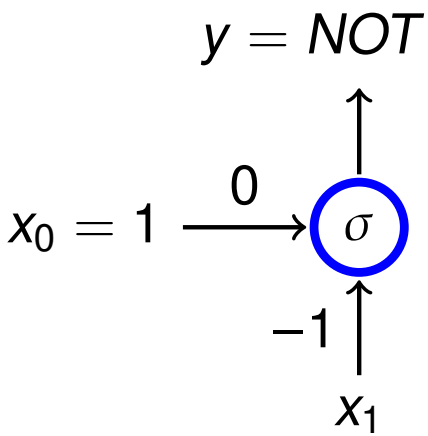

Boolean functions

Theorem

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 $F : \{0,1\}^n \to \{0,1\}$.

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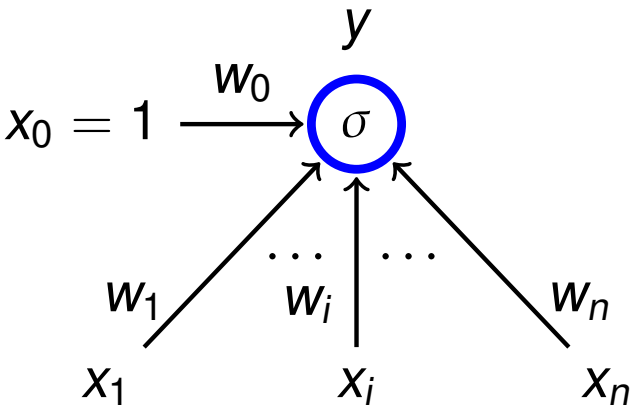
Proof.

- 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 $\vec{v}$:

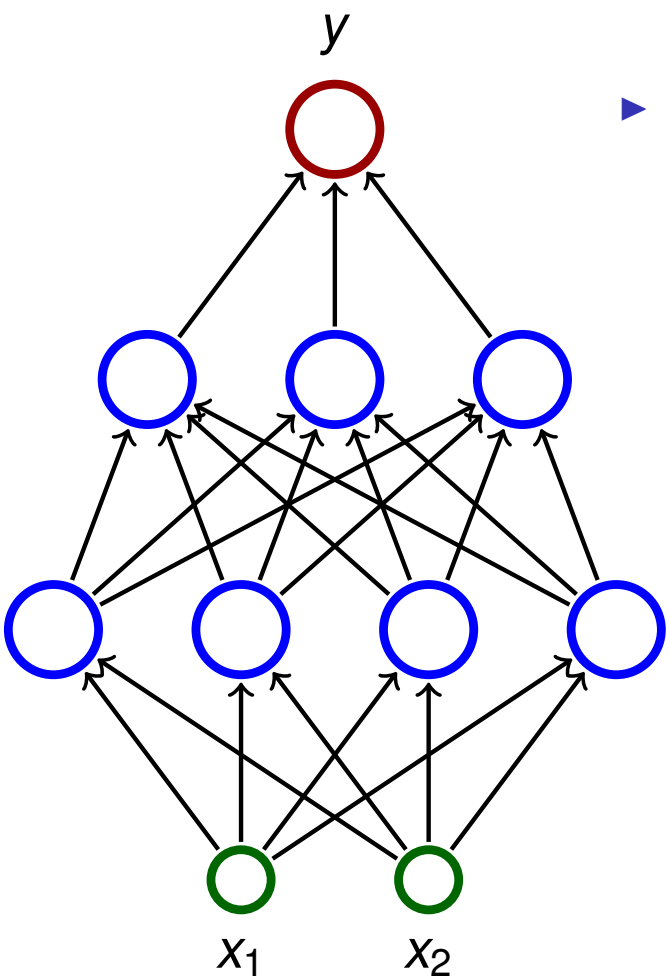


$$w_0 = -\sum_{i=1}^{n} v_i$$

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

- 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



- Consider a three layer network; each neuron has the unit step activation function.
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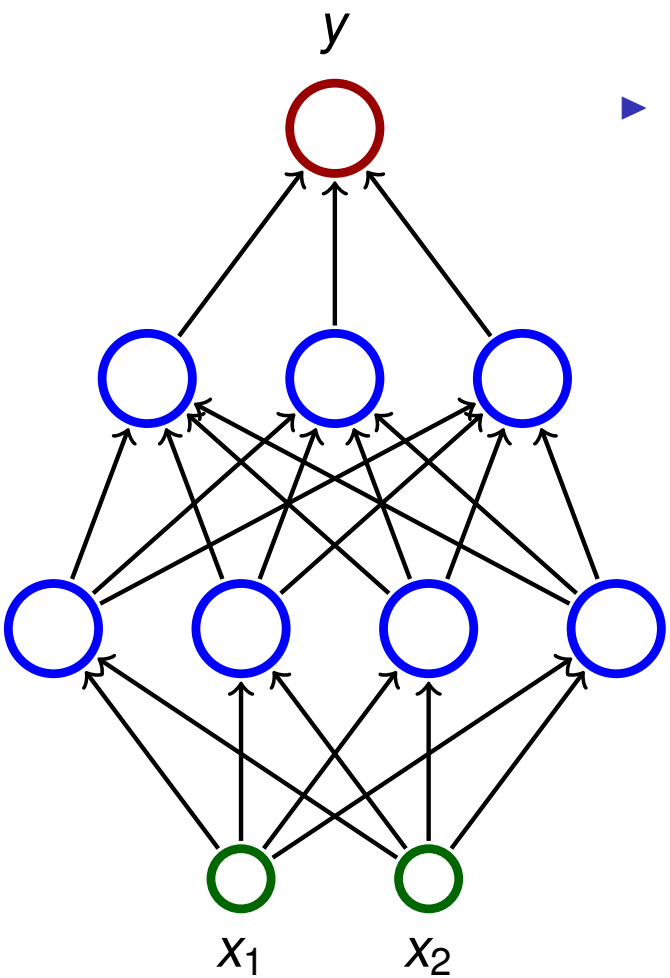

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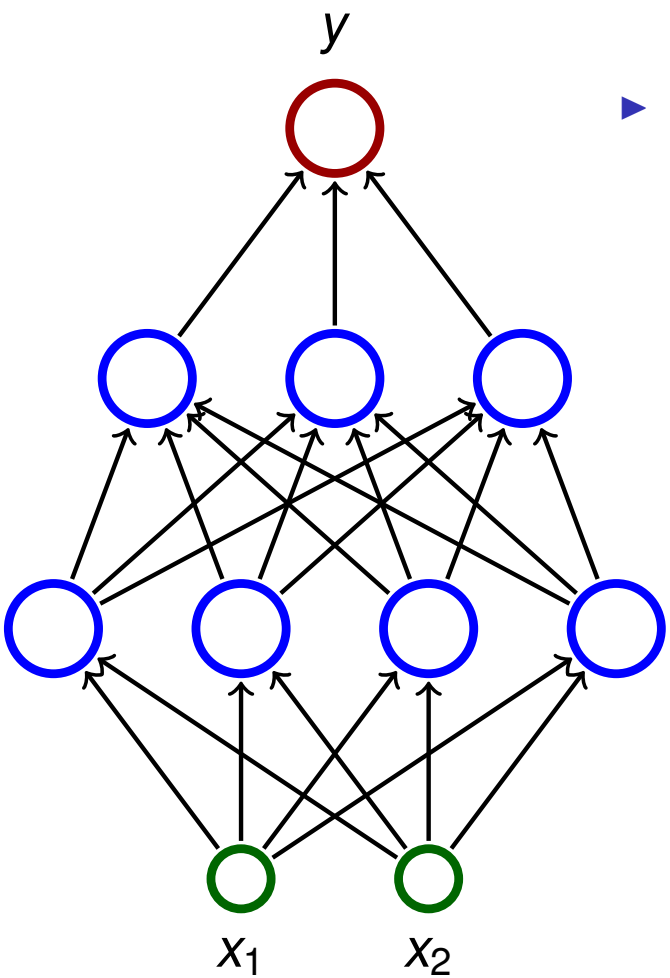

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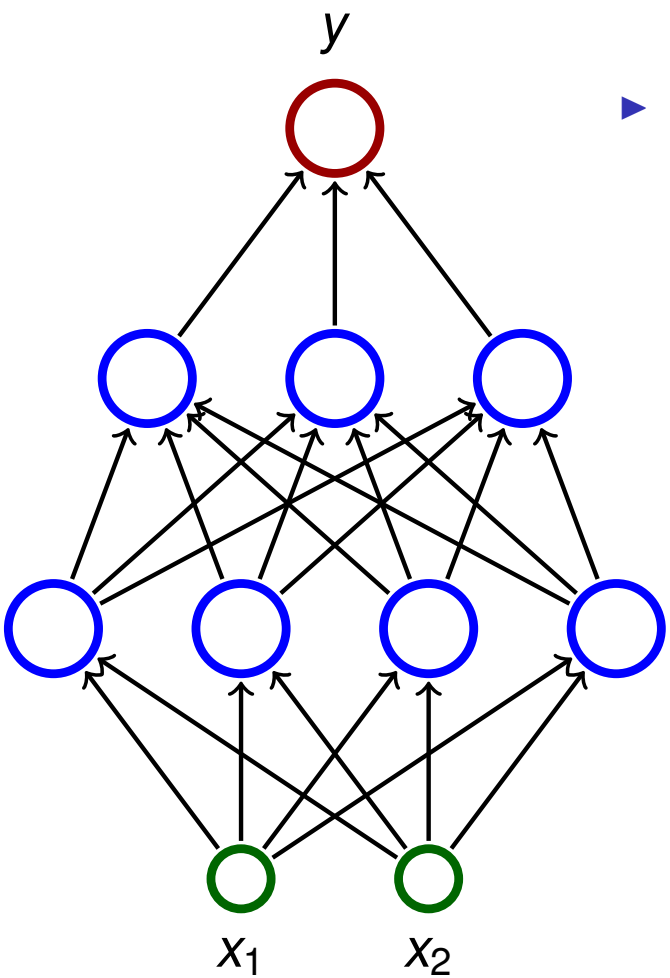

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  - The third layer may e.g. make unions of some convex sets.

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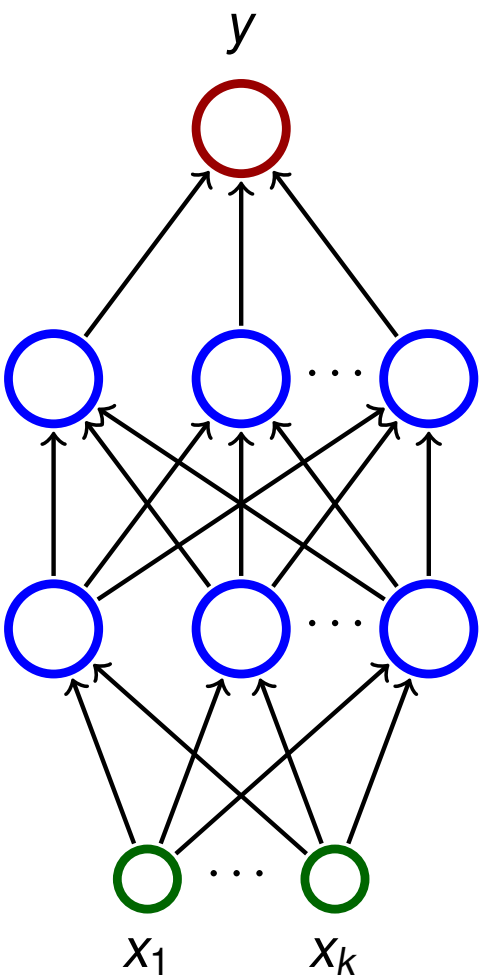

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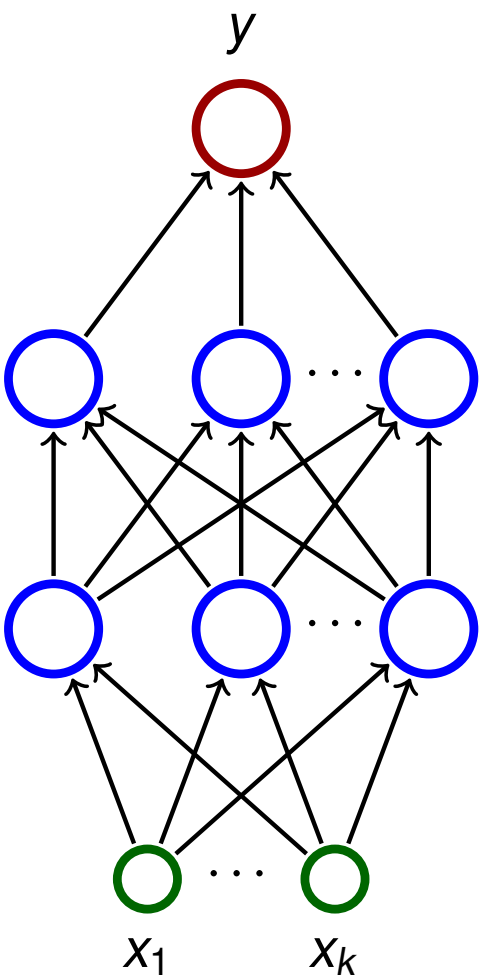

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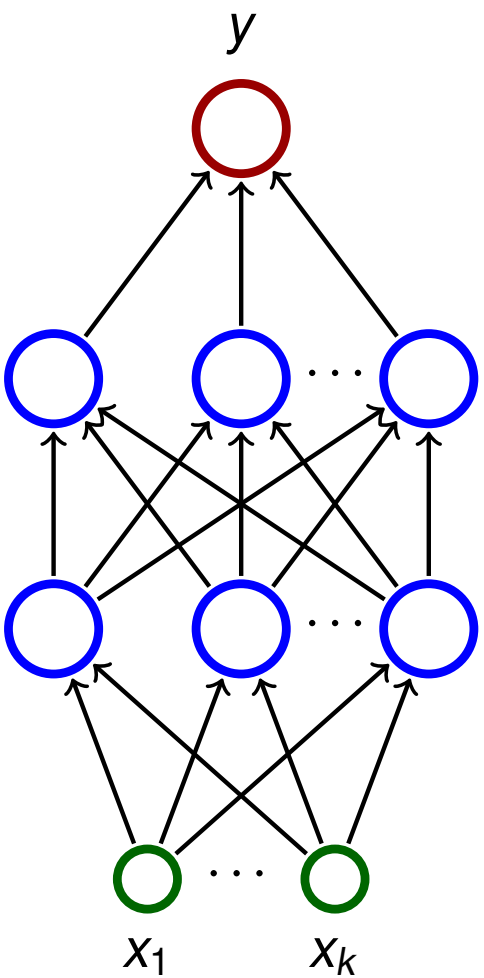

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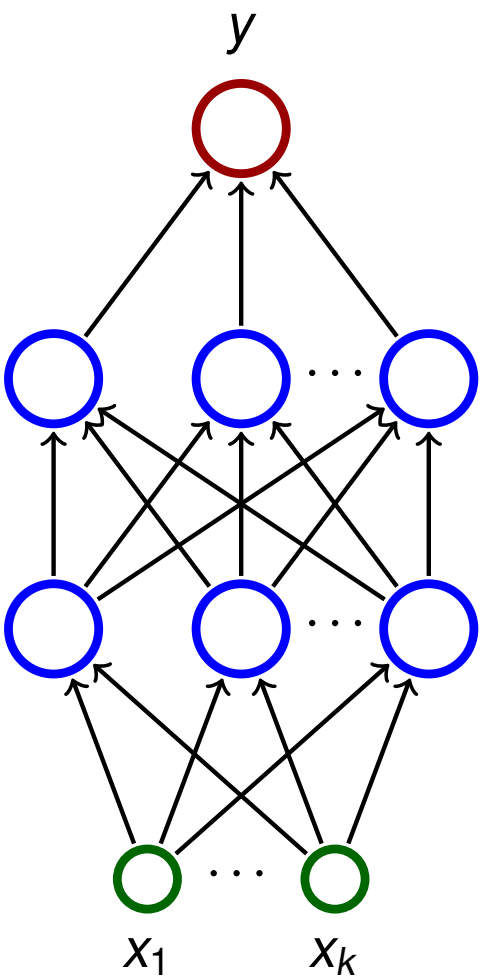

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Non-linear separation - sigmoid

Theorem (Cybenko 1989 - informal version)

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

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

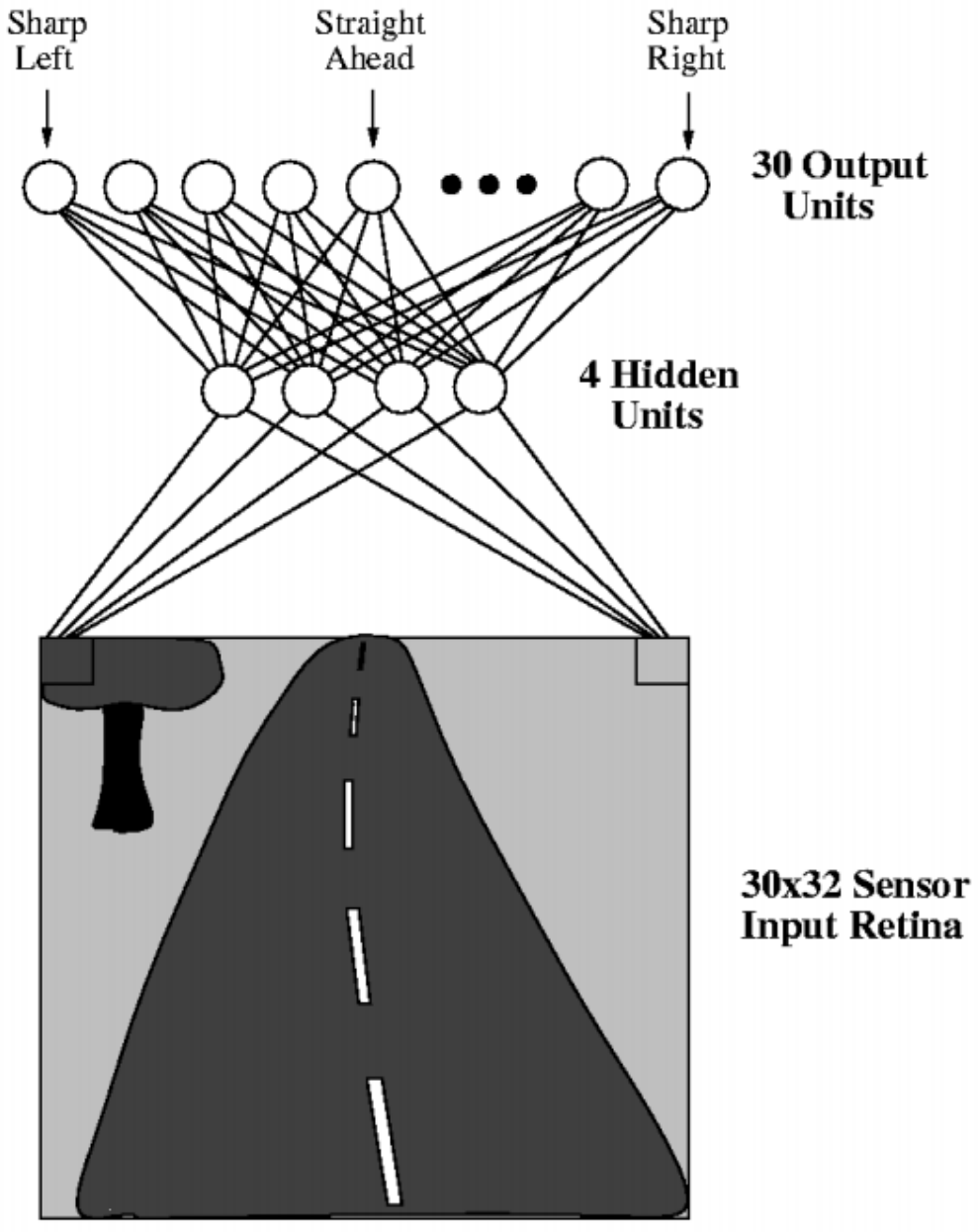
For every reasonable set $A \subseteq [0,1]^n$, there is a **two layer network** *where each hidden neuron has the activation function σ (output neurons are linear), that satisfies the following:*

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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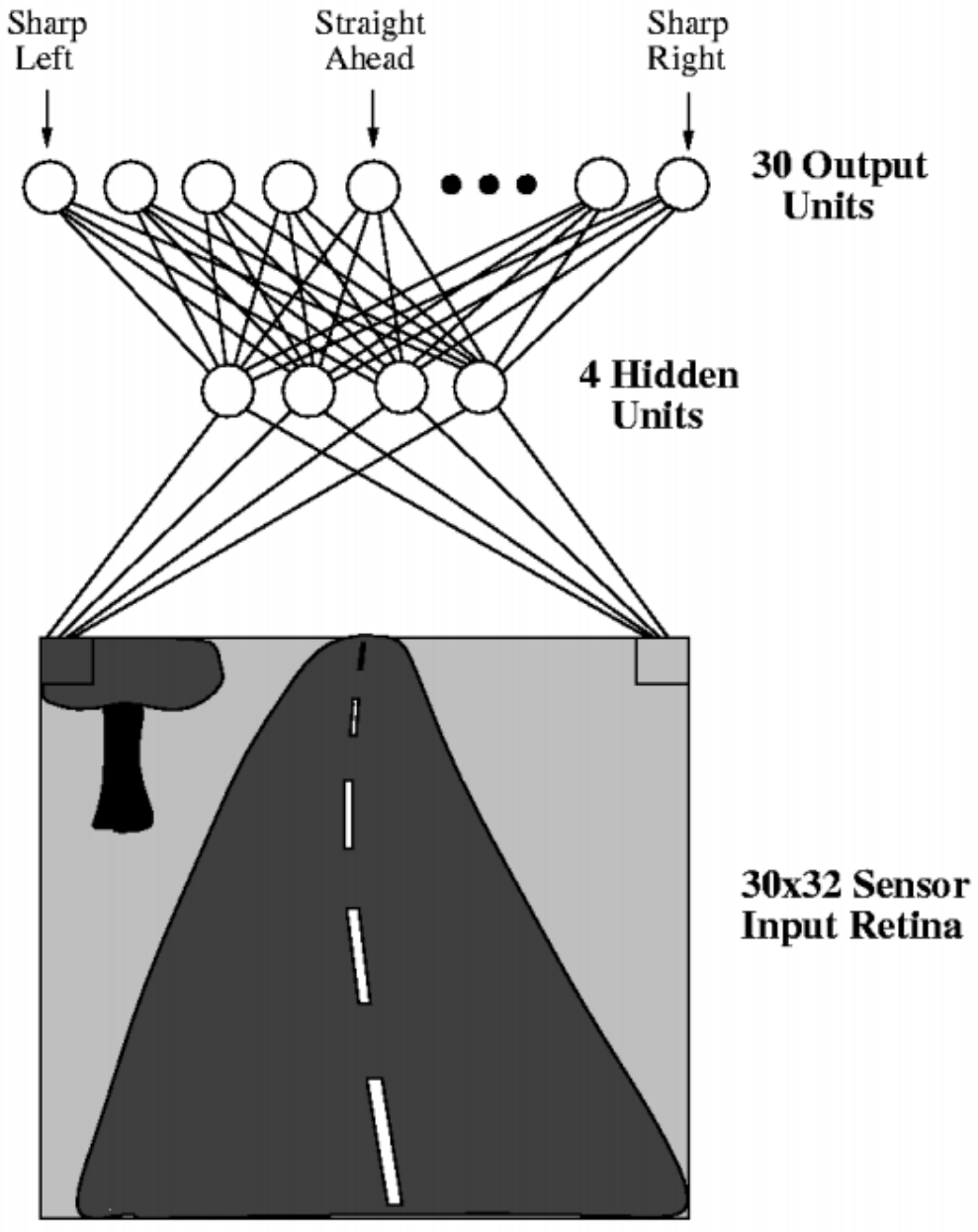

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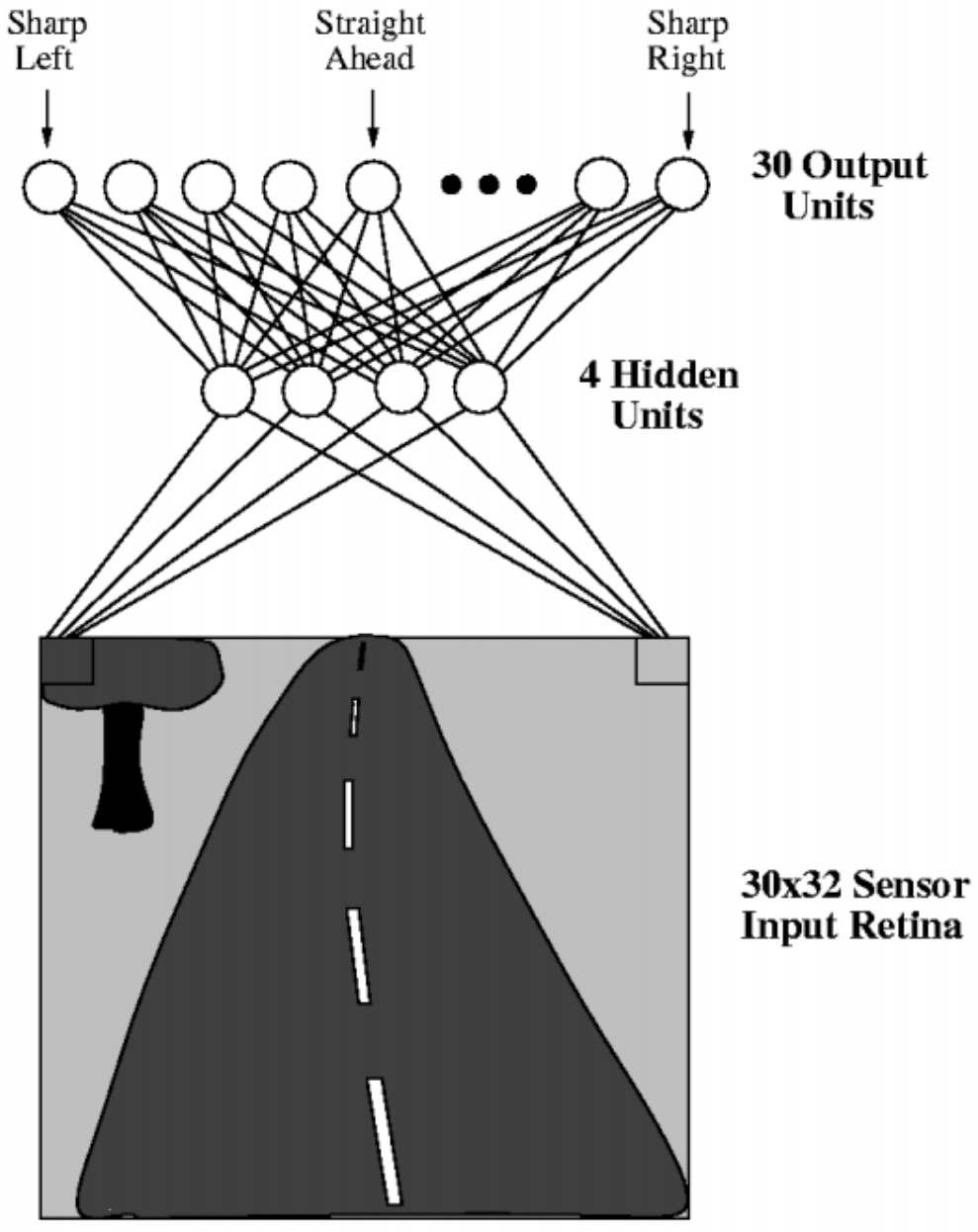

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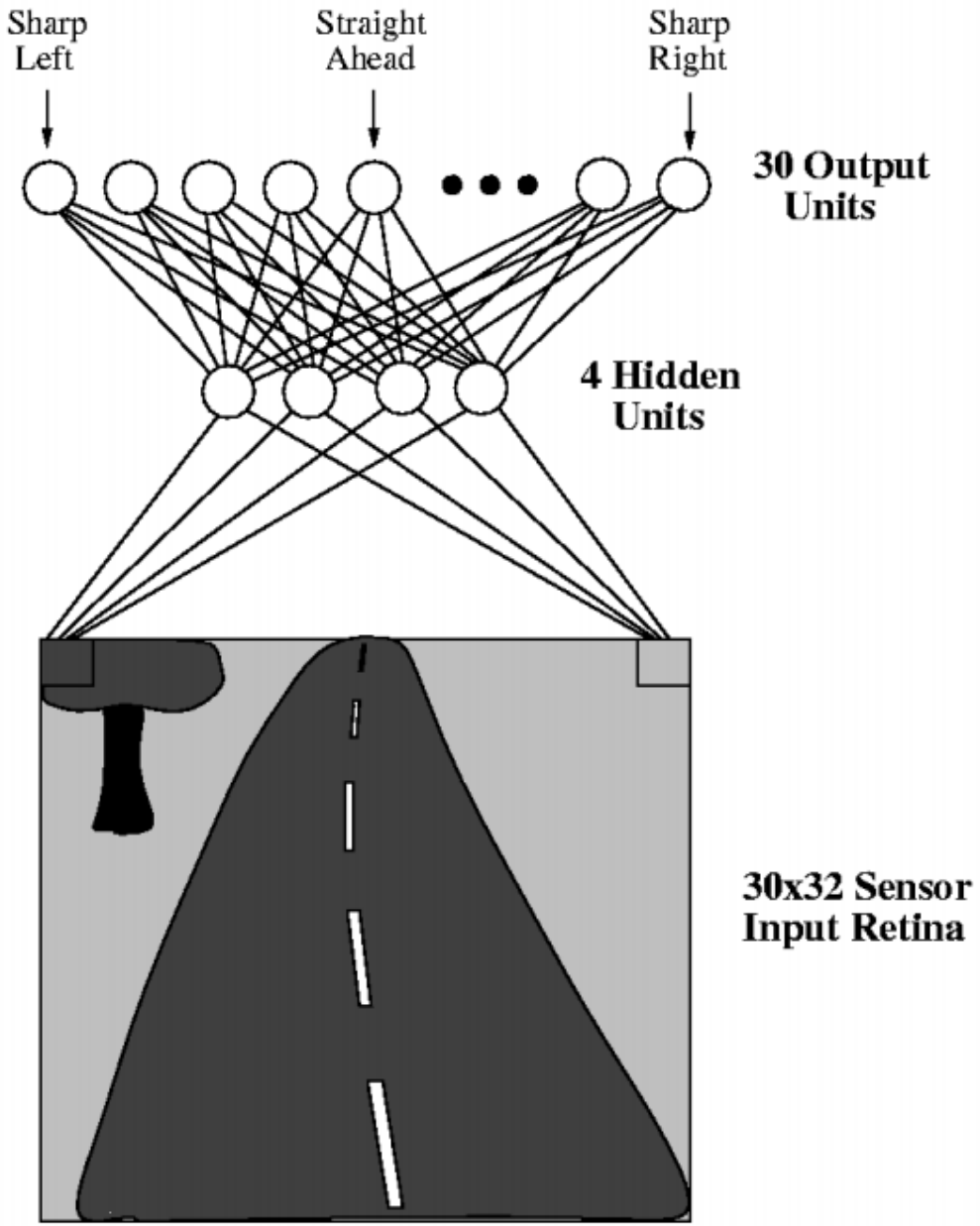

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- Output neurons "classify" images of the road based on their "curvature".

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

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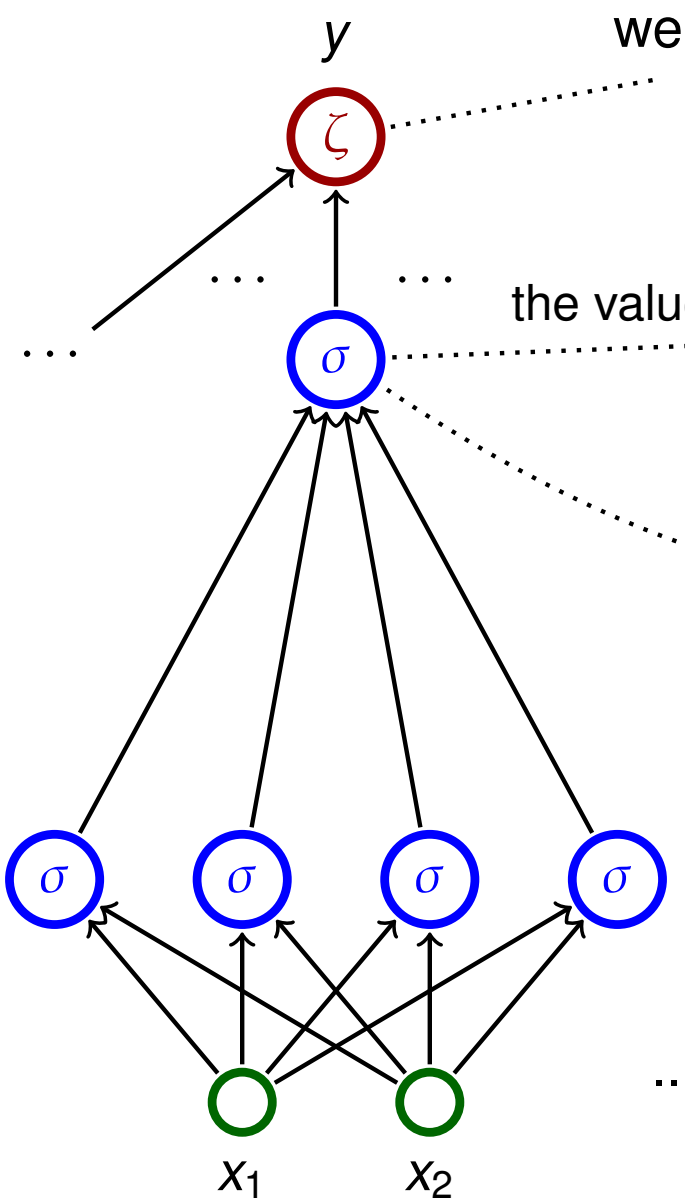
Function approximation – three layer networks



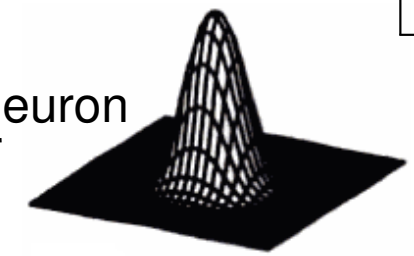
weighted sum of "spikes"

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

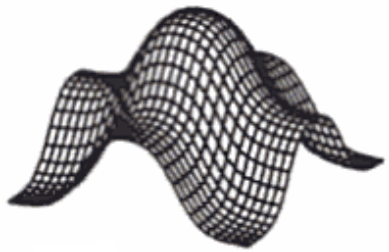
$$\zeta(\xi) = \xi$$

the value of the neuron

..... a "spike"



inner potential



... + the other two 90 degree rotations

Function approximation - two-layer networks

Theorem (Cybenko 1989)

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

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For every continuous function $f : [0,1]^n \to [0,1]$ and every $\varepsilon > 0$ there is a function $F : [0,1]^n \to [0,1]$ computed by a **two layer network** *where each hidden neuron has the activation function σ (output neurons are linear), that satisfies the following*

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

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- Consider recurrent networks (i.e. containing cycles)
  - with real weights (in general);
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Neural networks and computability

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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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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

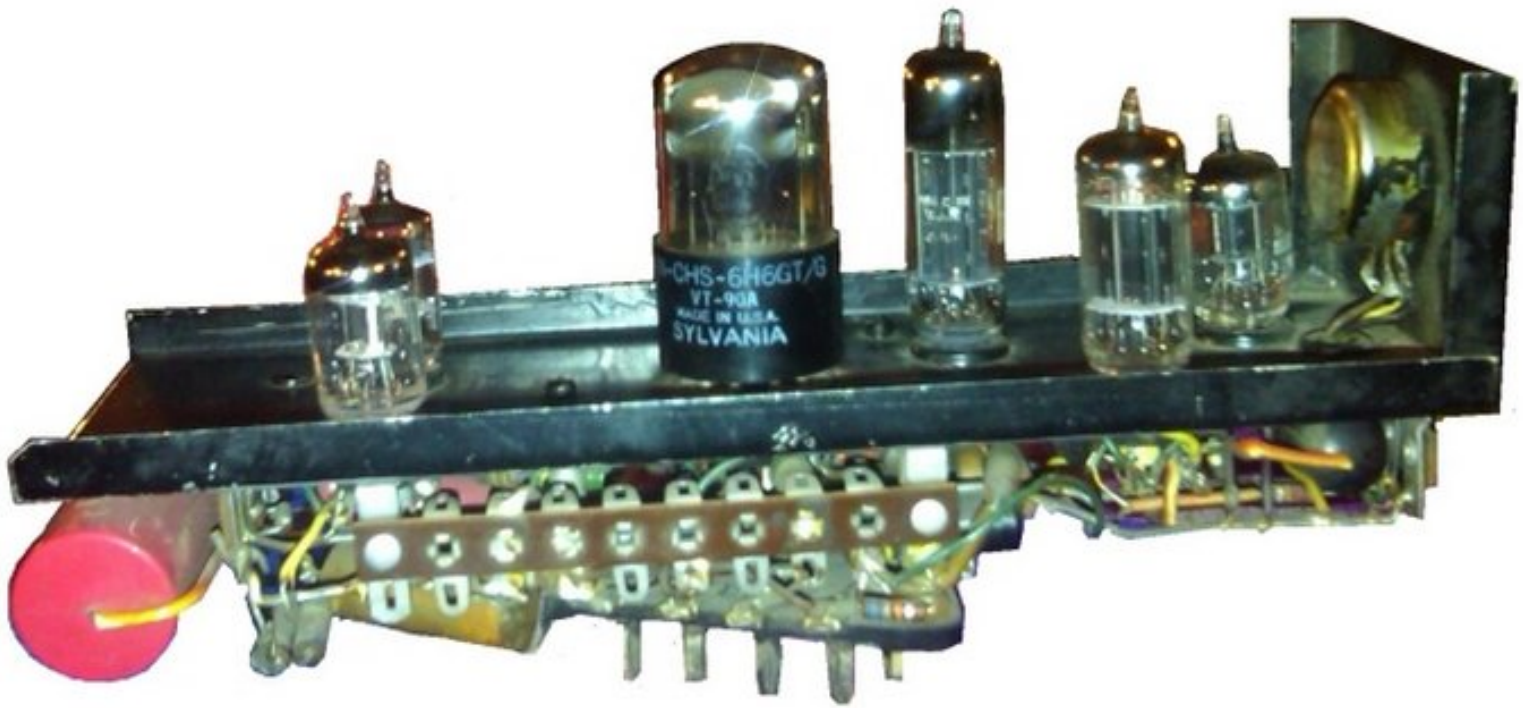
- Neural networks are very strong from the point of view of theory:
  - All Boolean functions can be expressed using two-layer networks.
  - Two-layer networks may approximate any continuous function.
  - Recurrent networks are at least as strong as Turing machines.
- These results are purely theoretical!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



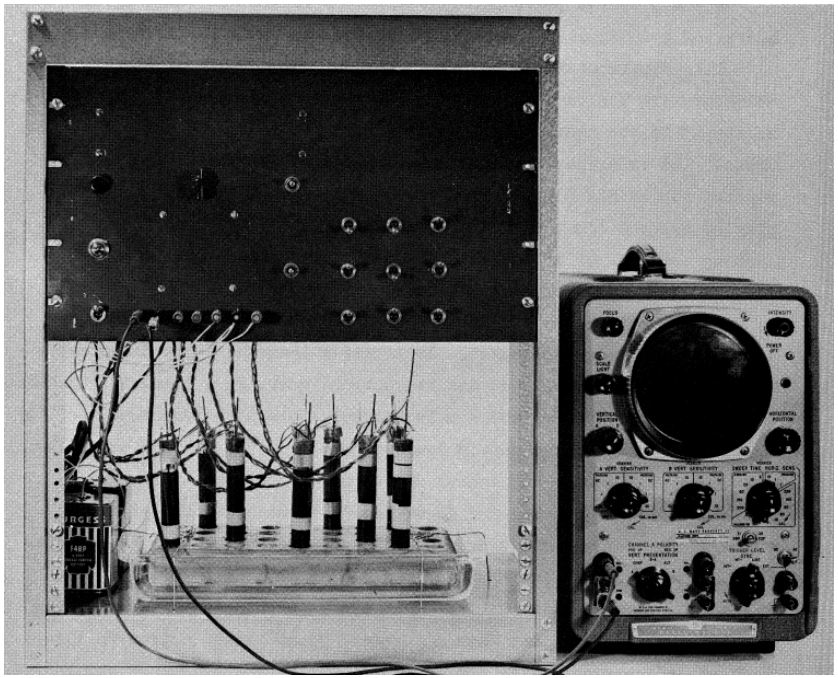
History of neurocomputers

- 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)

History in waves ...

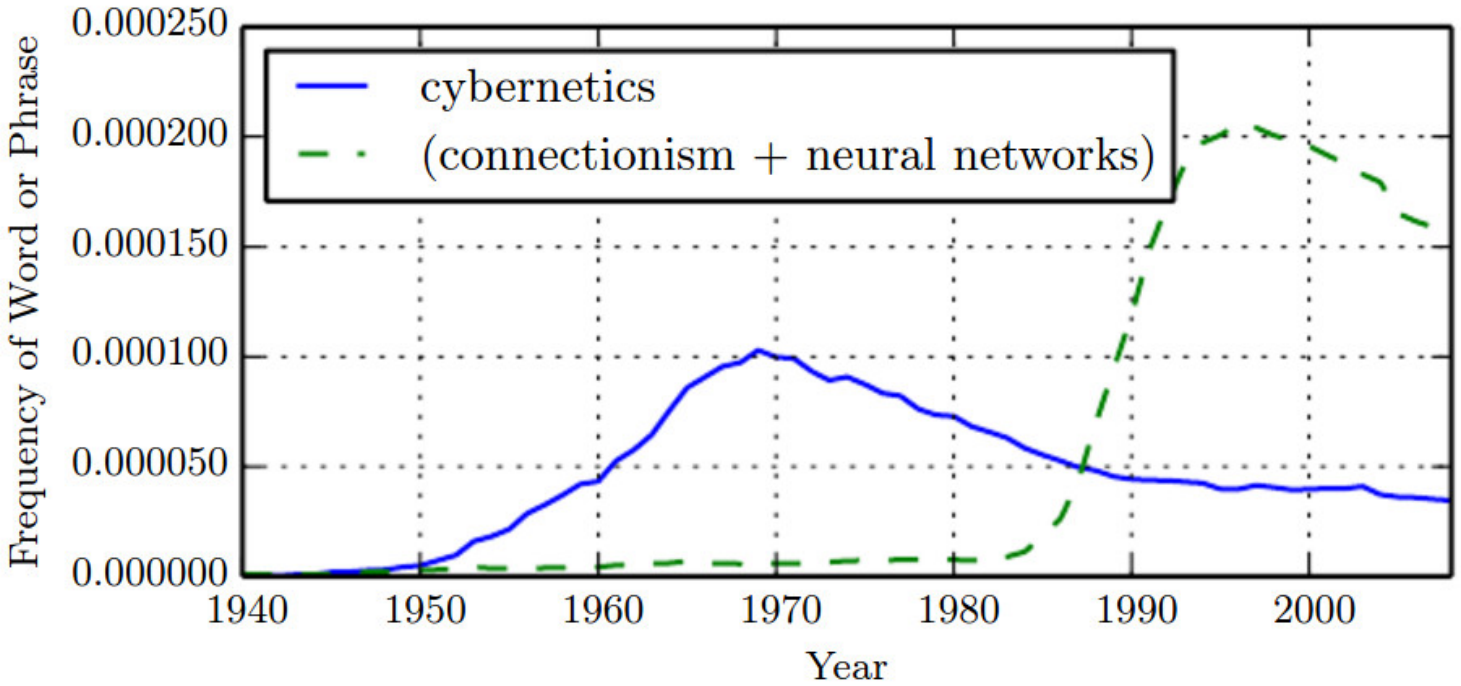
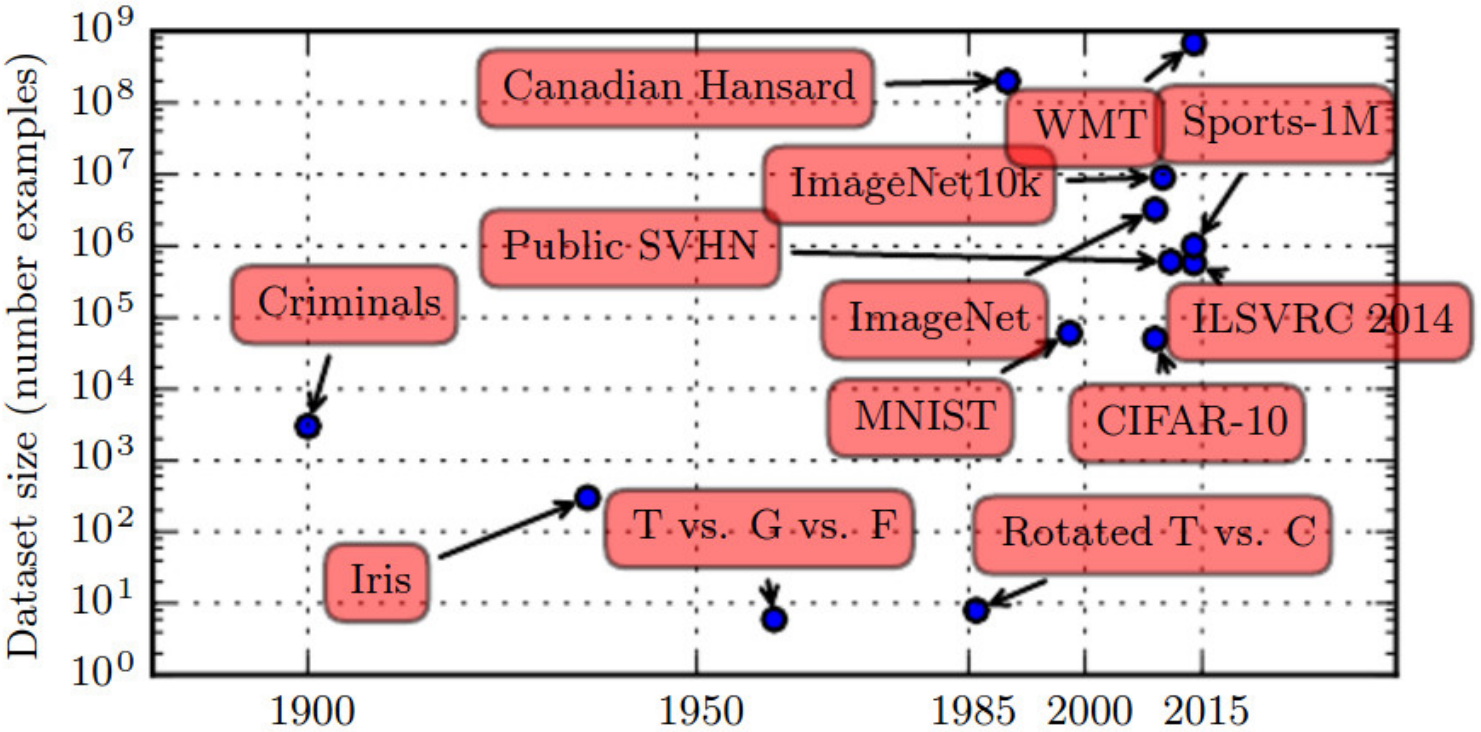


Figure: The figure shows two of the three historical waves of articial neural nets research, as measured by the frequency of the phrases "cybernetics" and "connectionism" or "neural networks" according to Google Books (the third wave is too recent to appear).

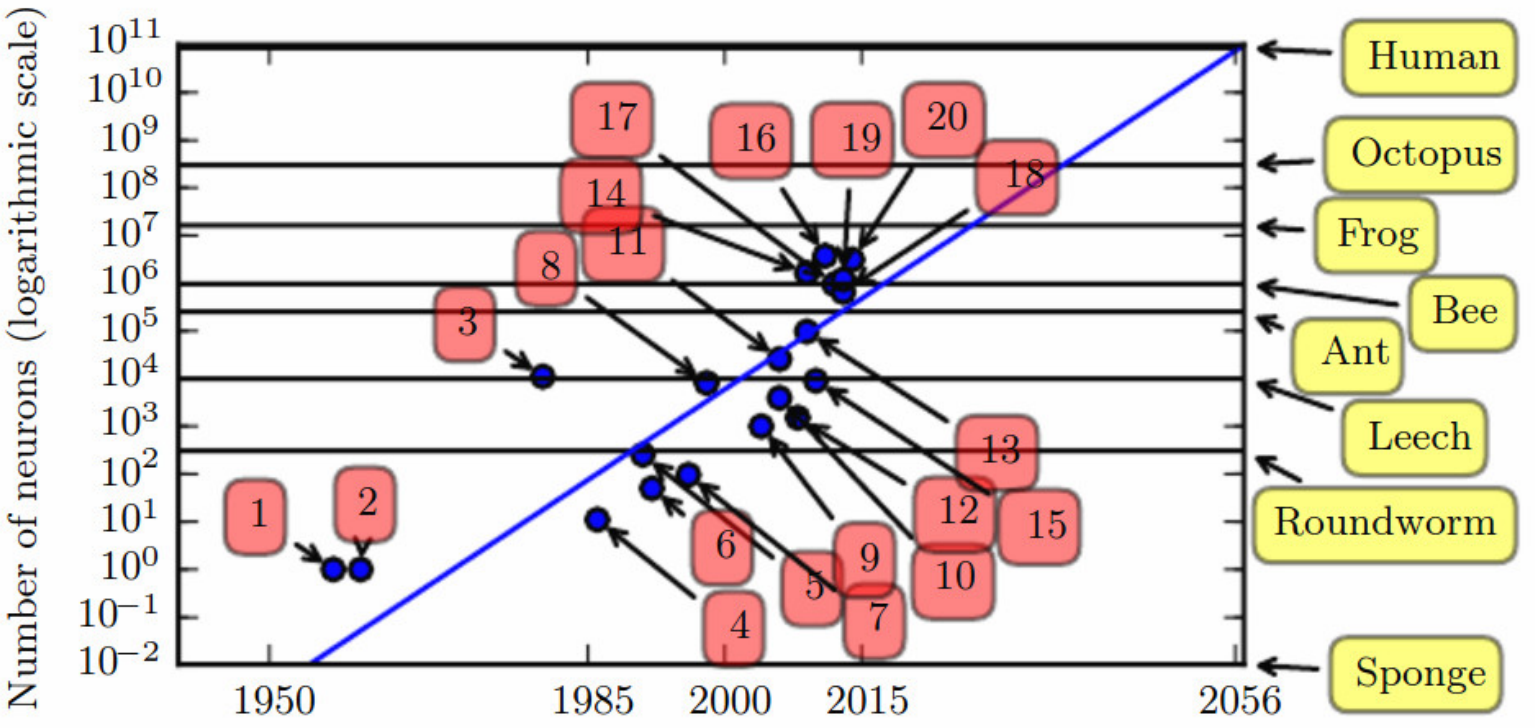
Current hardware – What do we face?

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 ...

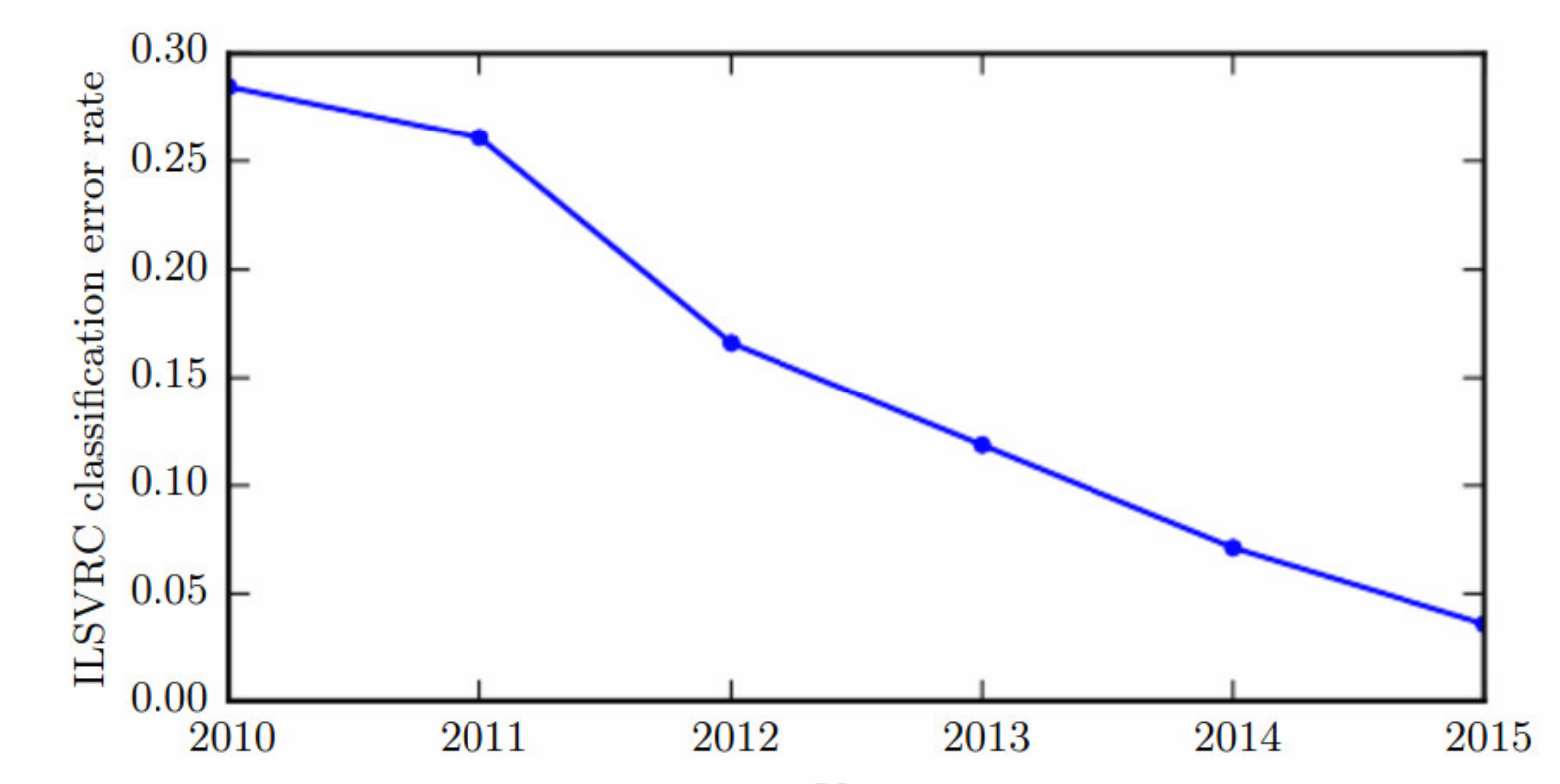


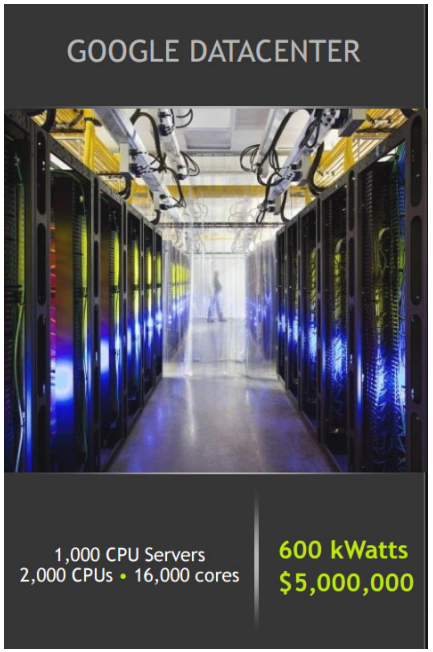
Figure: Since deep networks reached the scale necessary to compete in the ImageNetLarge Scale Visual Recognition Challenge, they have consistently won the competition every year, and yielded lower and lower error rates each time. Data from Russakovsky et al. (2014b) and He et al. (2015).

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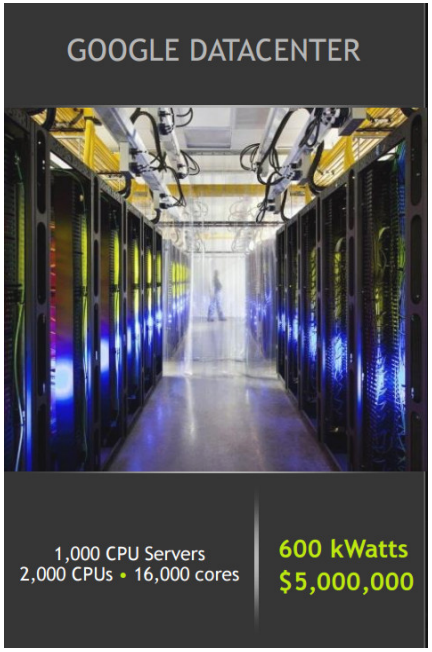
In 2014, similar task performed on Commodity Off-The-Shelf High Performance Computing (COTS HPC) technology: a cluster of GPU servers with Infiniband interconnects and MPI.

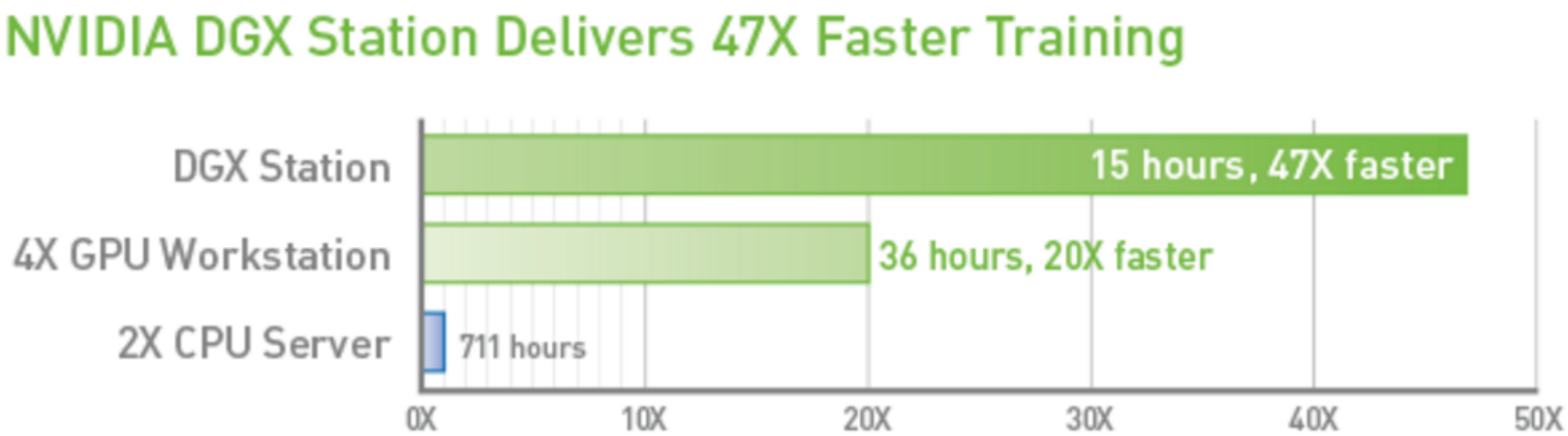
Able to train 1 billion parameter networks on just 3 machines in a couple of days.
Able to scale to 11 billion weights (approx. 6.5 times larger than the Google model) on 16 GPUs.



Current hardware – NVIDIA DGX Station

- 4x GPU (Tesla V100)
- TFLOPS = 480
- GPU memory 64GB total
- NVIDIA Tensor Cores: 2,560
- NVIDIA CUDA Cores: 20,480
- System memory: 256 GB
- Network: Dual 10 Gb LAN

- NVIDIA Deep Learning SDK



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 library on top of TensorFlow that allows easy description of most modern neural networks
- **CNTK** (Microsoft)
  - functionality similar to TensorFlow
  - special input language called BrainScript
- **Theano**:
  - 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, Torch (Facebook), 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)
```

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.

SyNAPSE (USA)

- Big research project, partially funded by DARPA
- Among the main subjects IBM a HRL, collaboraton with top US universities, e.g. Boston, Stanford
- The project started in 2008
- Invested tens of millions USD.

The goal

- Develop a neural network comparable with a real brain of a mammal
- The resulting hw chip should simulate 10 billion neurons, 100 trillion synaptic connections, consume 1 kilowatt ($\sim$ a small heater), size 2 dm^3
- Oriented towards development of a new parallel computer architecture rather than neuroscience.

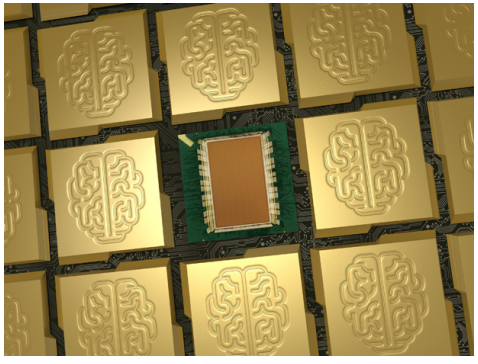
SyNAPSE (USA) – some results

A cat brain simulation (2009)

- A simulation of a network with 10^9 neurons, 10^{13} synapses
- Simulated on a supercomputer Dawn (Blue Gene/P), 147,450 CPU, 144 tB of memory
- 643 times slower than the real brain
- The network modelled according to the real-brain structure (hierarchical model of a visual cortex, 4 layers)
- The authors claim that they observed some behaviour similar to the behaviour of the real brain (signal propagation, α, γ waves)

... simulation was heavily criticised (see latter)
... in 2012 the number of neurons increased to 530 bn neurons a 100 tn synapses

SyNAPSE (USA) – TrueNorth



- A chip with 5.4 billion elements
- 4096 neurosynaptic cores connected by a network, implementing 1 million programmable "spiking" neurons, 256 million programmable synaptic connections
- global frequency 1-kHz
- low energy consumption, approx. 63mW

- Offline learning, implemented some known algorithms (convolutional networks, RBM etc.)
- Applied to simple image recognition tasks.

Human Brain Project, HBP (Europe)

- Funded by EU, budget 10^9 EUR for 10 years
- Successor of Blue Brain Project at EPFL Lausanne
- Blue Brain started in 2005, ended in 2012, Human Brain Project started in 2013

The original goal: Deeper understanding of human brain

- **networking in neuroscience**
- diagnosis of brain diseases
- thinking machine

The approach:

- study of brain tissue using current technology
- modelling of biological neurons
- simulation of the models (program NEURON)

HBP (Europe

Blue brain project (2008)

- Model of a part of the brain cortex of a rat (approx. 10,000 neurons), much more complex model of neurons than in SyNAPSE
- Simulated on a supercomputer of the type Blue Gene/P (provided by IBM on discount), 16,384 CPU, 56 teraflops, 16 terabytů paměti, 1 PB disk space
- Simulation 300x slower than the real brain

Human brain project (2015):

- Simplified model of the nervous system of a rat (approx. 200 000 neurons)

SyNAPSE vs HBP

2011: IBM Simulates 4.5 percent of the Human Brain, and All of the Cat Brain (Scientific American)

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"This is a mega public relations stunt – a clear case of scientific deception of the public"

"Their so called "neurons" are the tiniest of points you can imagine, a microscopic dot"

"Neurons contain 10's of thousands of proteins that form a network with 10's of millions of interactions. These interactions are incredibly complex and will require solving millions of differential equations. They have none of that."

SyNAPSE vs HBP

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But did Mohda not collaborate with neuroscientists?
"I would be very surprised if any neuroscientists that he may have had in his DARPA consortium realized he was going to make such an outrageous claim. I can't imagine that the San Fransisco neuroscientists knew he was going to make such a stupid claim. Modha himself is a software engineer with no knowledge of the brain."

... and in the meantime in Europe

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Peter Dayan, director of the computational neuroscience unit at UCL:

“The main apparent goal of building the capacity to construct a larger-scale simulation of the human brain is radically premature.”

“We are left with a project that can’t but fail from a scientific perspective. It is a waste of money, it will suck out funds from valuable neuroscience research, and would leave the public, who fund this work, justifiably upset.”

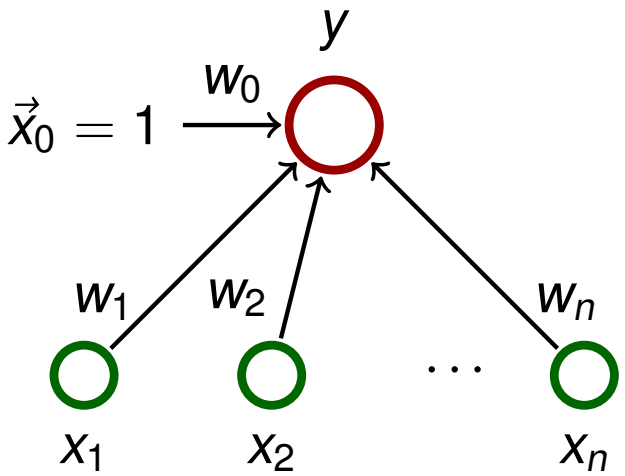
... and in 2016

The European Commission and the Human Brain Project Coordinator, the École Polytechnique Fédérale de Lausanne (EPFL), have signed the first Specific Grant Agreement (SGA1), releasing EUR 89 million in funding retroactively from 1st April 2016 until the end of March 2018. The signature of SGA1 means that the HBP and the European Commision have agreed on the HBP Work Plan for this two year period.

The SGA1 work plan will move the Project closer to achieving its aim of establishing a cutting-edge, ICT-based scientific Research Infrastructure for brain research, cognitive neuroscience and brain-inspired computing.

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: $y[\vec{w}](\vec{x}) = \sigma(\xi) = \vec{w} \cdot \vec{x}$

ADALINE

Learning:

- Given a **training set**

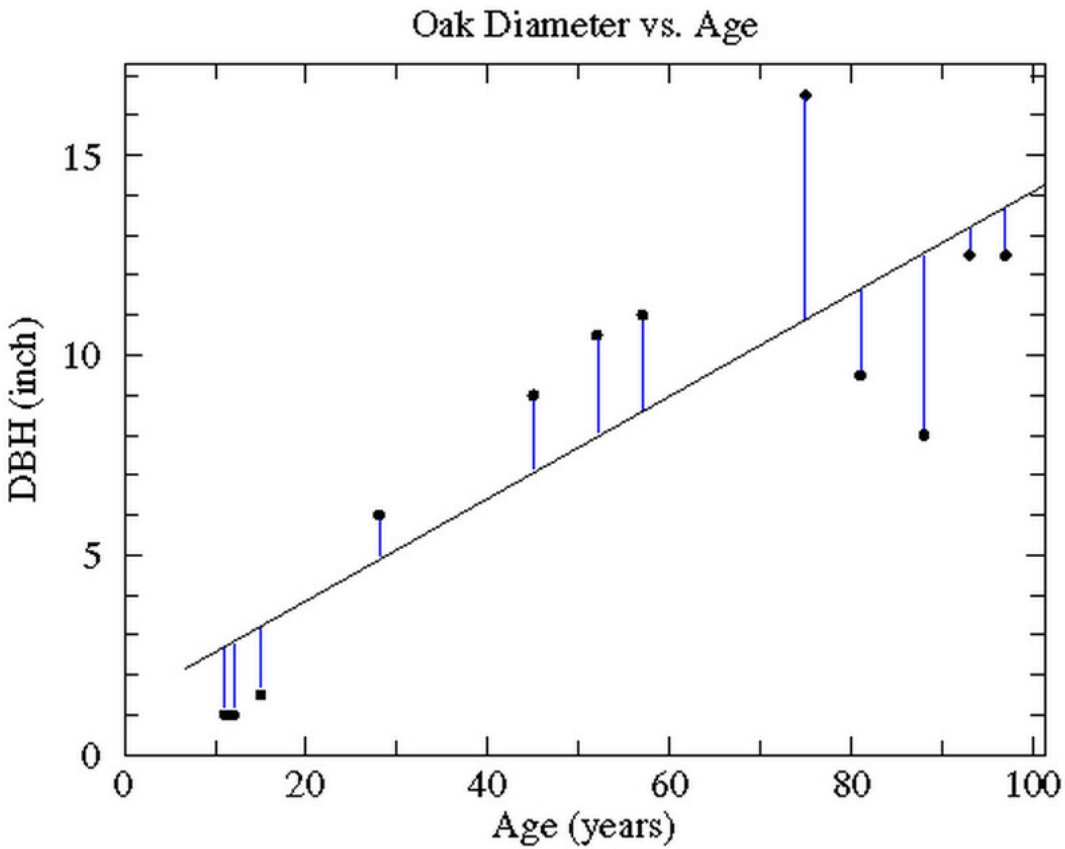
$$\mathcal{T} = \left\{\left(\vec{x}_1, d_1\right), \left(\vec{x}_2, d_2\right), \ldots, \left(\vec{x}_p, d_p\right)\right\}$$

  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 $d_k \in \mathbb{R}$ 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



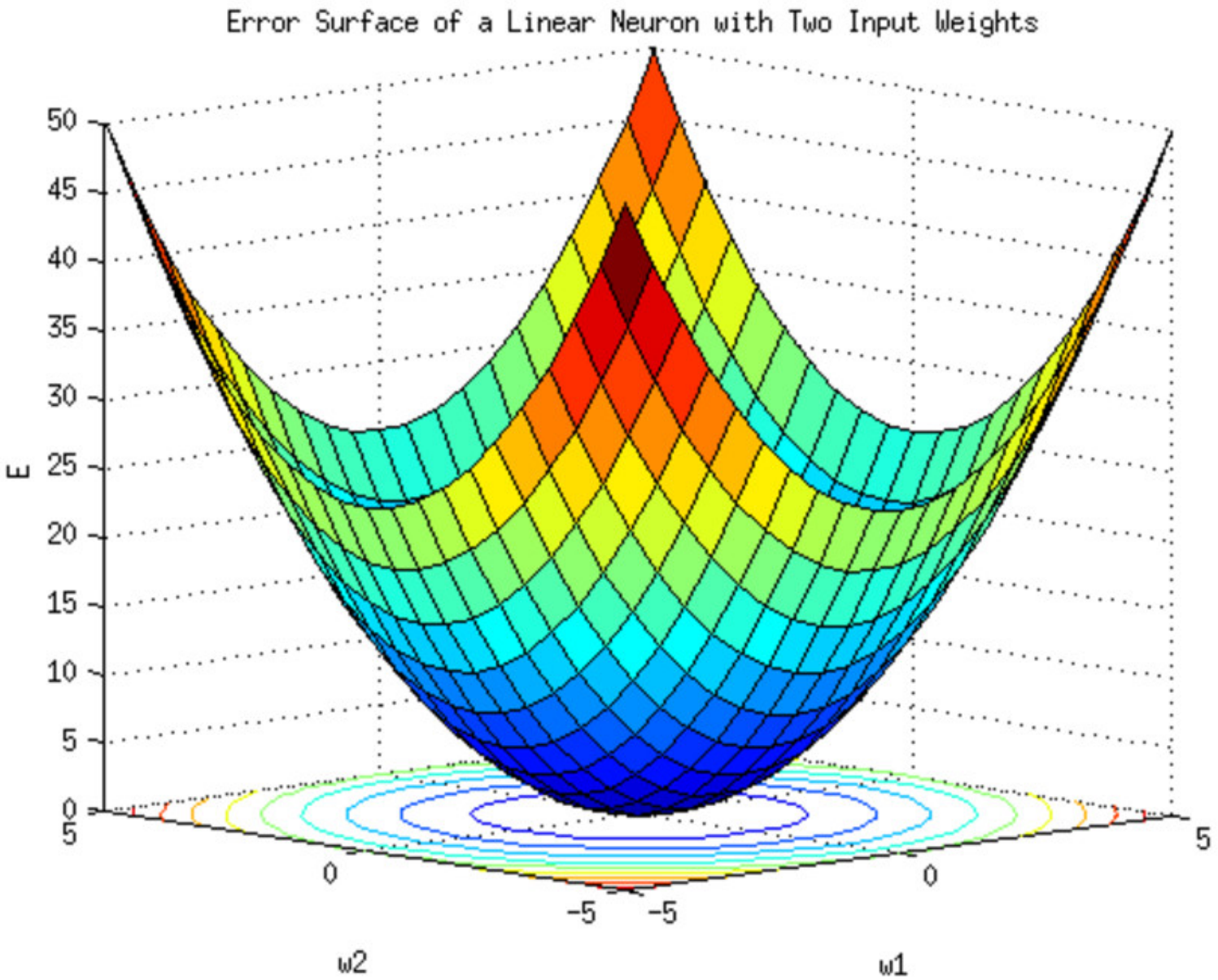
ADALINE

- **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!

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.

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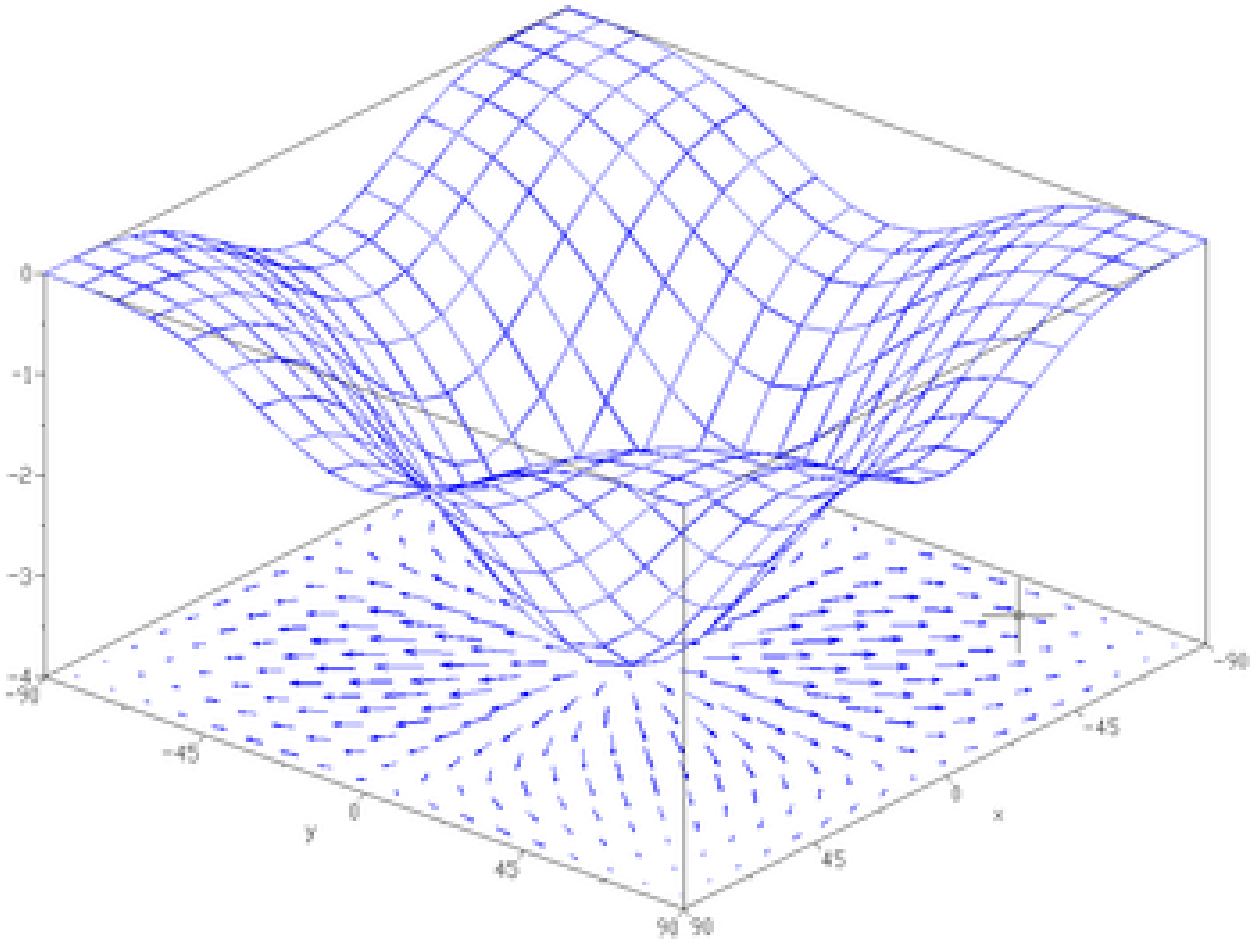
Fact

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 (ADALINE)

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

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&= \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}$$

Gradient of the error function (ADALINE)

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\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) \\
&= \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}
$$

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

Batch algorithm (gradient descent):

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

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

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

$$\begin{aligned} \vec{w}^{(t+1)} &= \vec{w}^{(t)} - \varepsilon \cdot \nabla E(\vec{w}^{(t)}) \\ &= \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(\vec{w}^{(t)} \cdot \vec{x}_k - d_k \right) \cdot \vec{x}_k \end{aligned}$$

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

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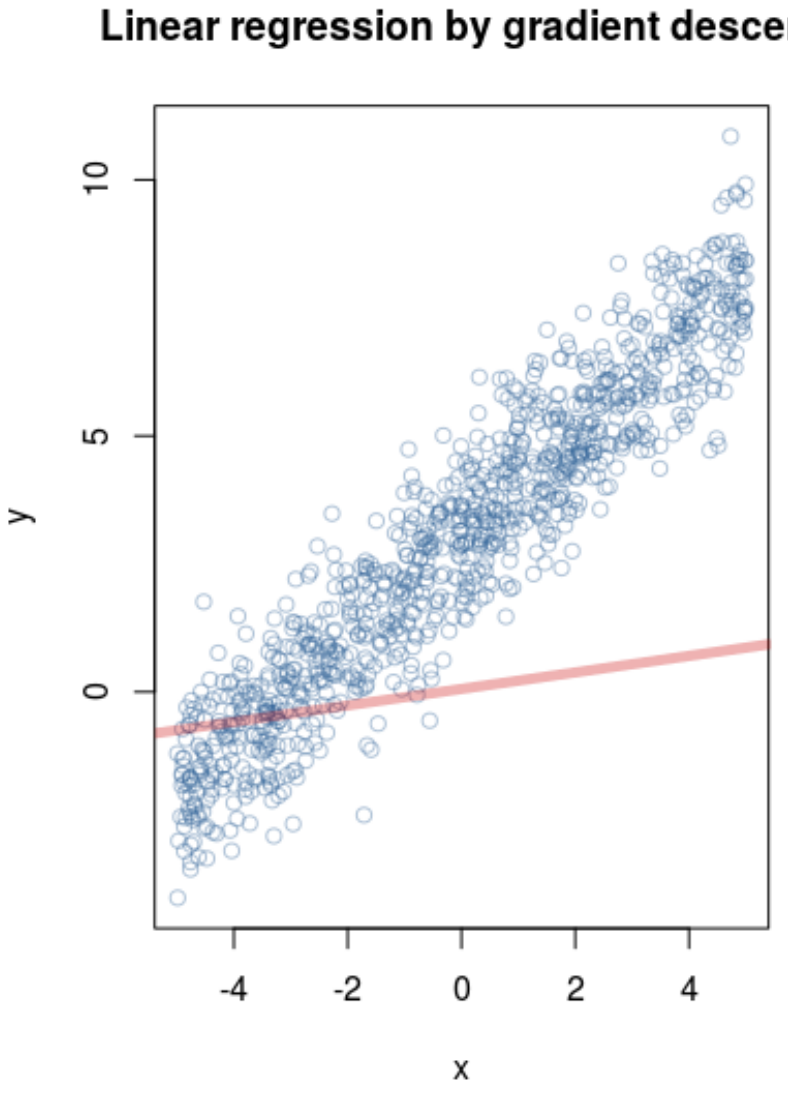
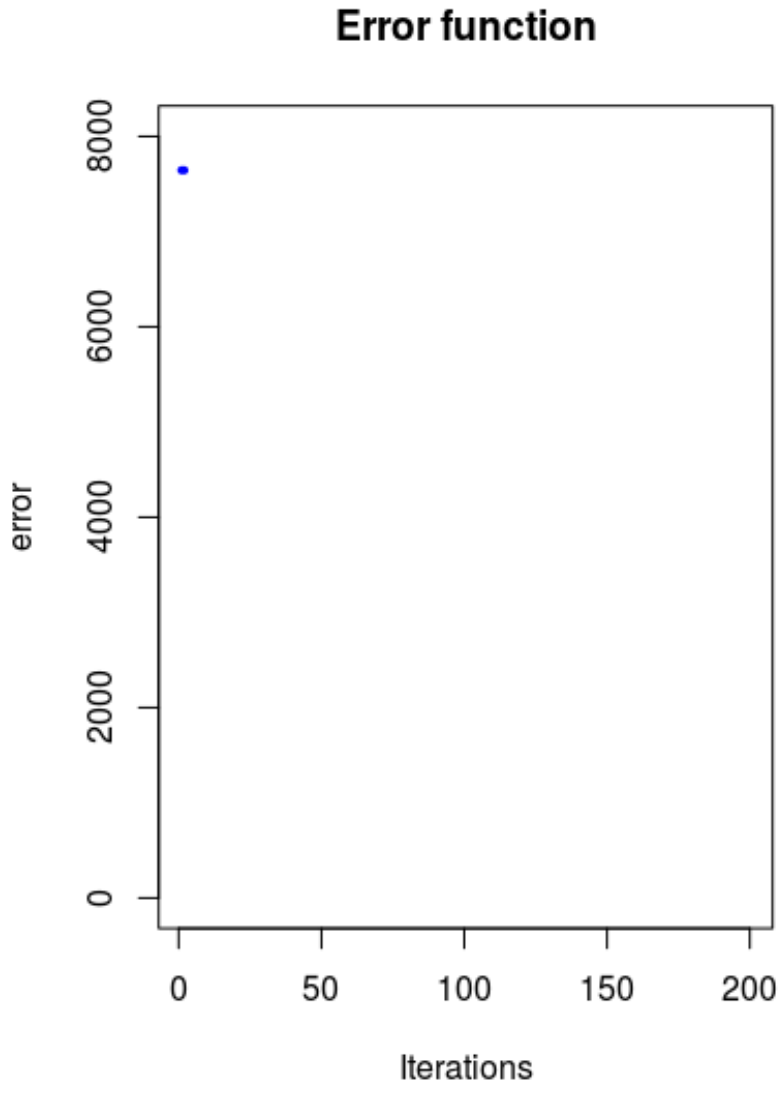
Proposition

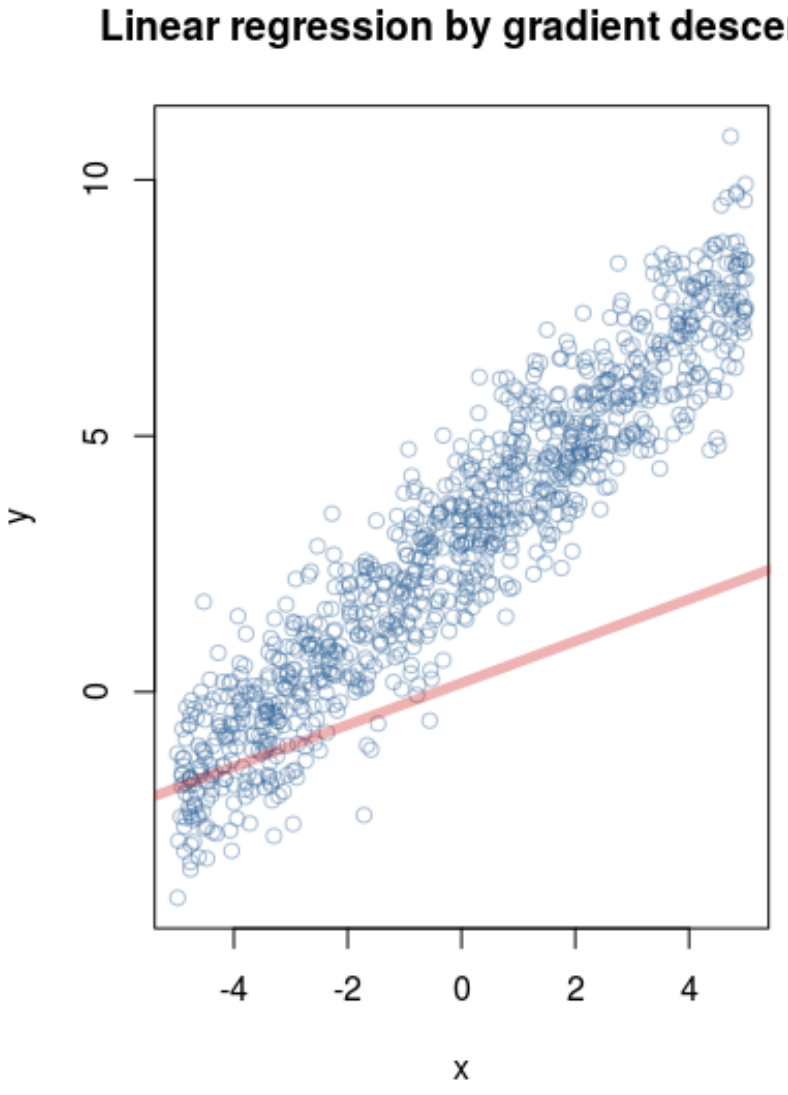
For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (componentwise) to the global minimum of E (i.e. to the vector $\vec{w}$ satisfying $\nabla E(\vec{w}) = \vec{0}$).

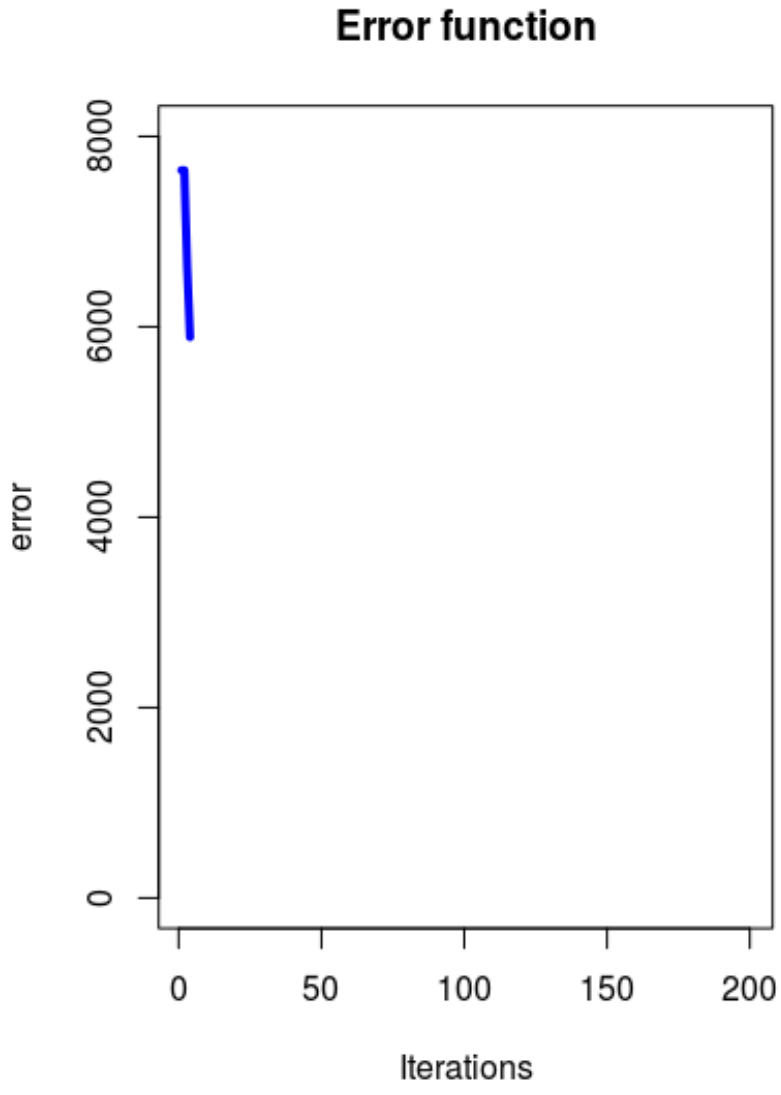
ADALINE – Animation





ADALINE – Animation





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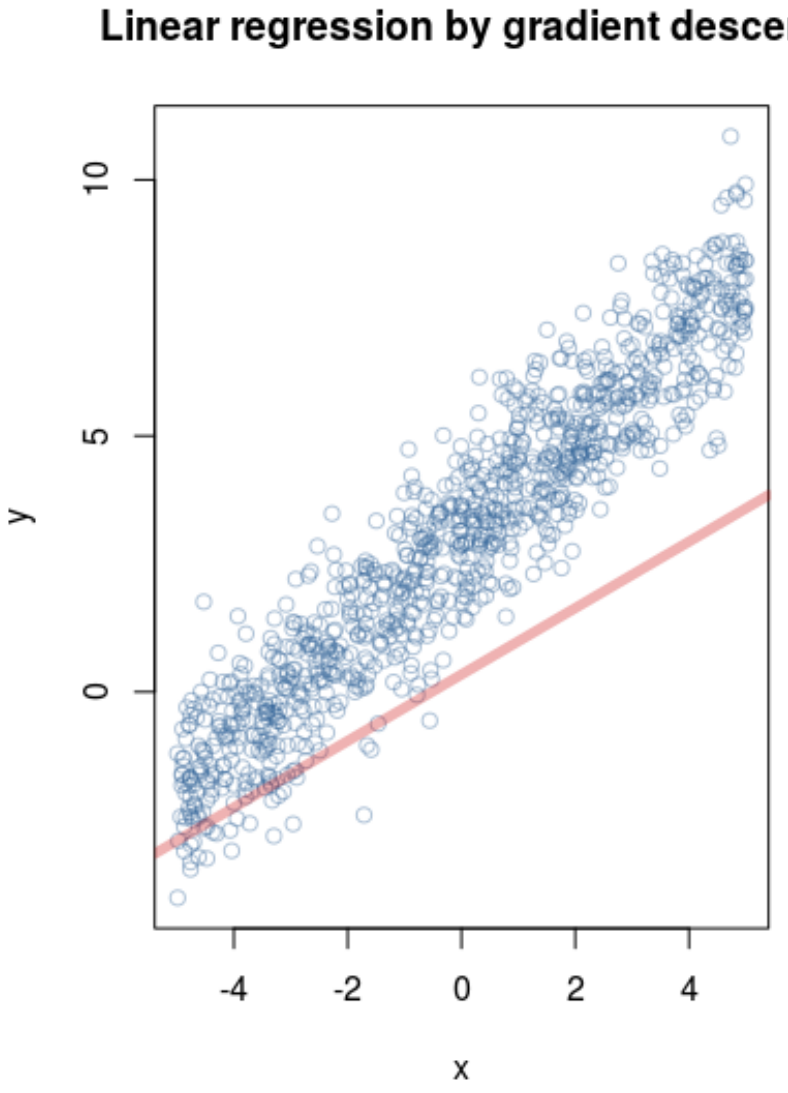

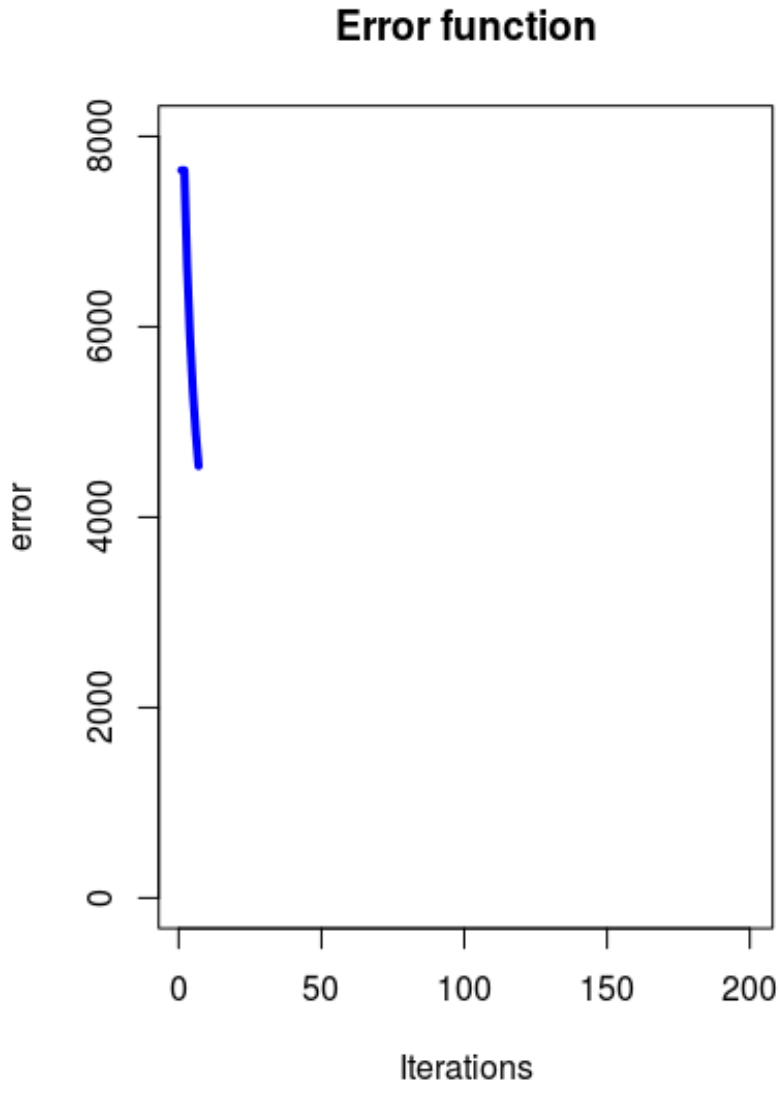

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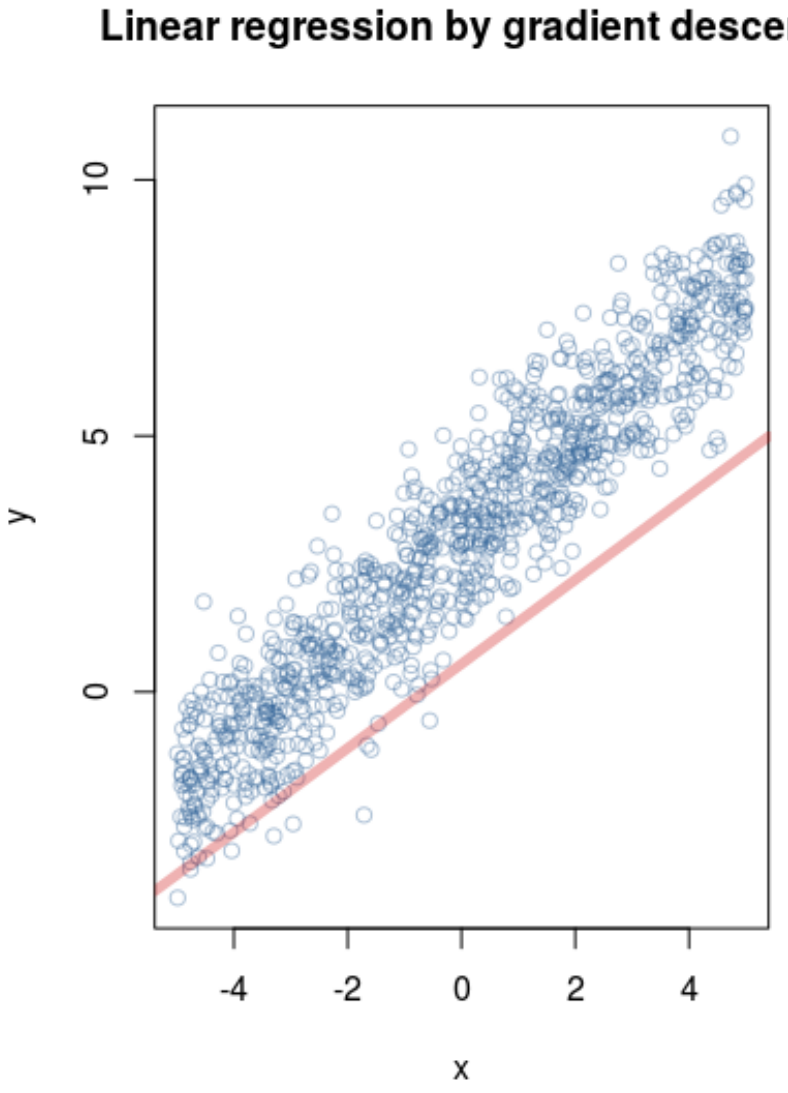

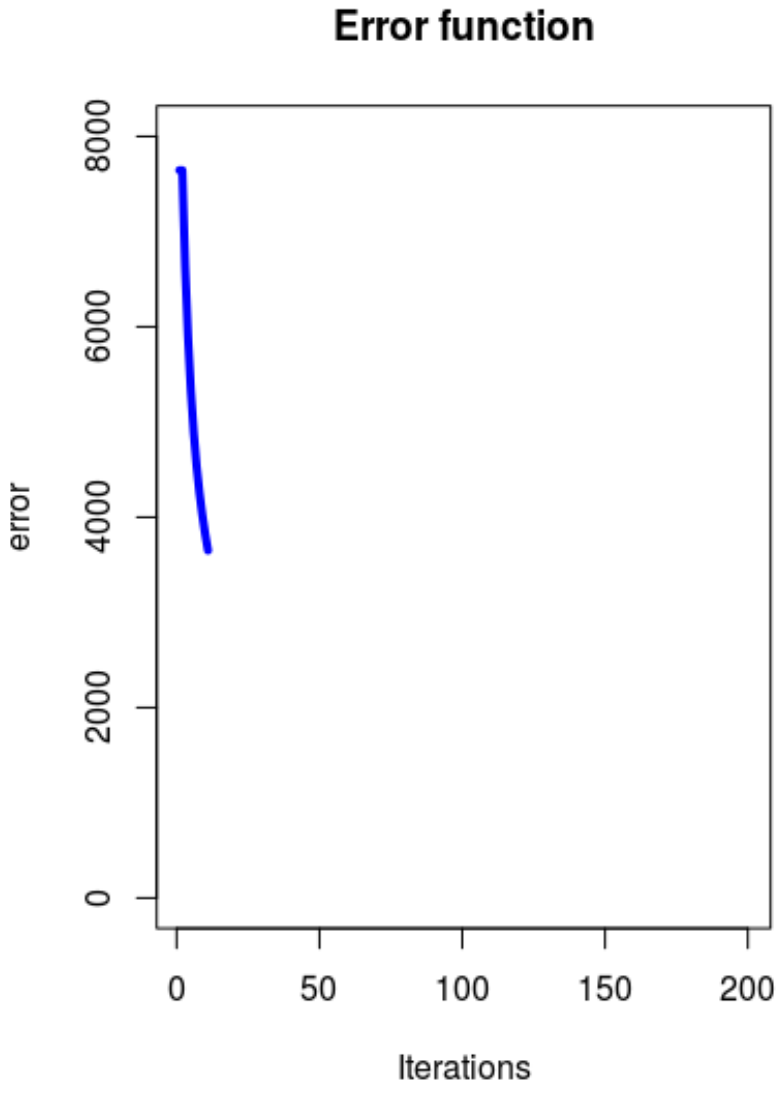

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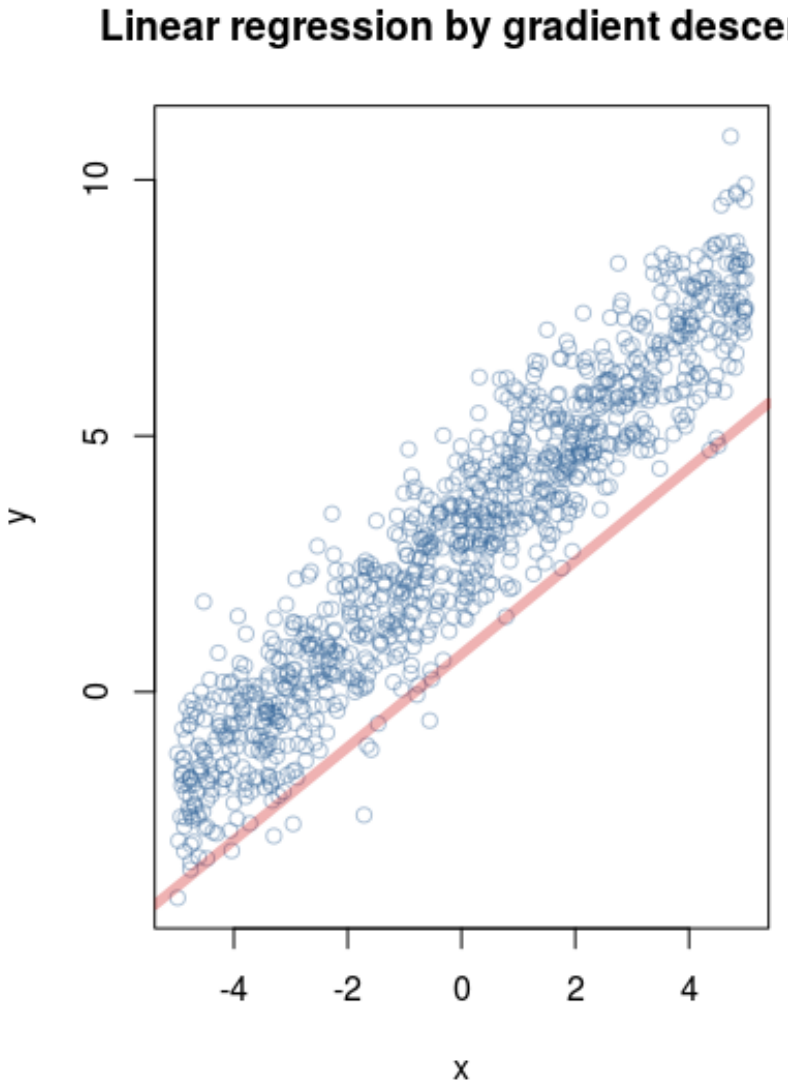

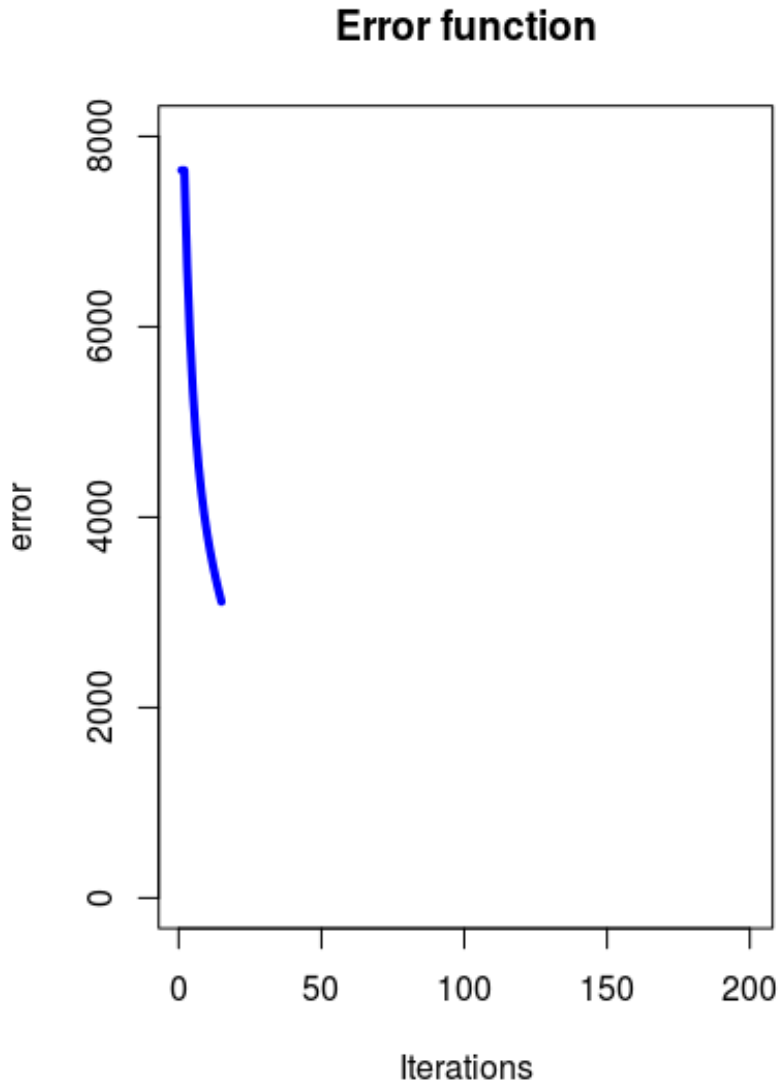

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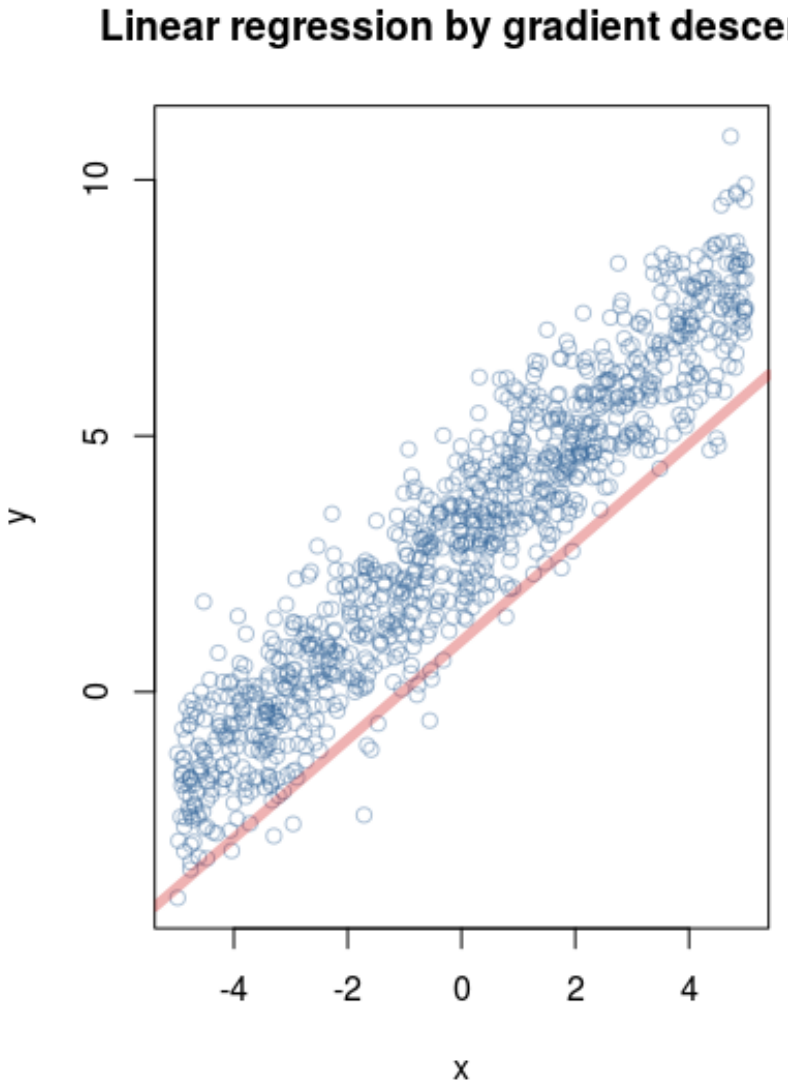

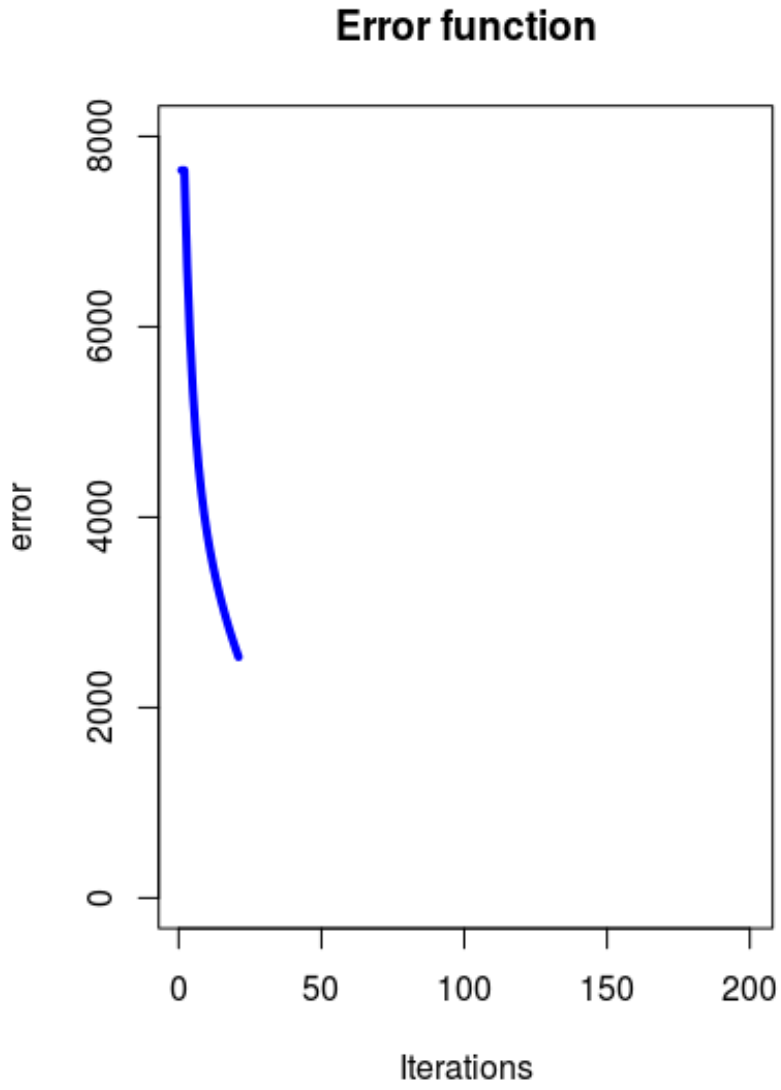

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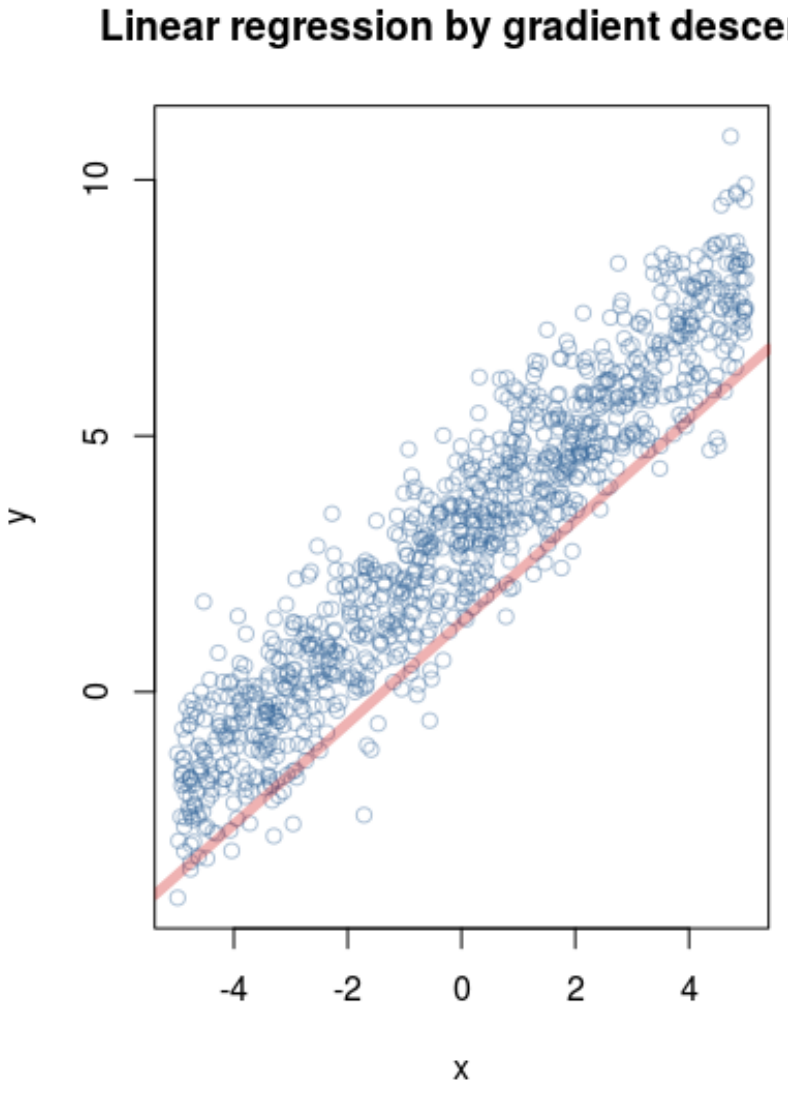

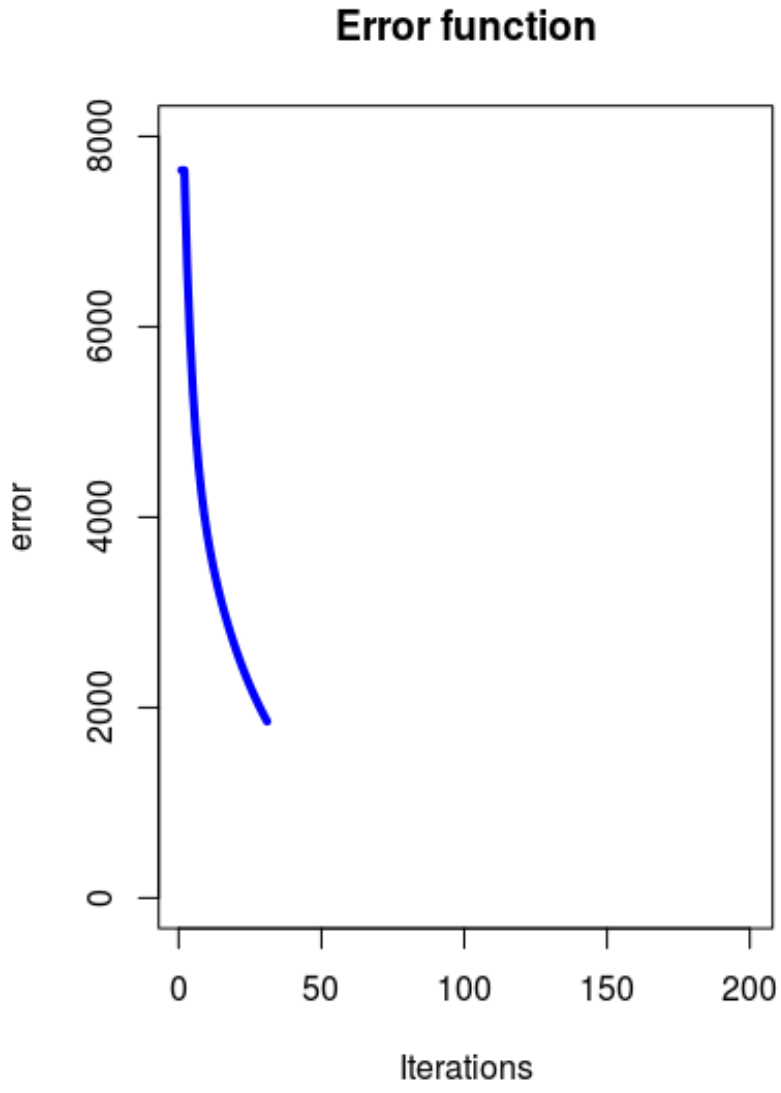

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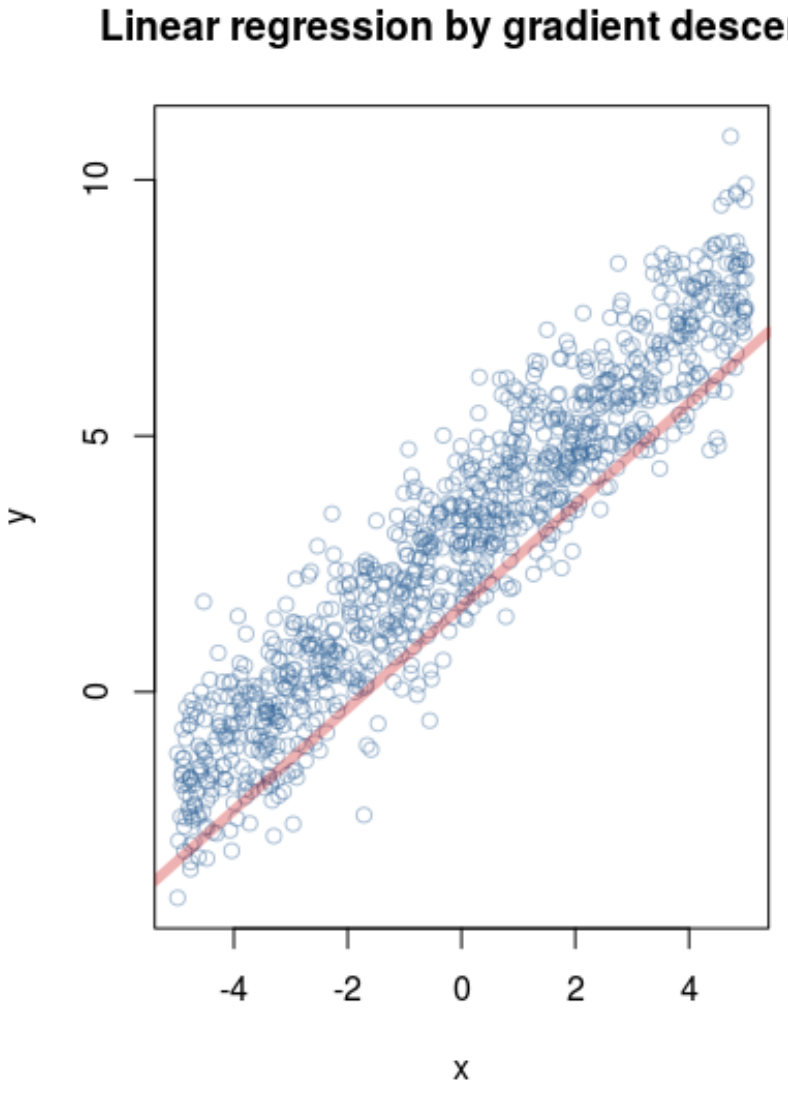

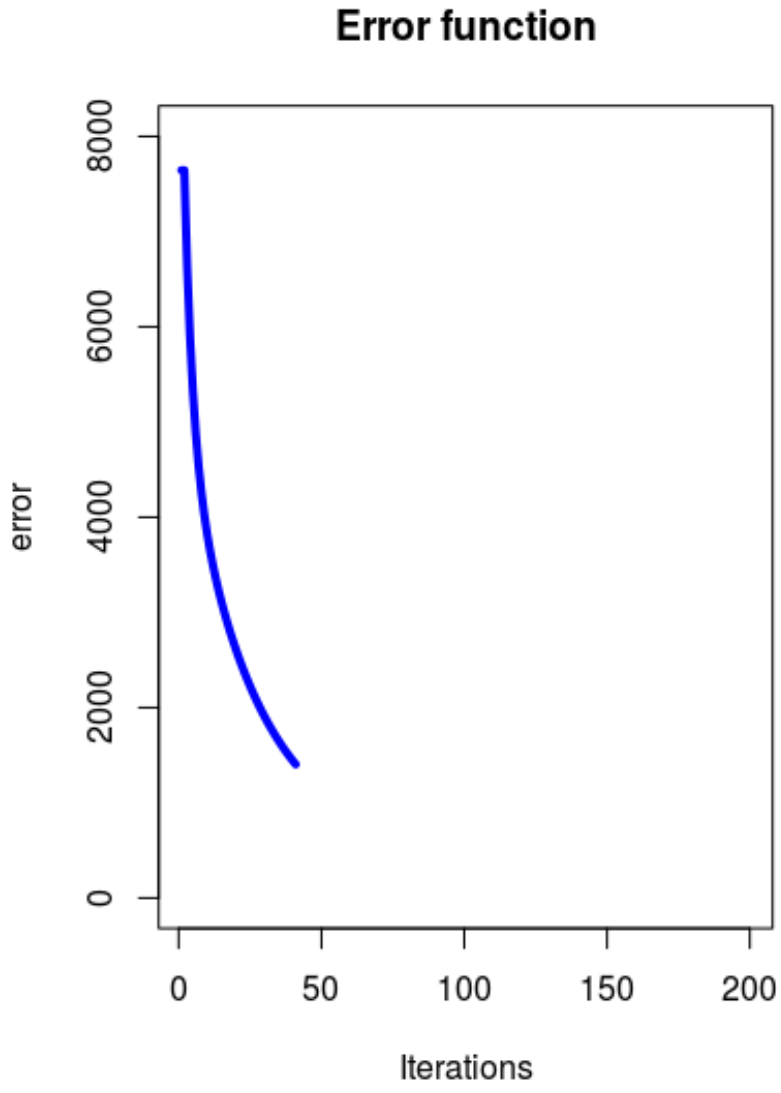

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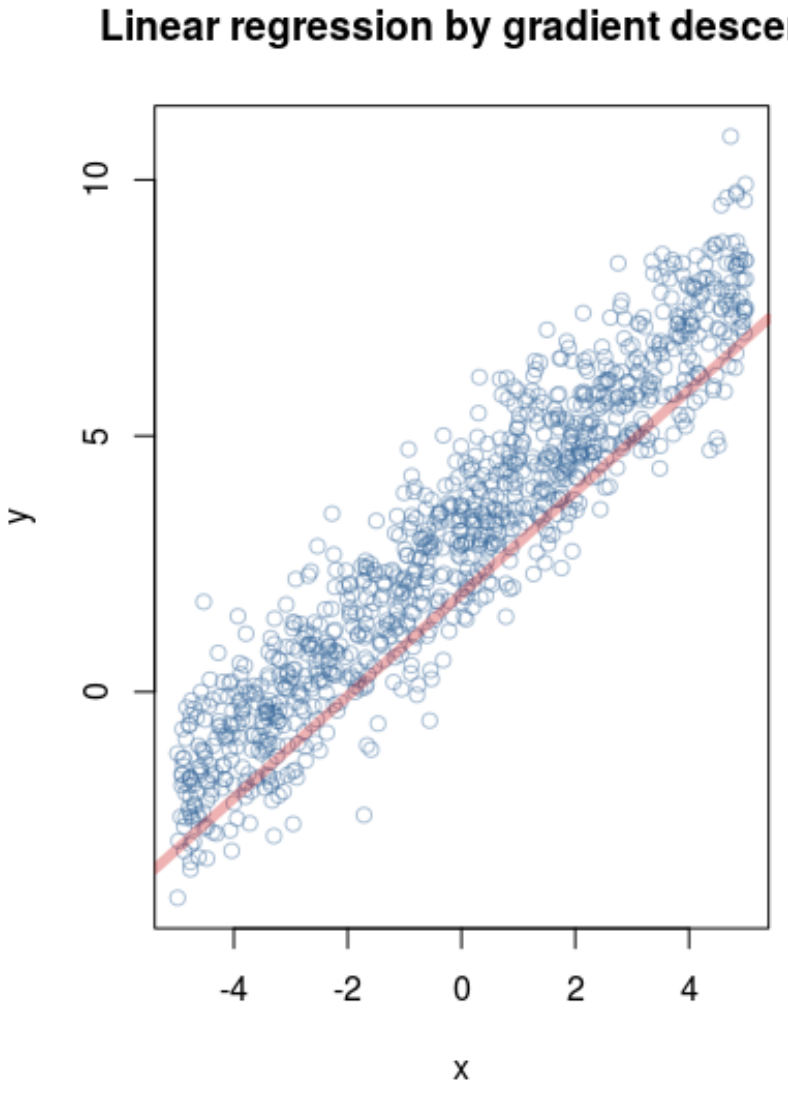

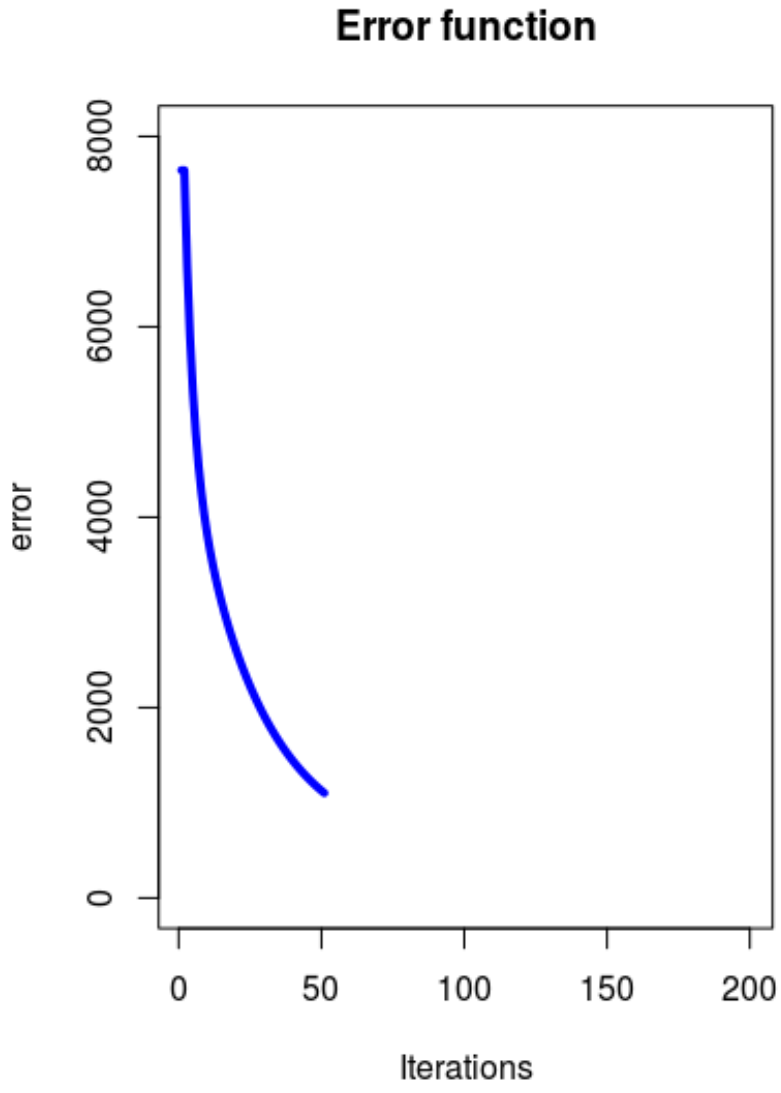

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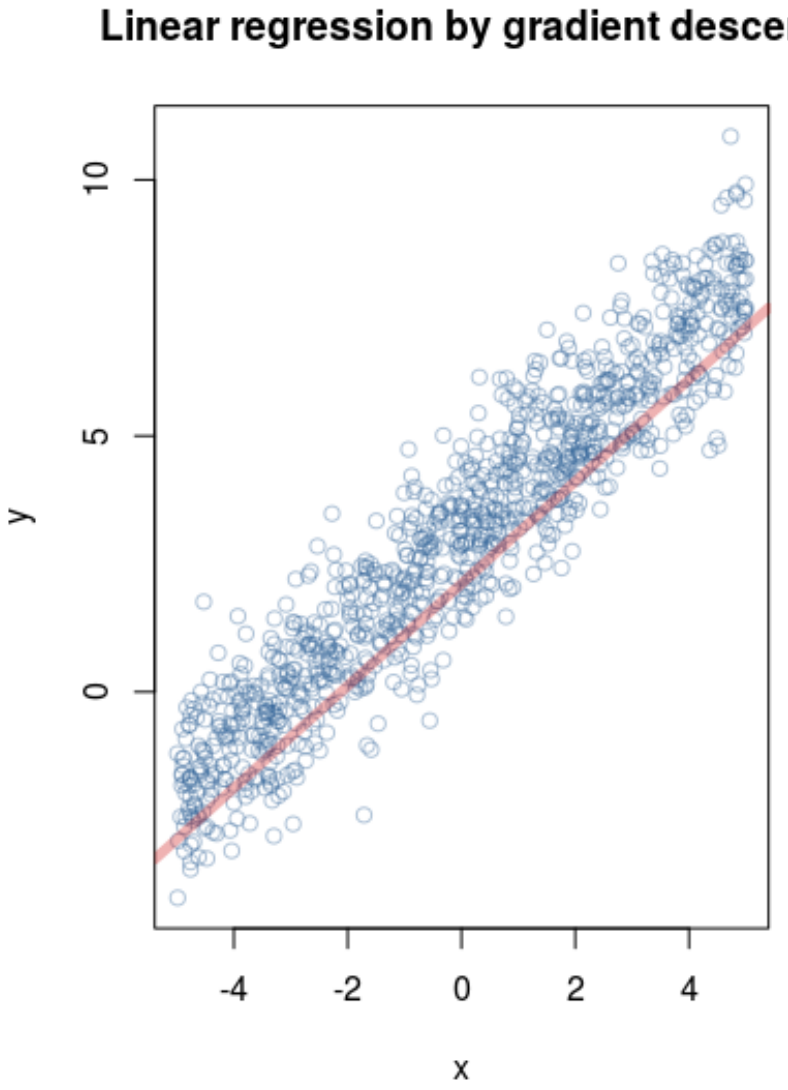

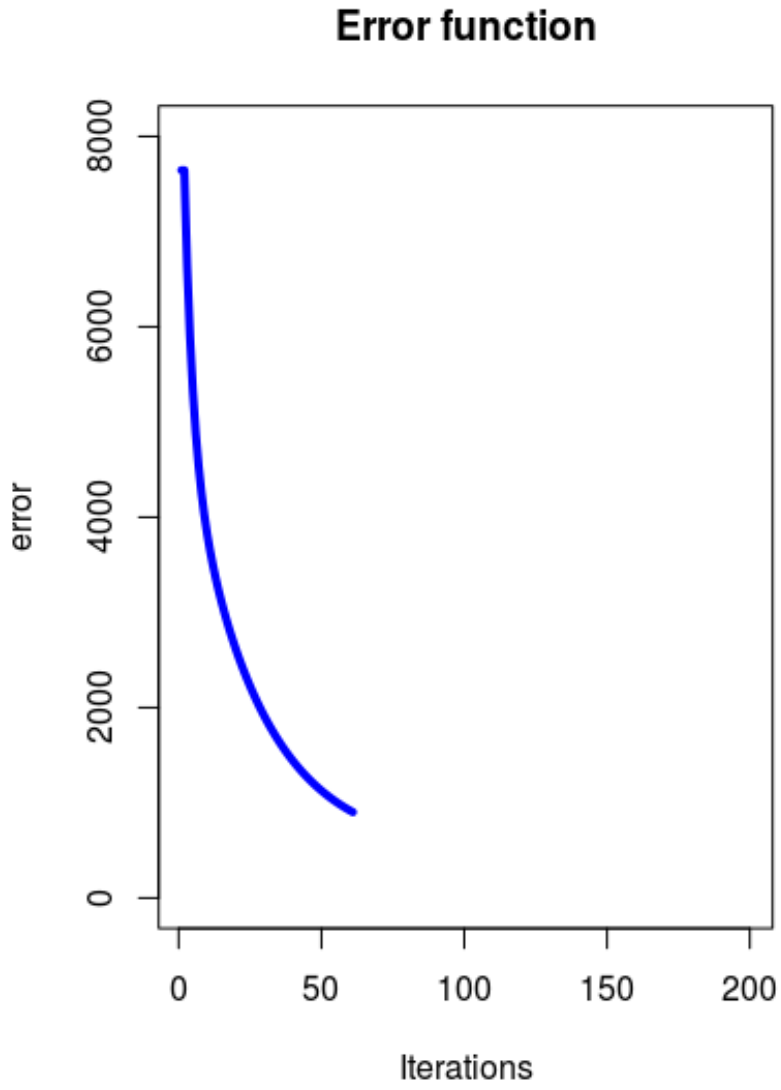

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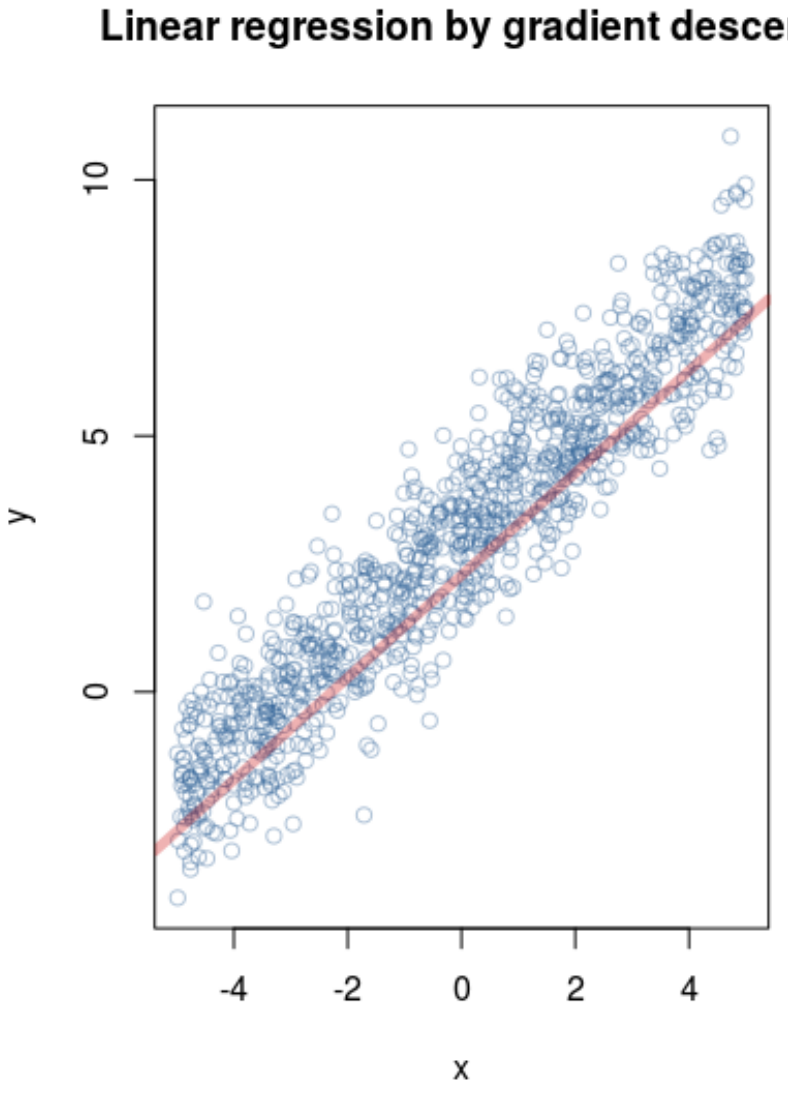

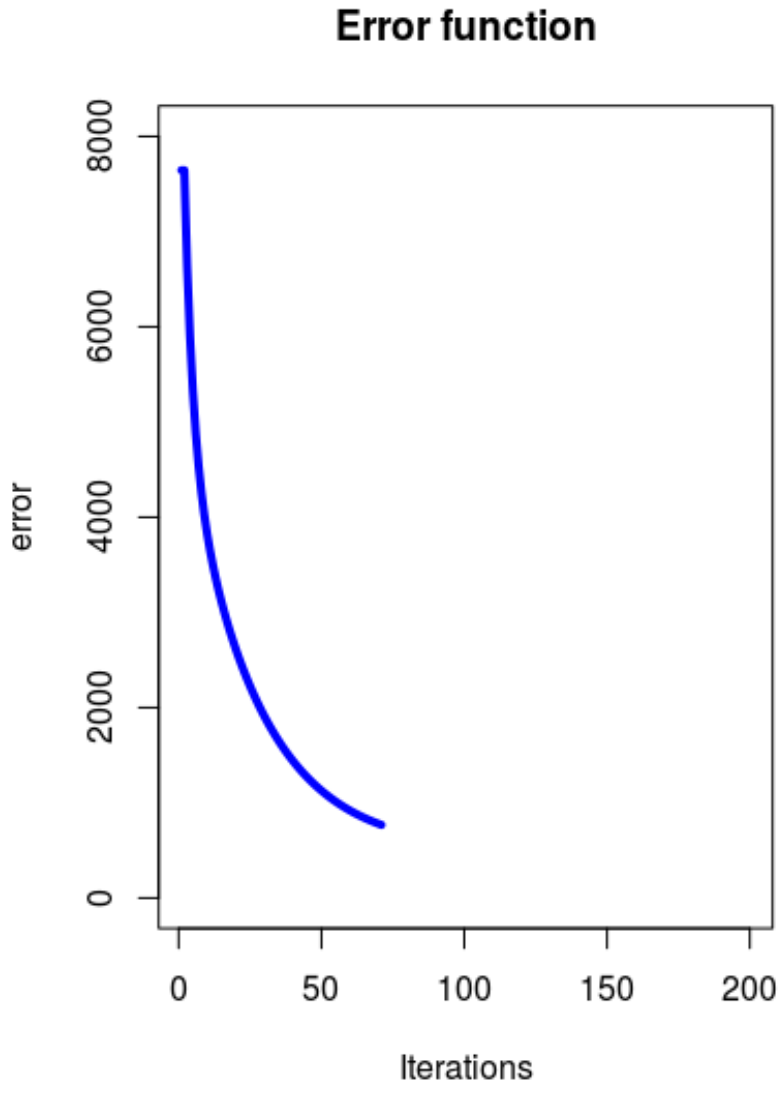

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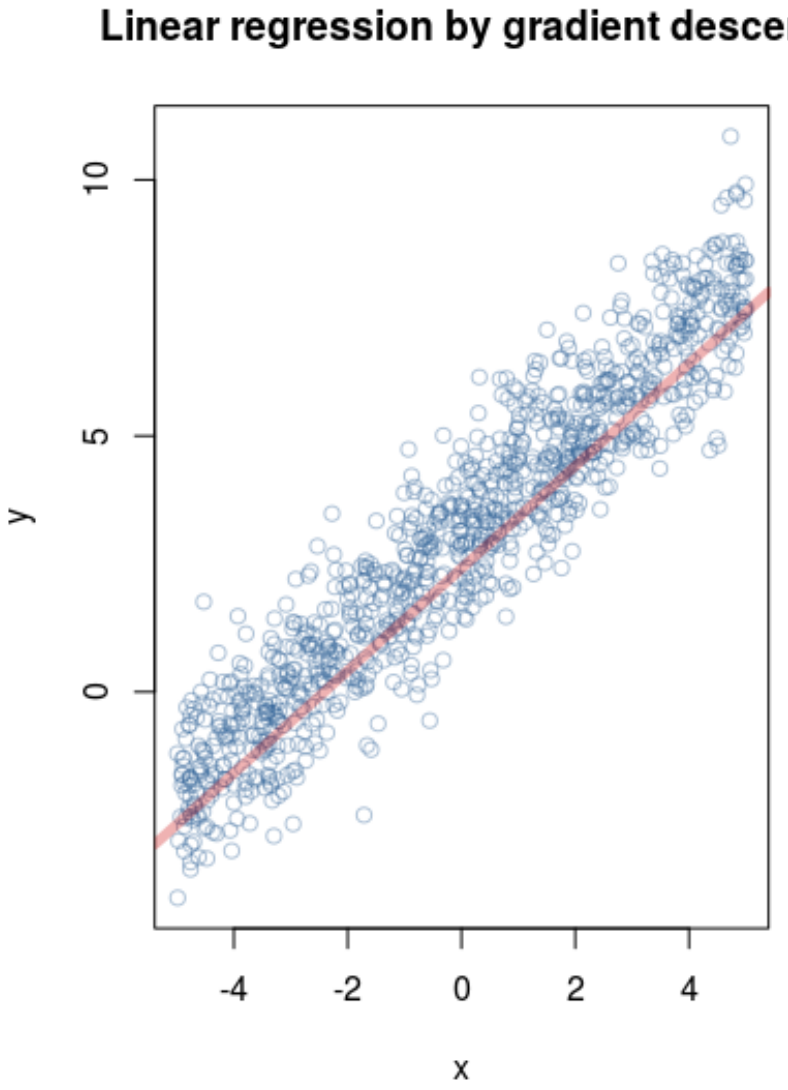

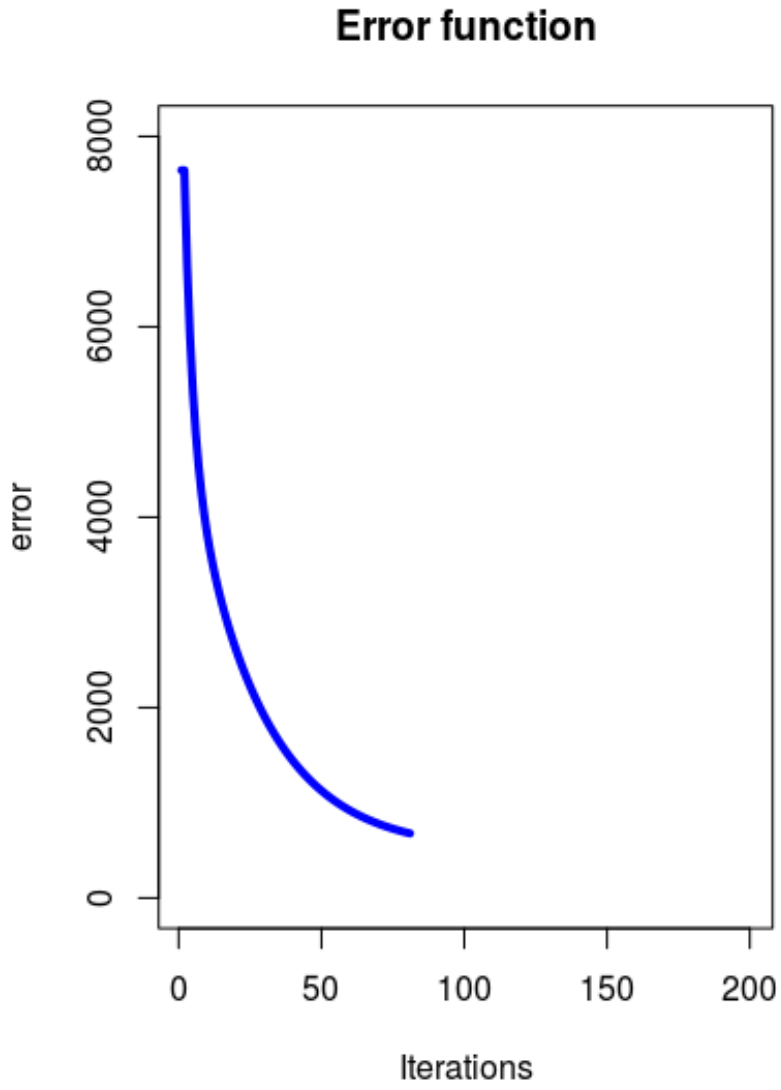

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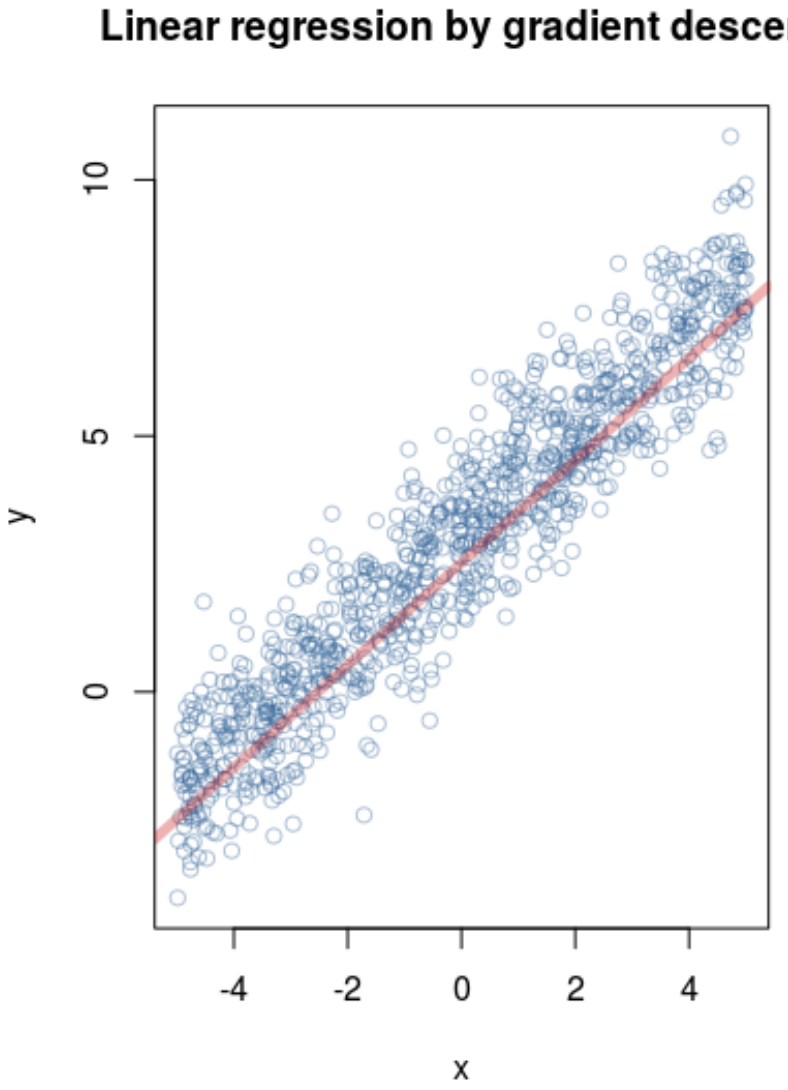

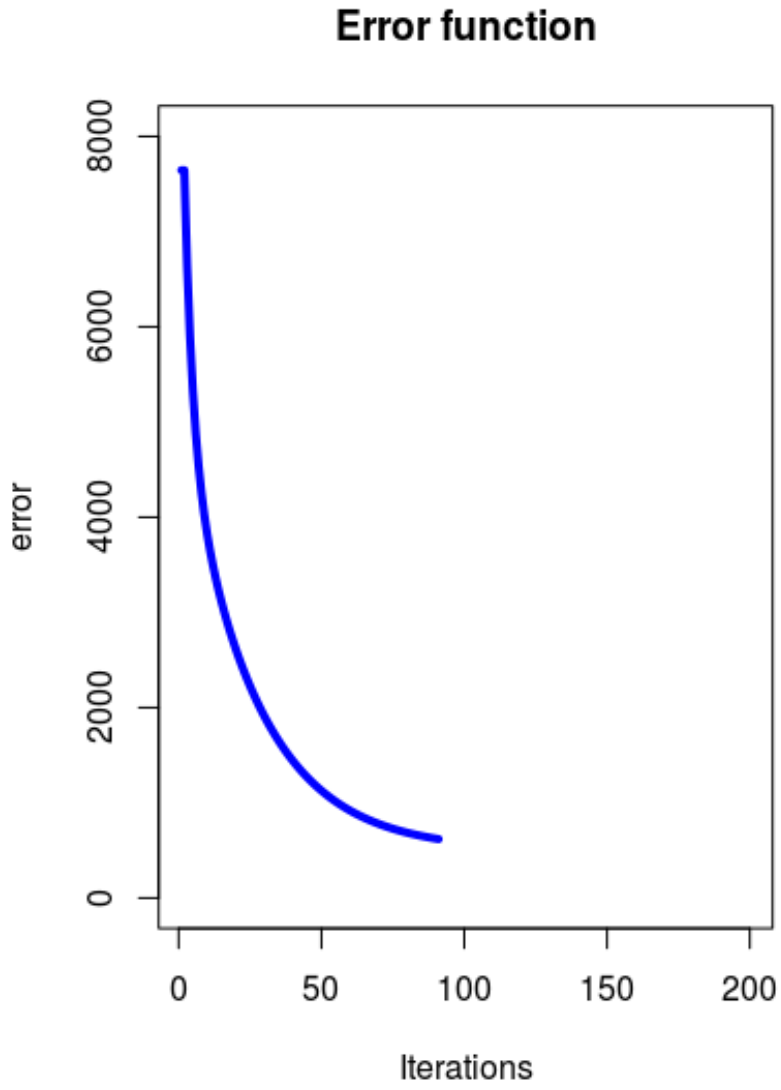

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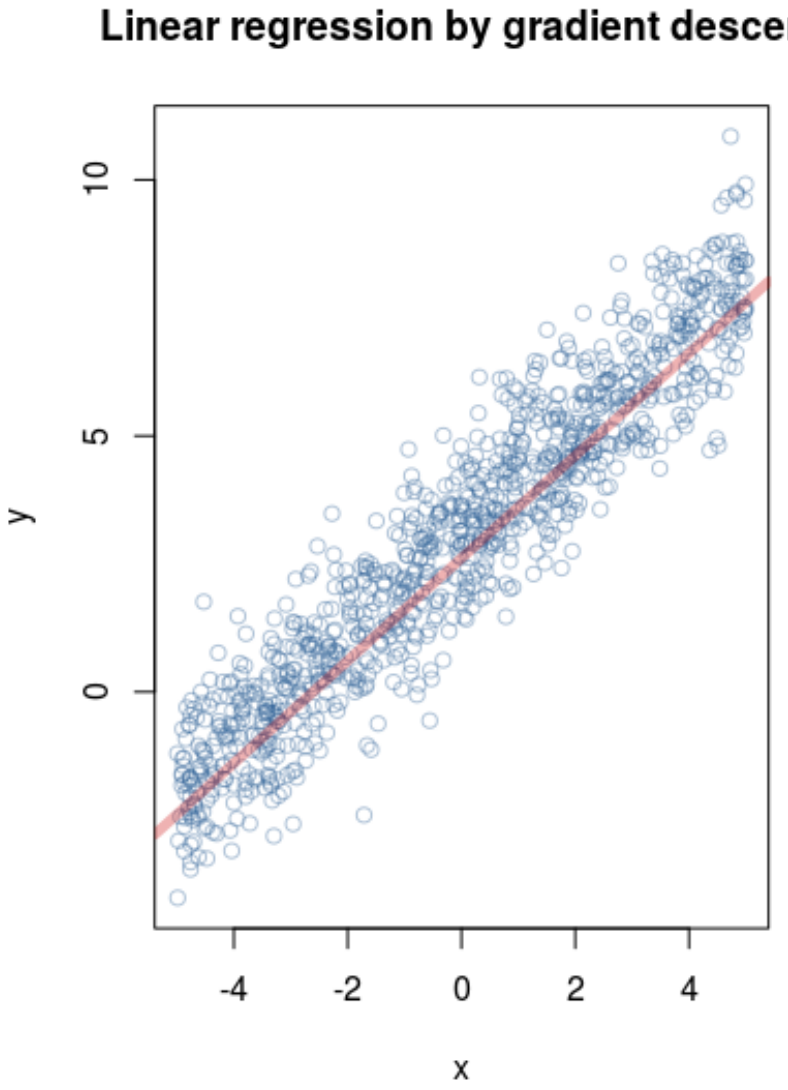

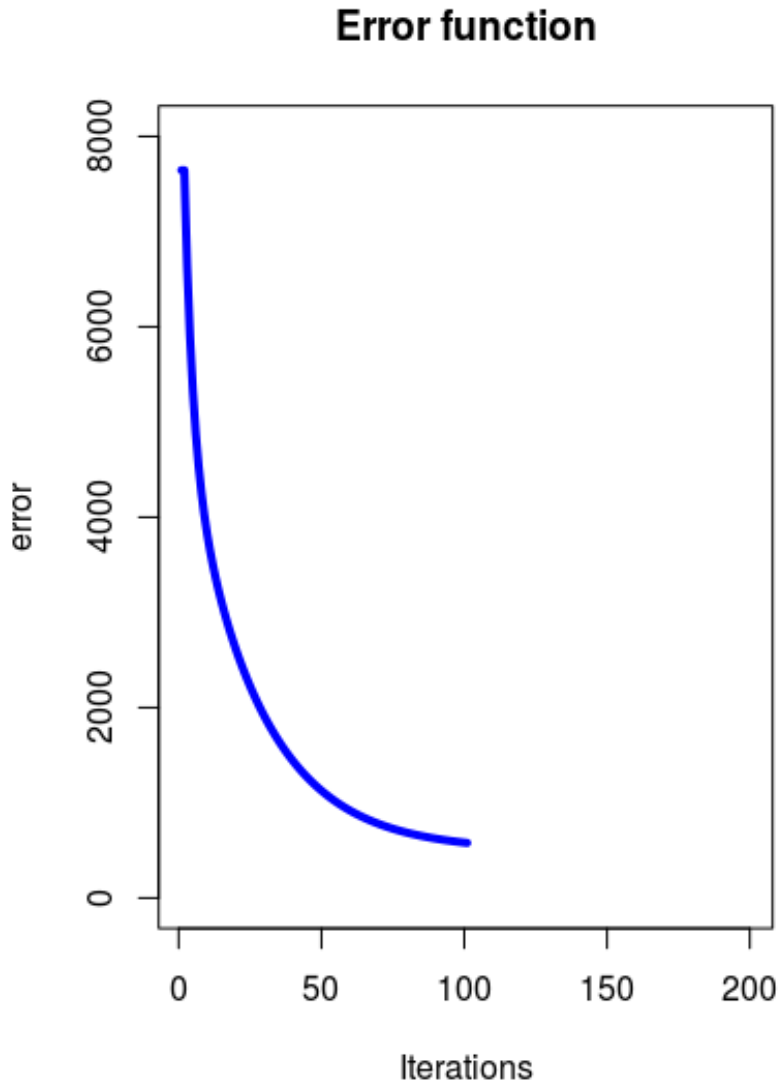

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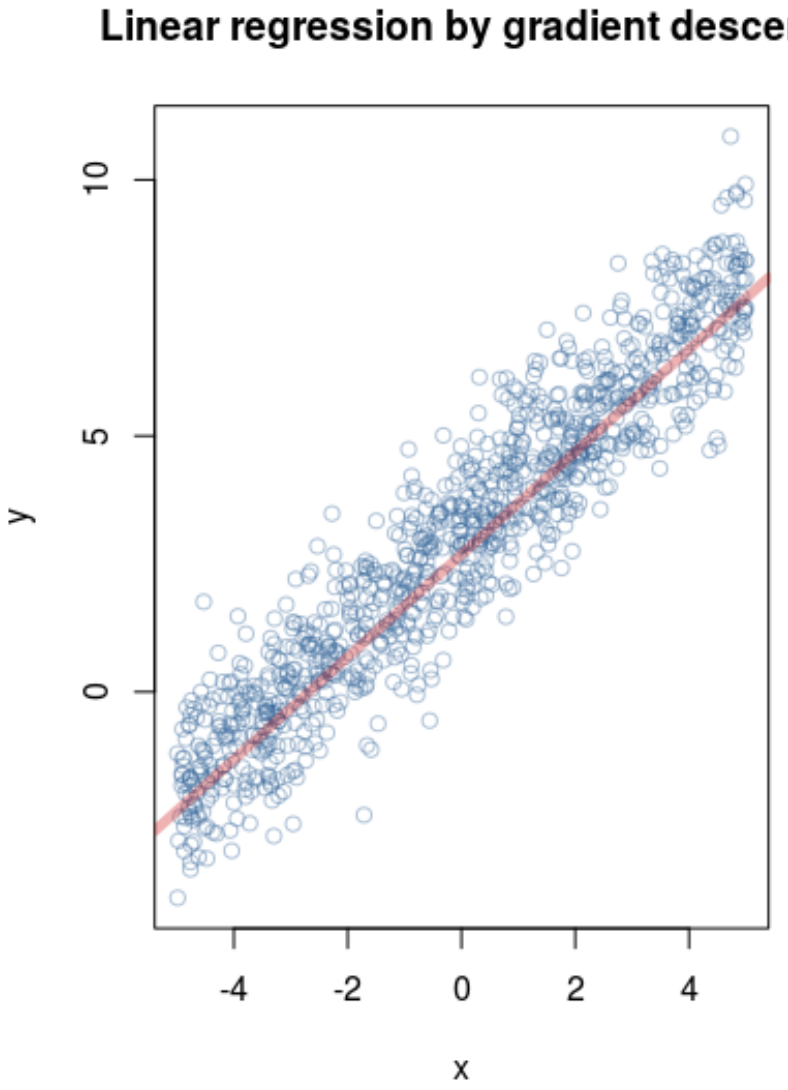

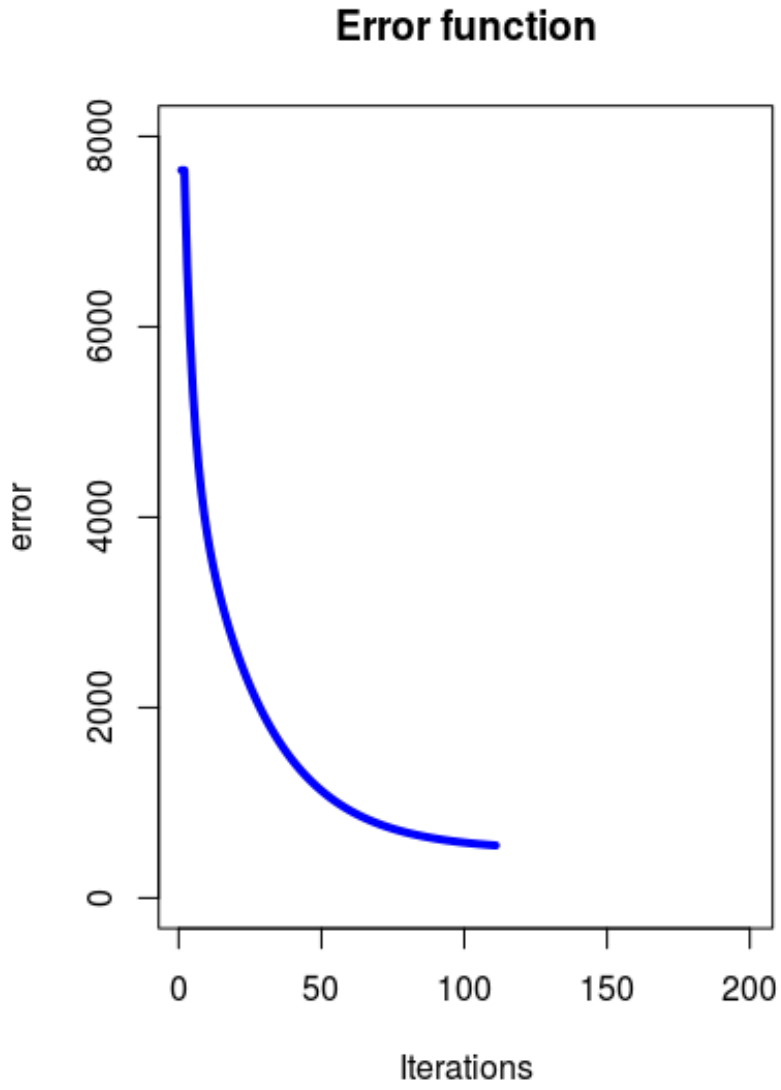

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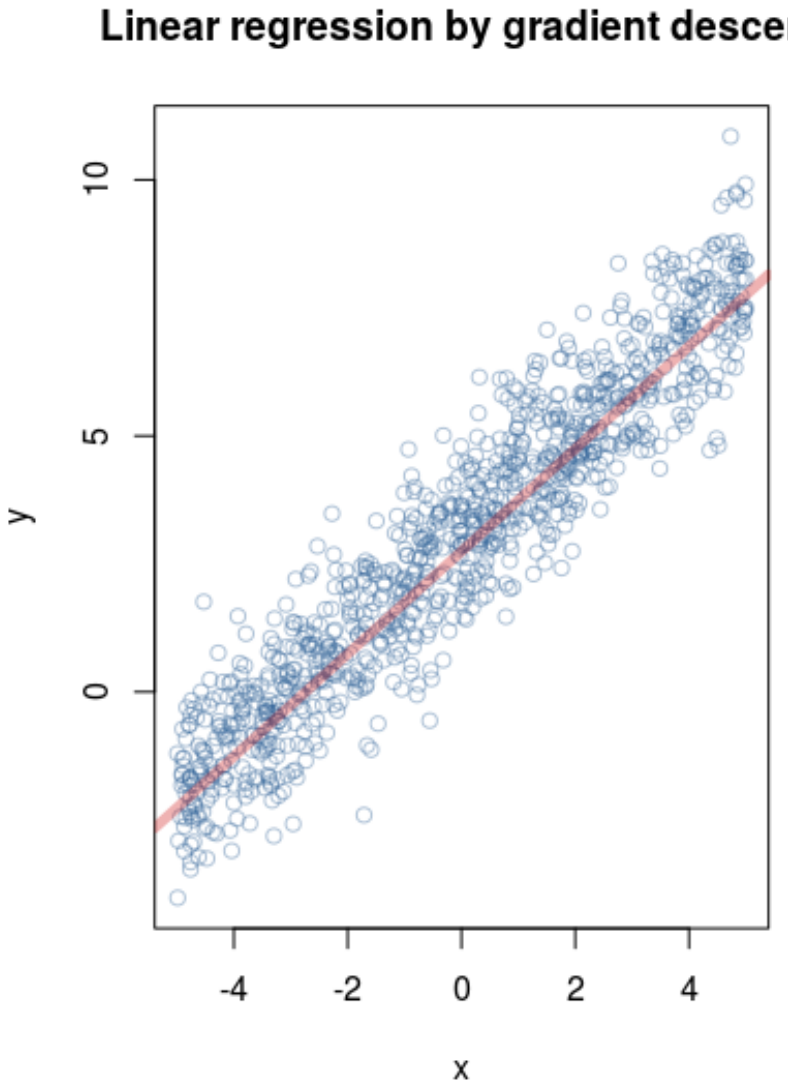
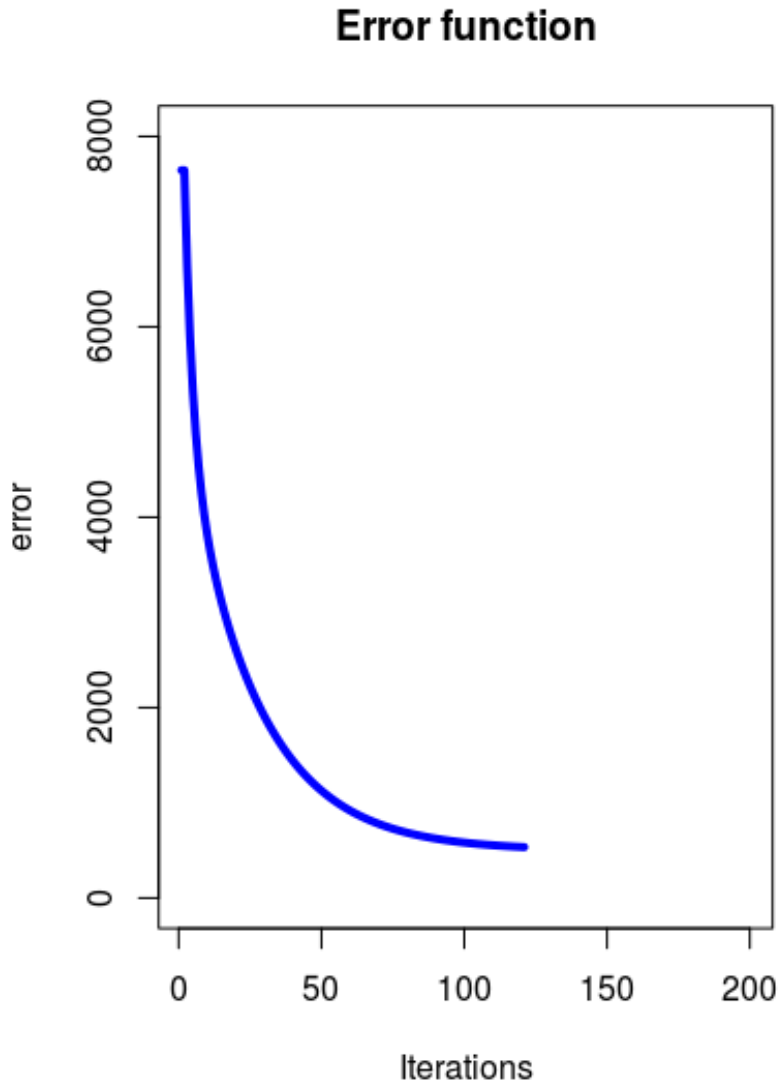
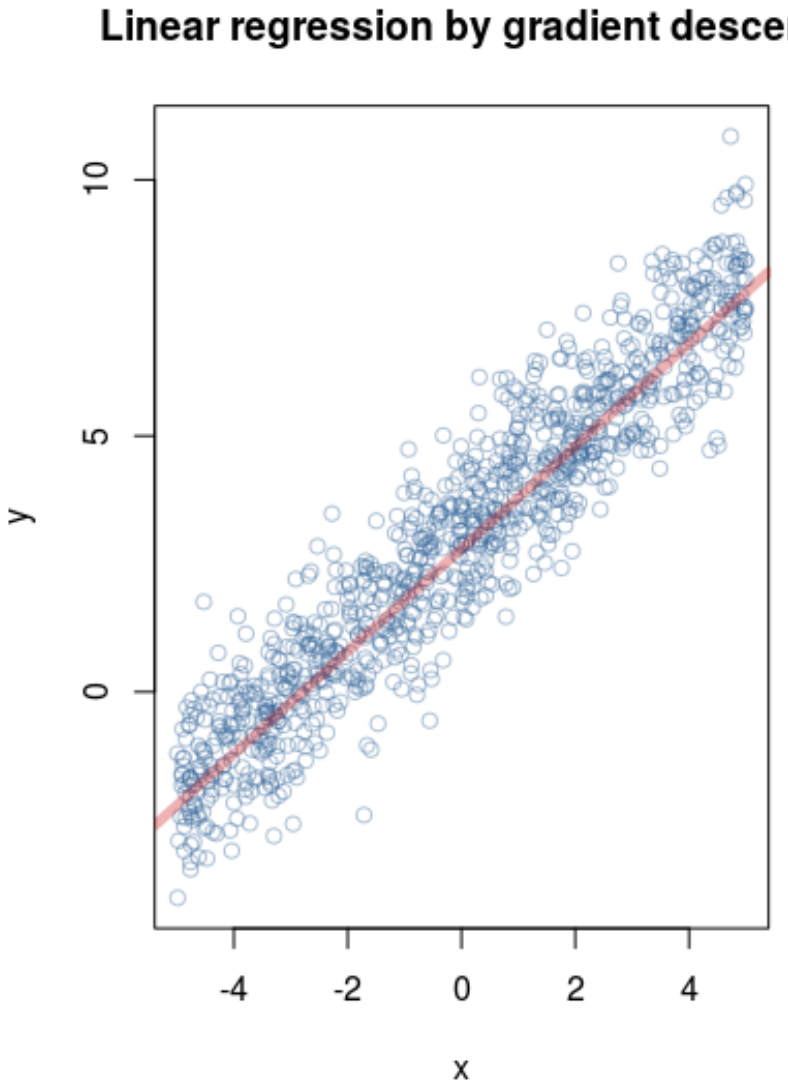
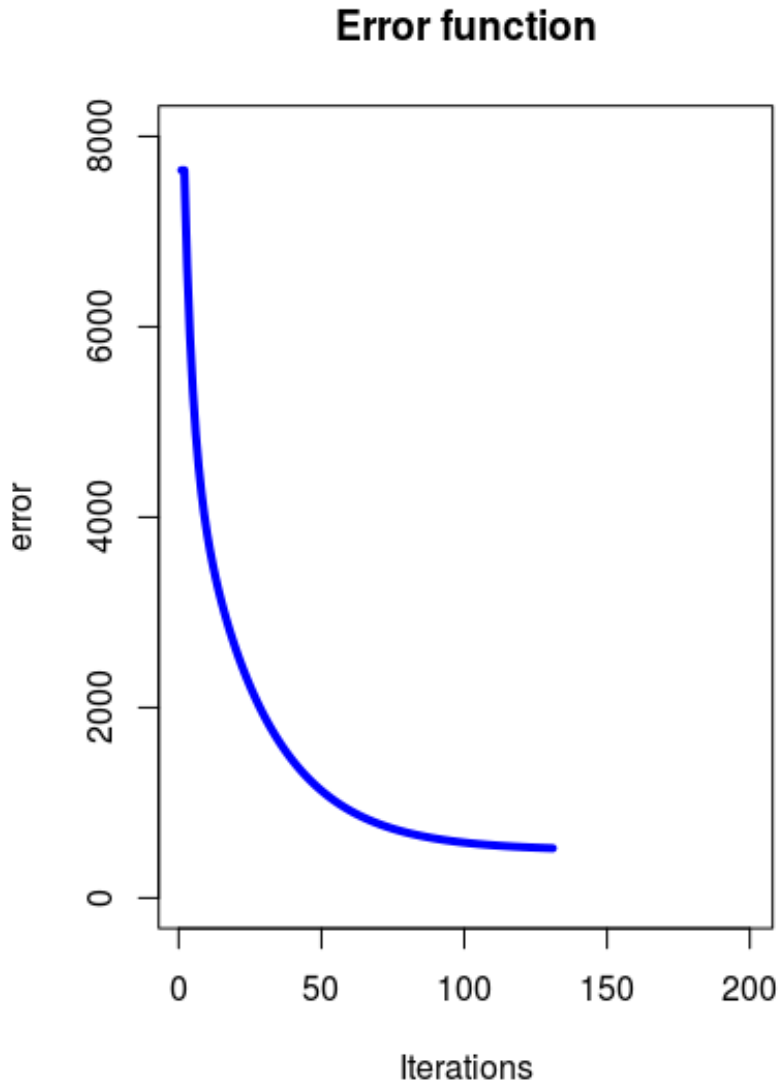


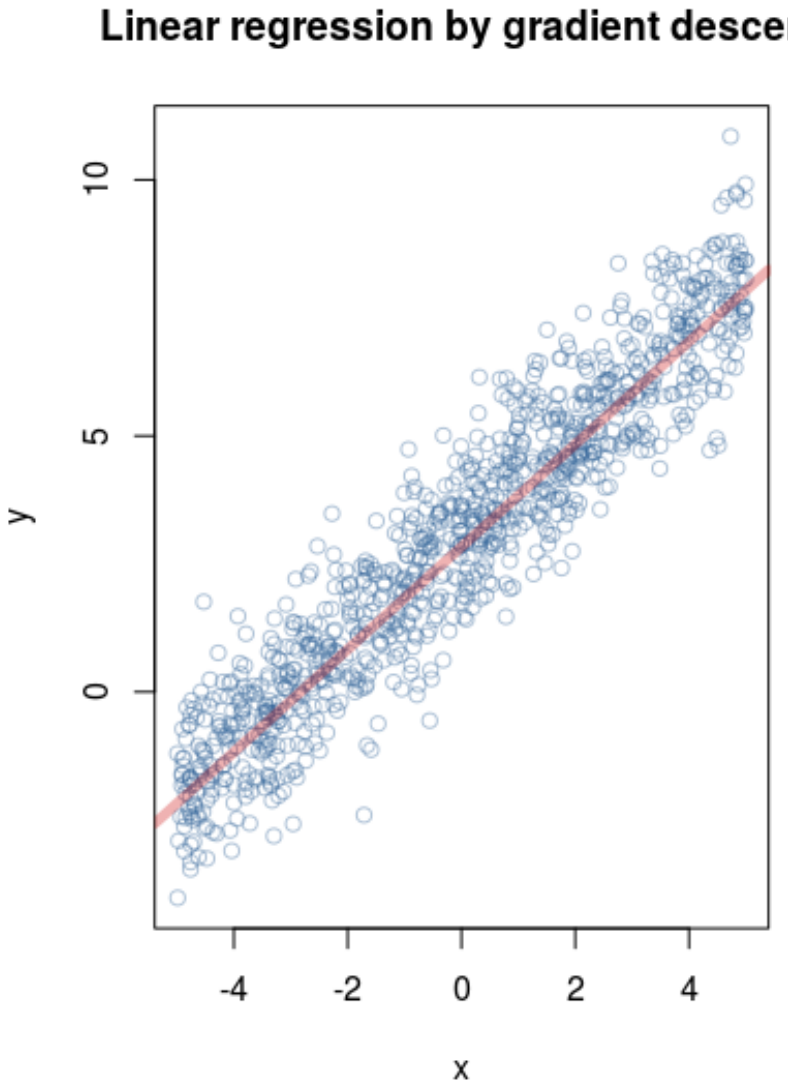


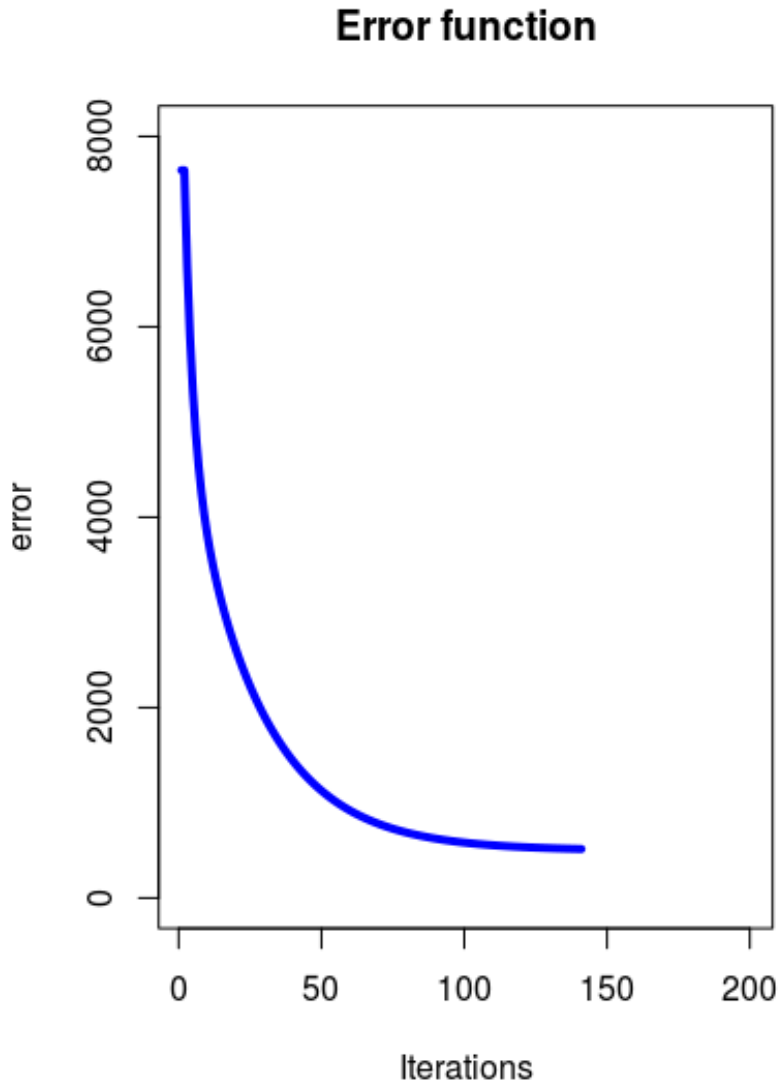
ADALINE – Animation





ADALINE – Animation





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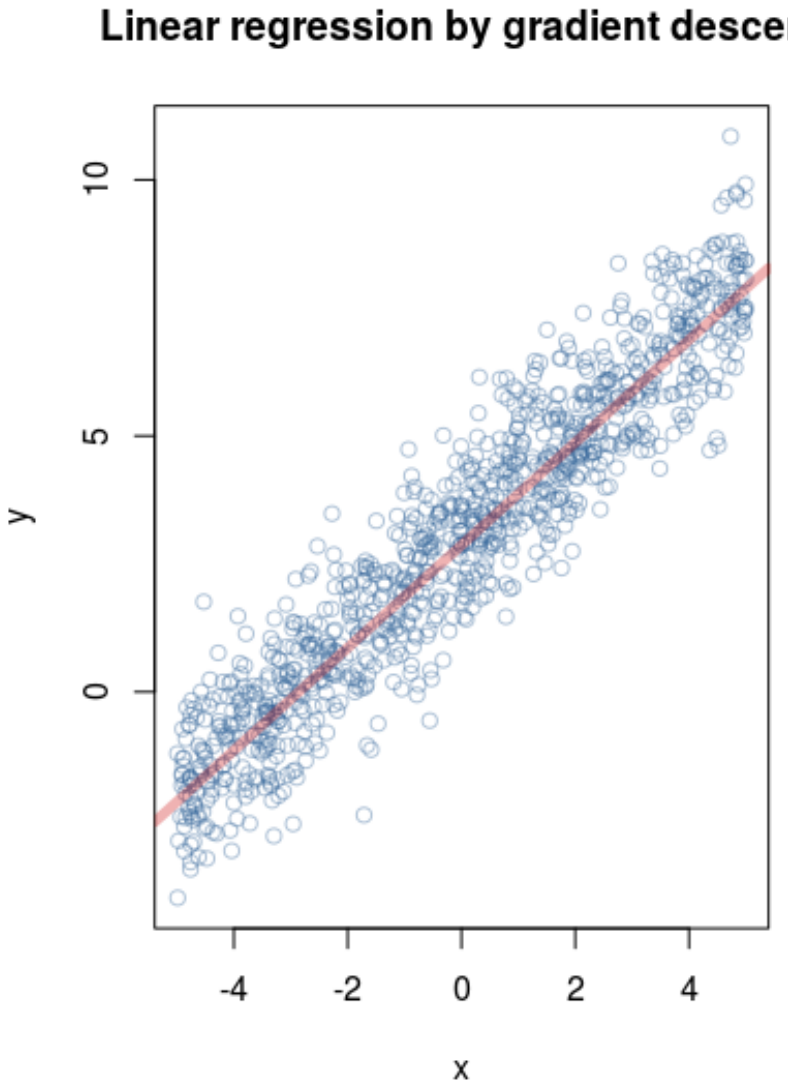

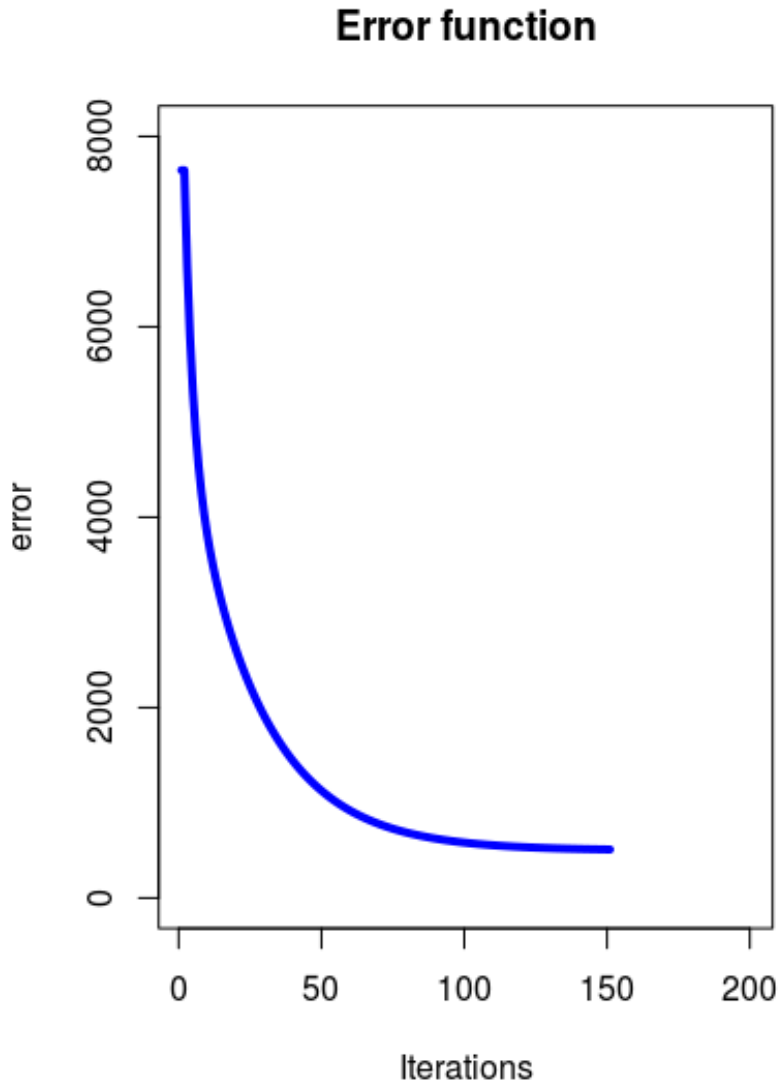

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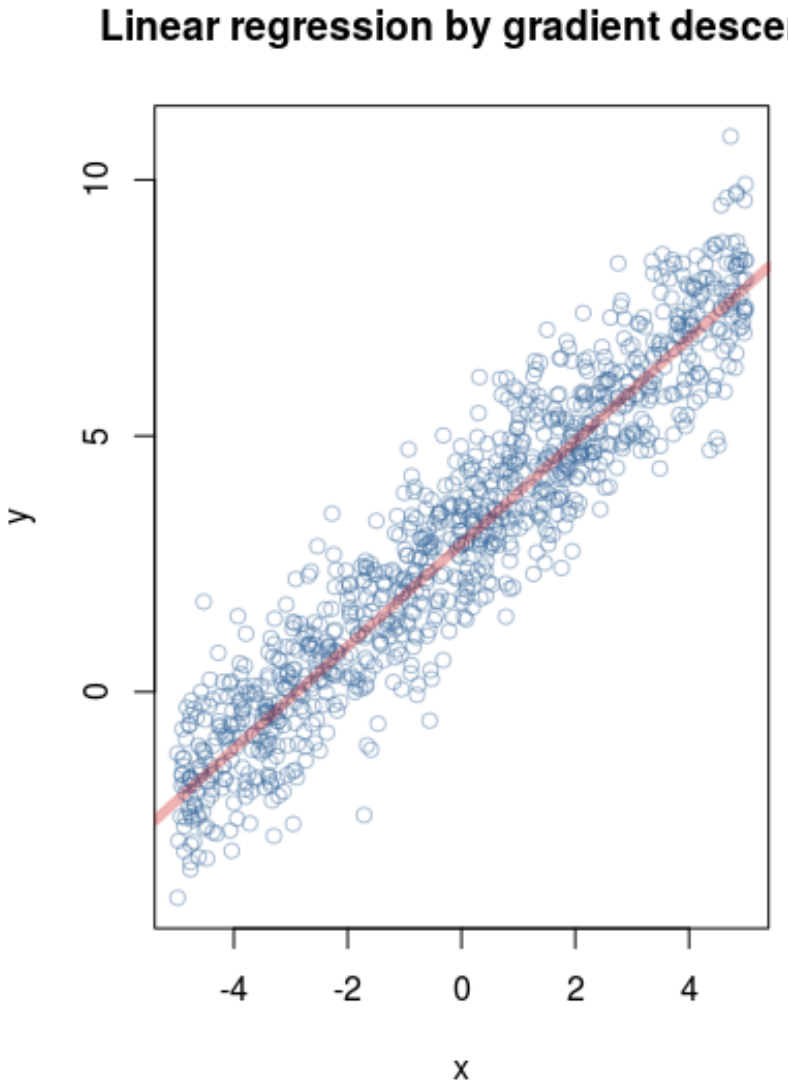

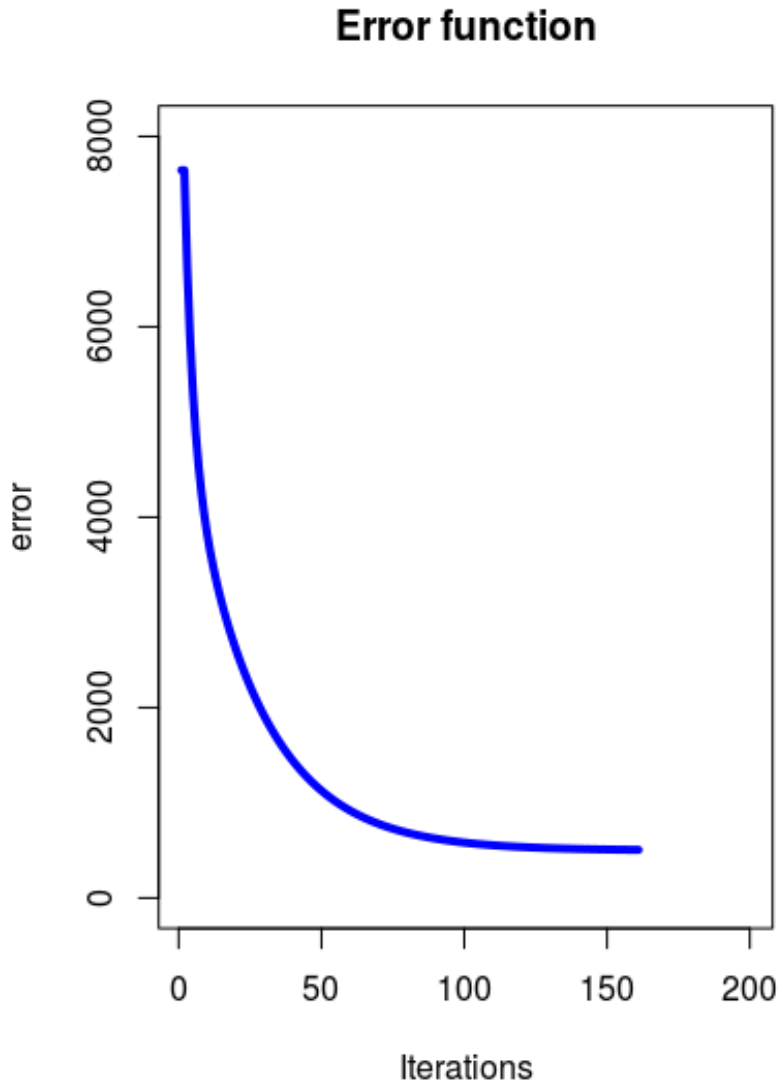

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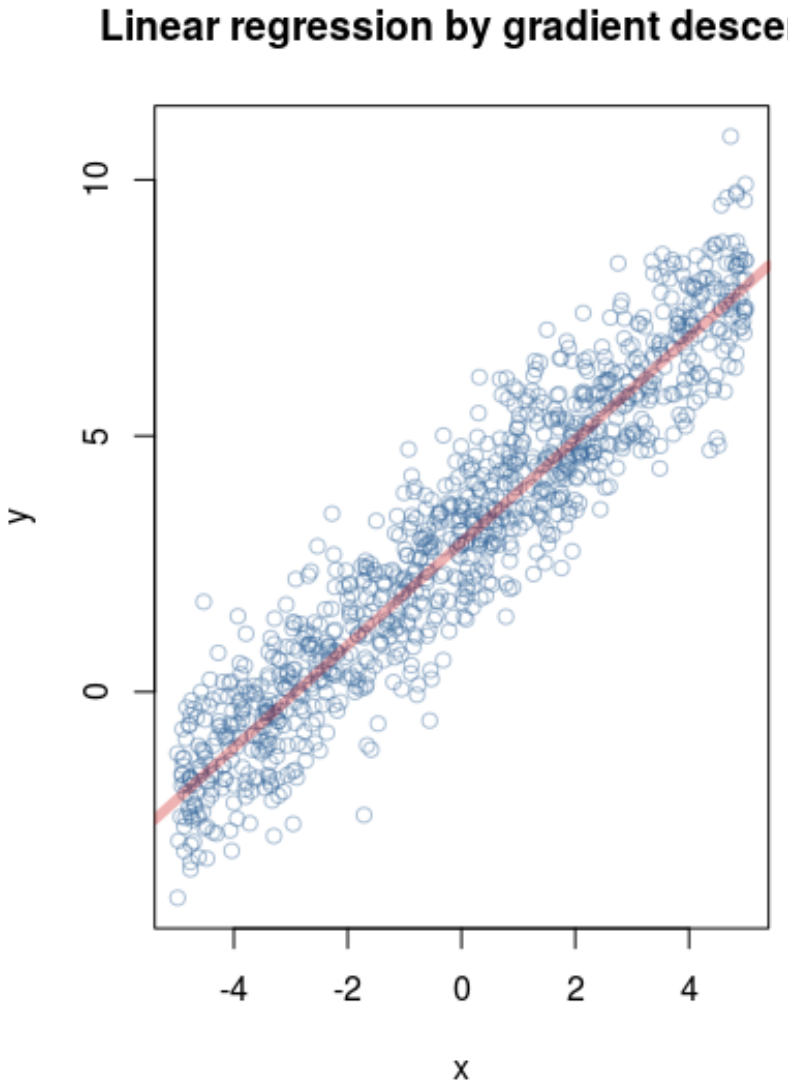

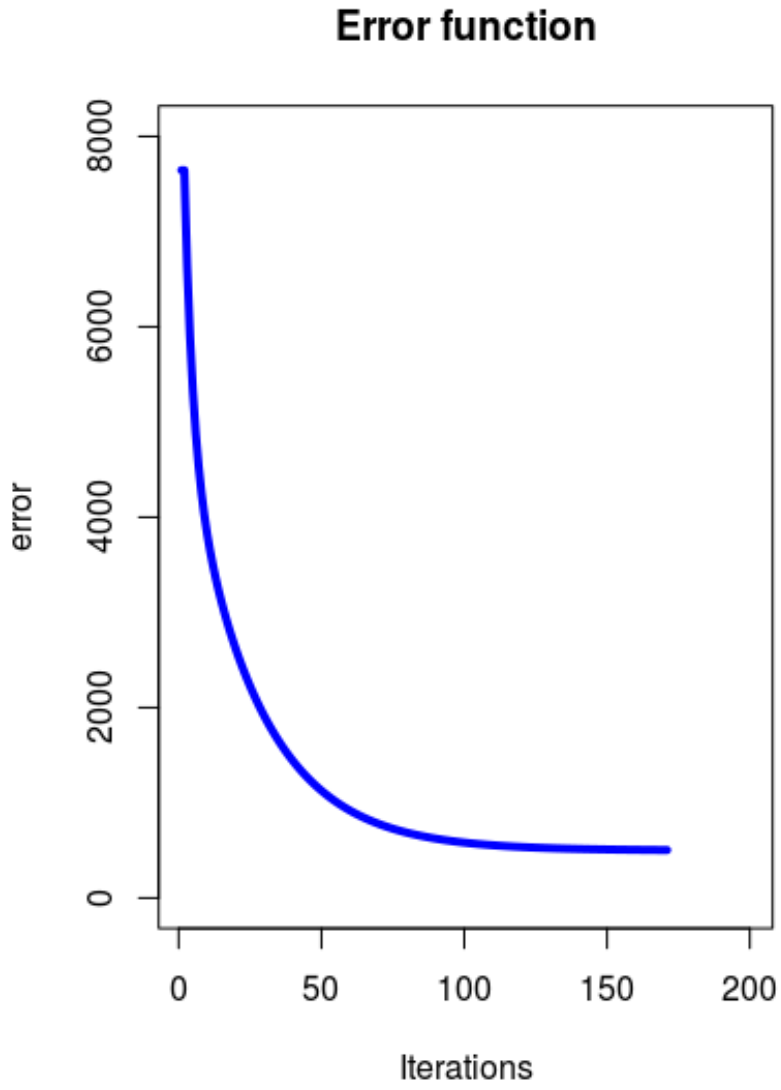

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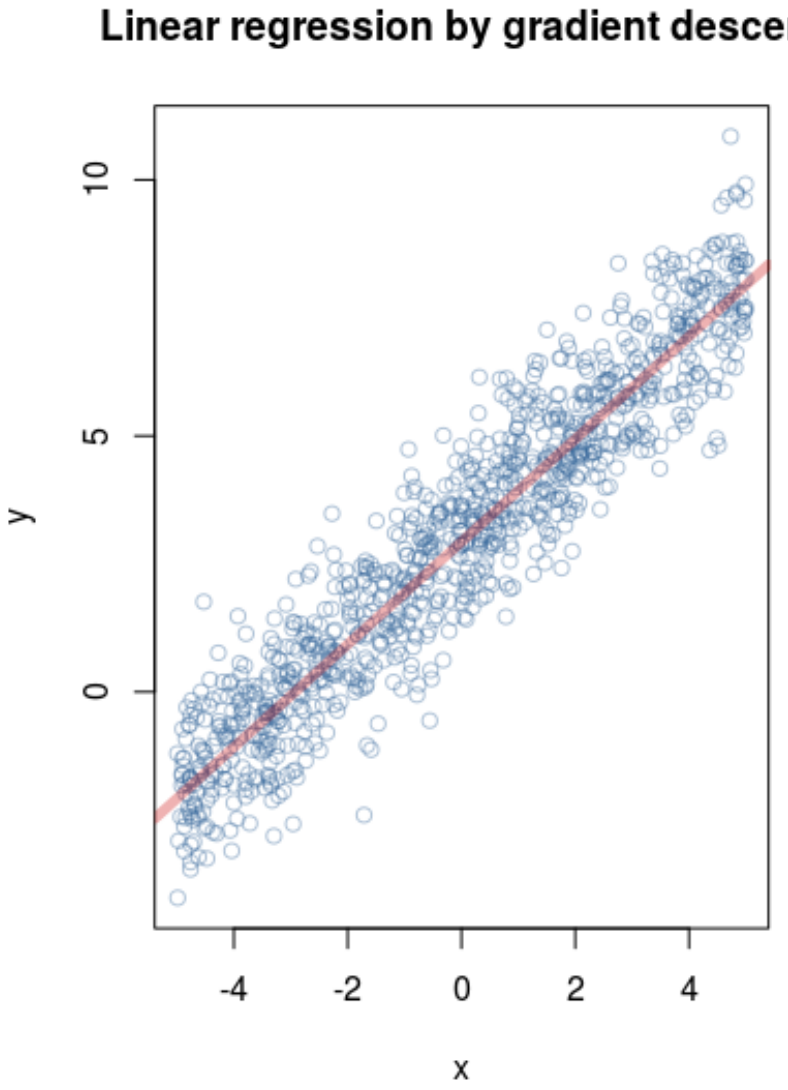

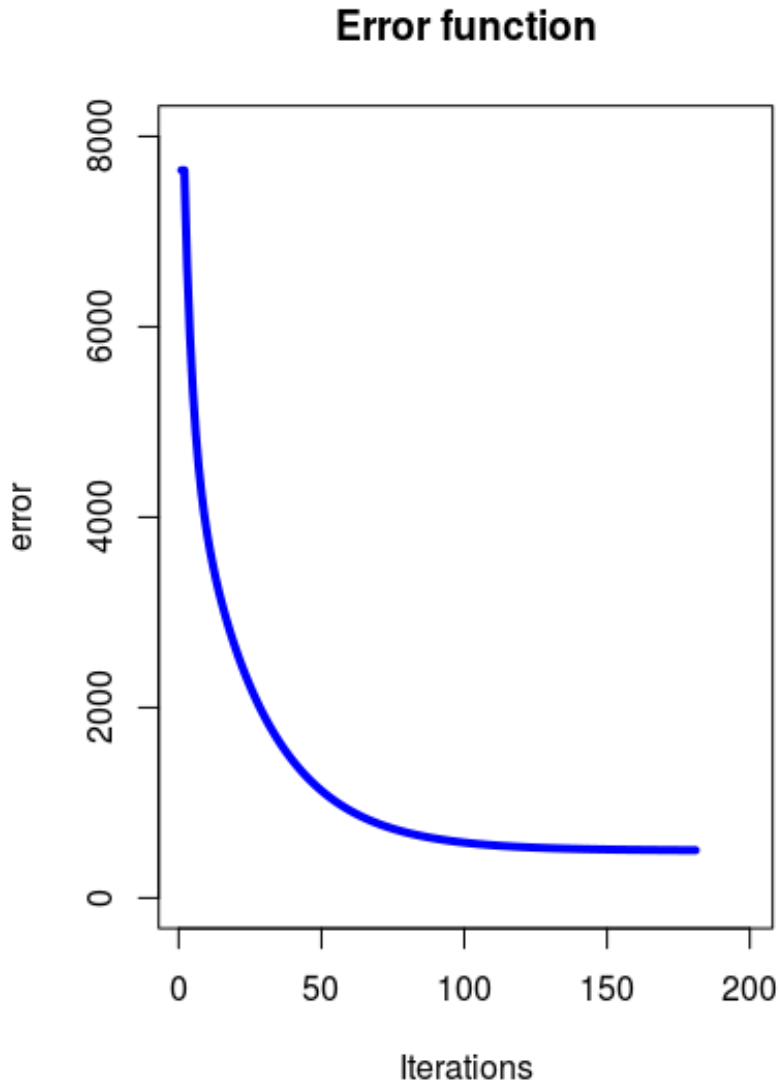

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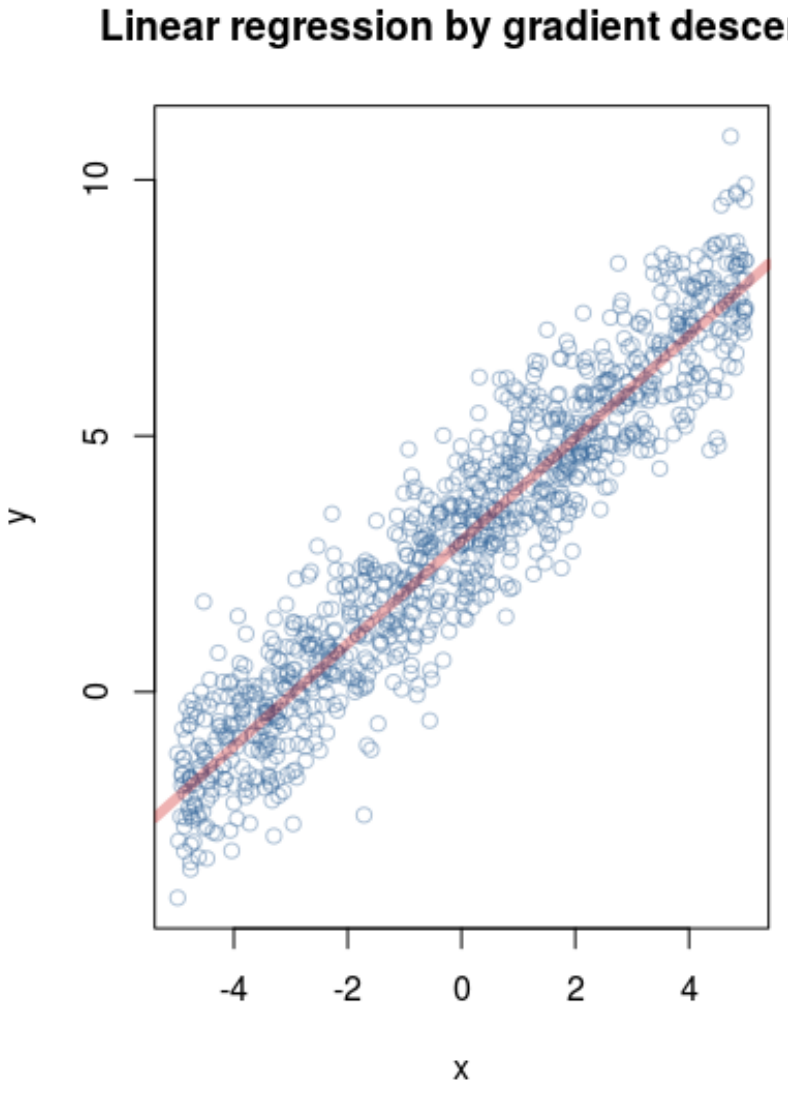

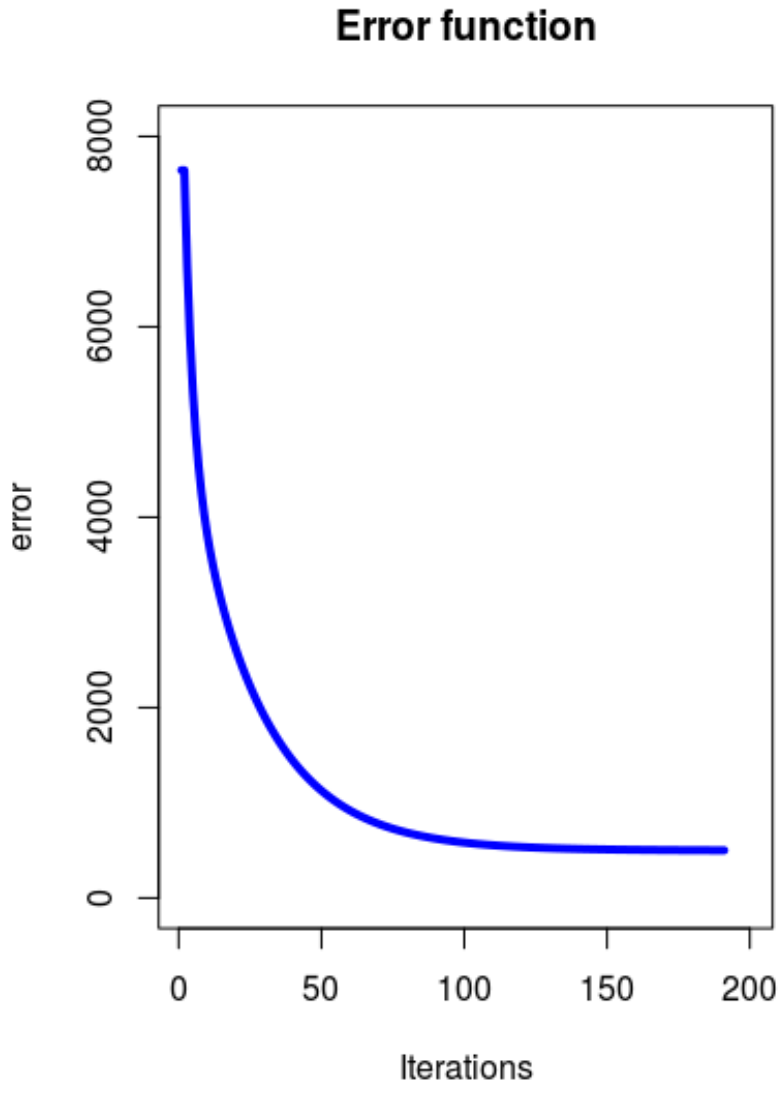

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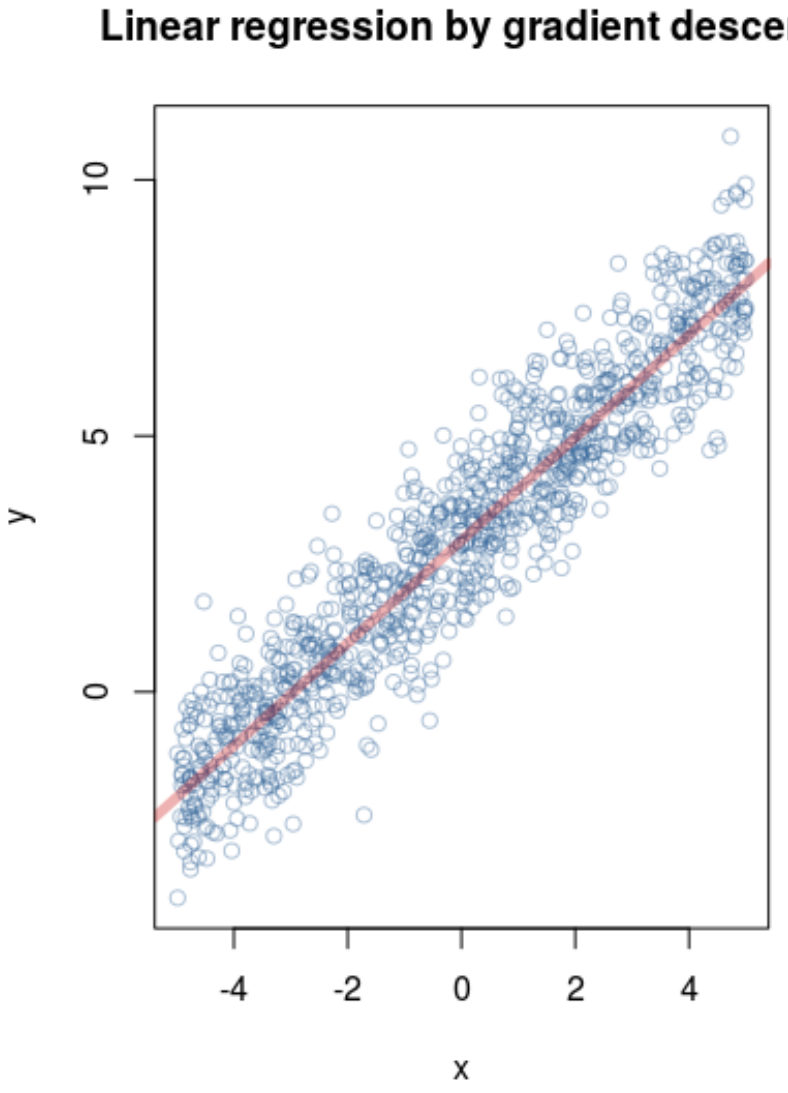

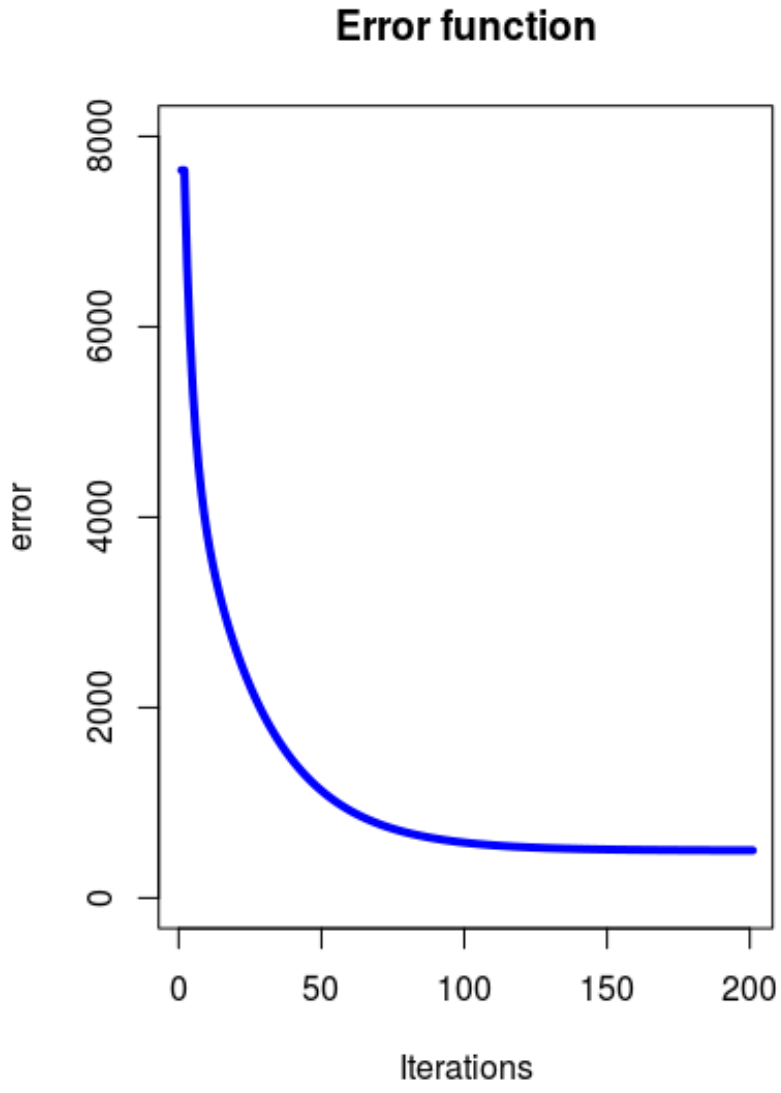

ADALINE - learning

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 $t+1$.

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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.

ADALINE - classification

How to use the ADALINE for classification?

- The training set is

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

kde $\vec{x}_k = (x_{k0}, x_{k1}, \ldots, x_{kn}) \in \mathbb{R}^{n+1}$ a $d_k \in \{1, -1\}$.
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- We may expect the following:
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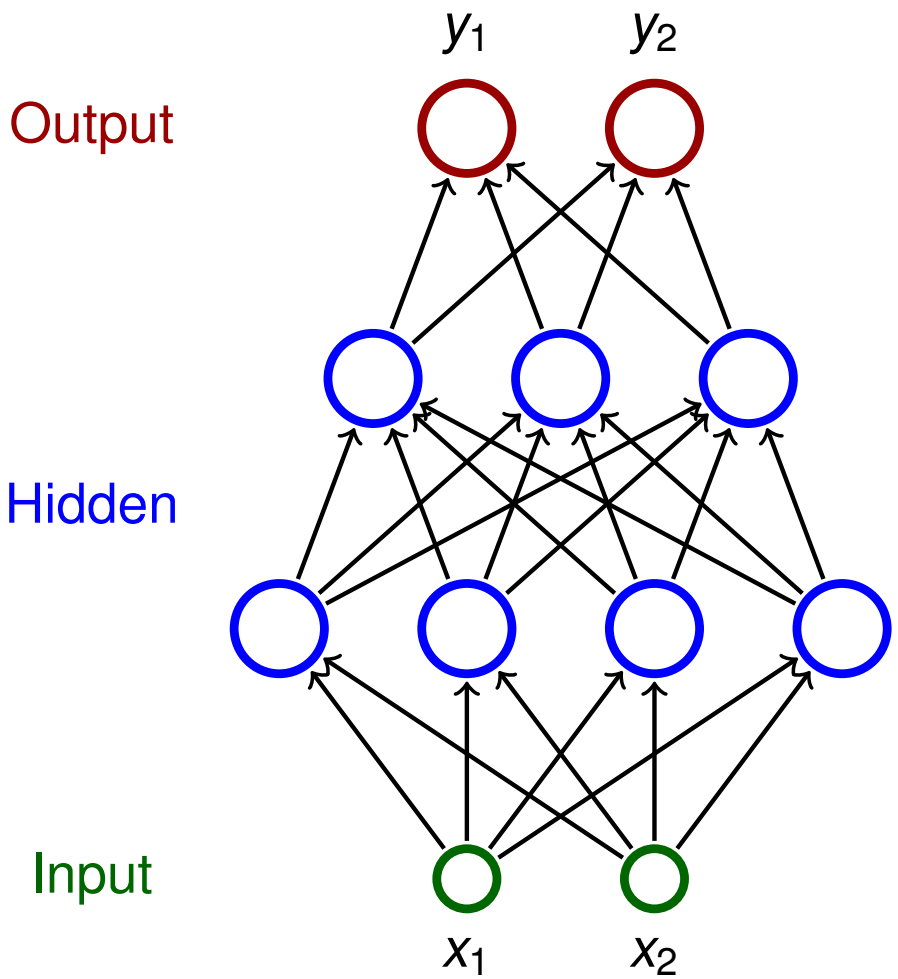
- This does not have to be always true but if the training set is reasonably linearly separable, then the algorithm typically gives satisfactory results.

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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Activity:

- inner potential of neuron j:

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

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- State of non-input neuron $j \in Z \setminus X$ after the computation stops:

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  (y_j depends on the configuration $\vec{w}$ and the input $\vec{x}$, so we sometimes write $y_j(\vec{w}, \vec{x})$)
- 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

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

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 $\left(d_{kj}\right)_{j \in Y}$).

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

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

MLP – error function gradient

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

$$\sigma_j'(\xi_j) = \lambda_j y_j (1 - y_j)$$

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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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1. **forward pass:** compute $y_j = y_j(\vec{w}, \vec{x}_k)$ for all $j \in Z$

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1. **forward pass:** compute $y_j = y_j(\vec{w}, \vec{x}_k)$ for all $j \in Z$
2. **backward pass:** compute $\frac{\partial E_k}{\partial y_j}$ for all $j \in Z$ using *backpropagation* (see the next slide!)

MLP – computing the gradient

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

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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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Compute $\frac{\partial E_k}{\partial y_j}$ for all $j \in Z$ as follows:

- 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.

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The steps 1. - 3. take linear time.

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

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:

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

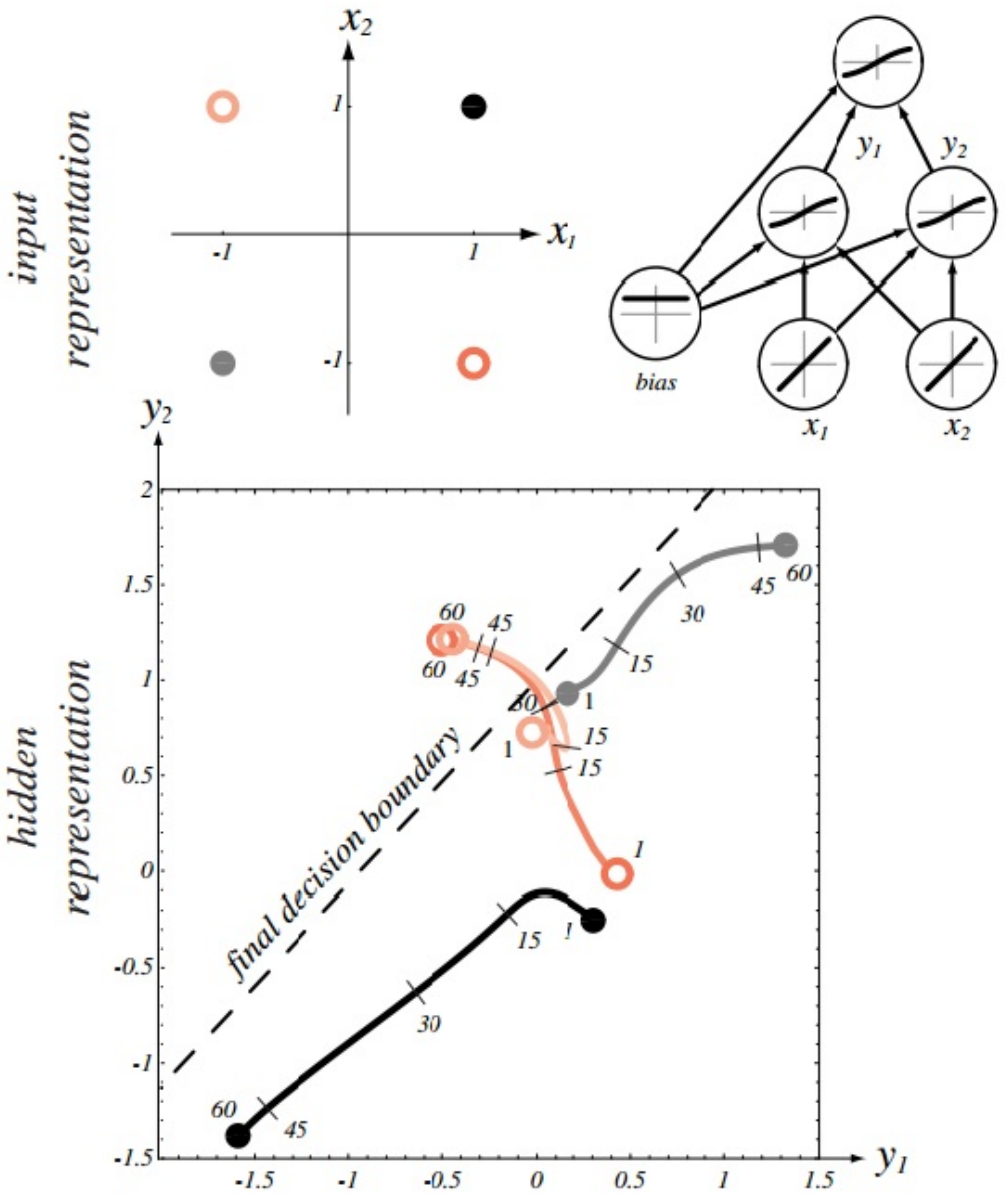
where

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

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).

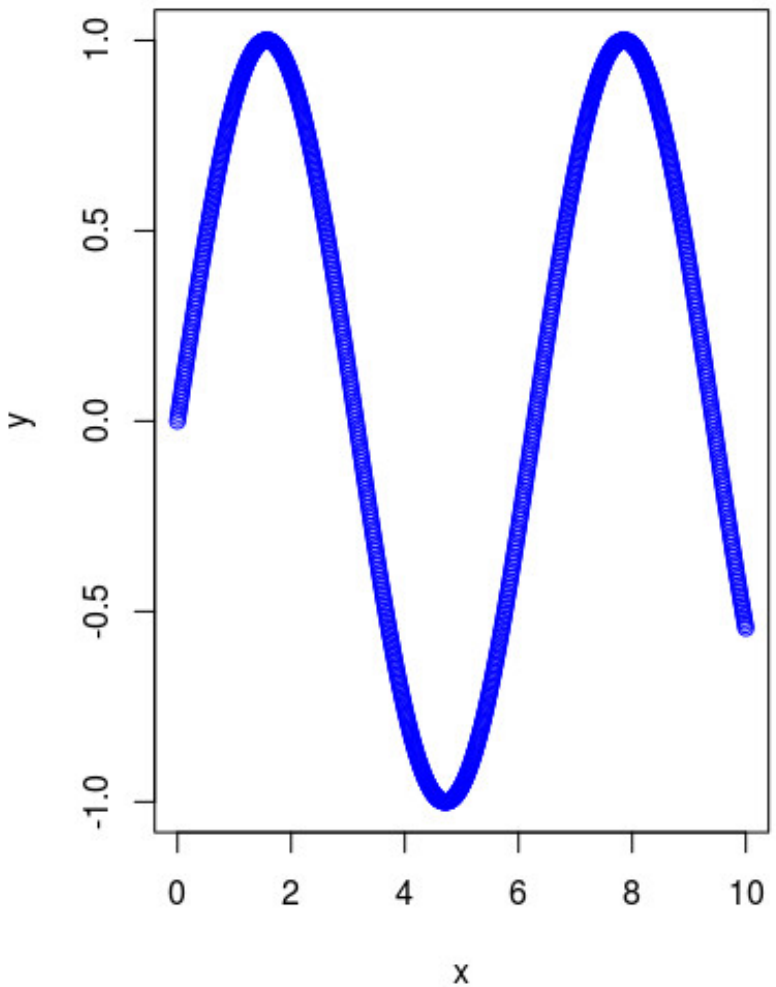
Illustration of the gradient descent – XOR

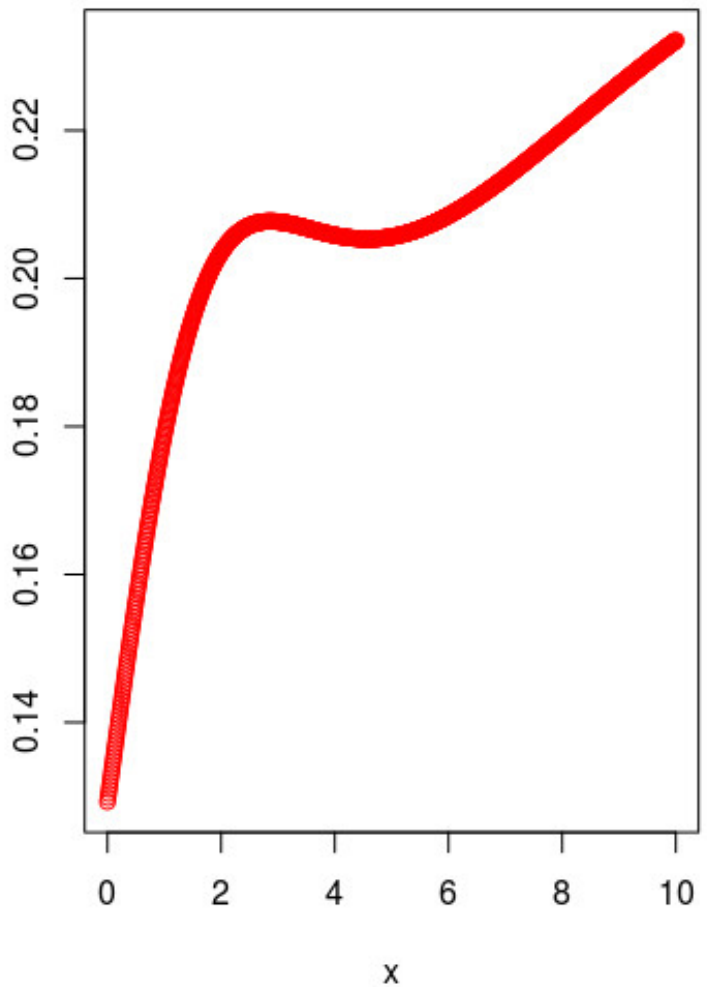


Source: Pattern Classification (2nd Edition); Richard O. Duda, Peter E. Hart, David G. Stork

Animation (sin(x)), network 1-5-1)

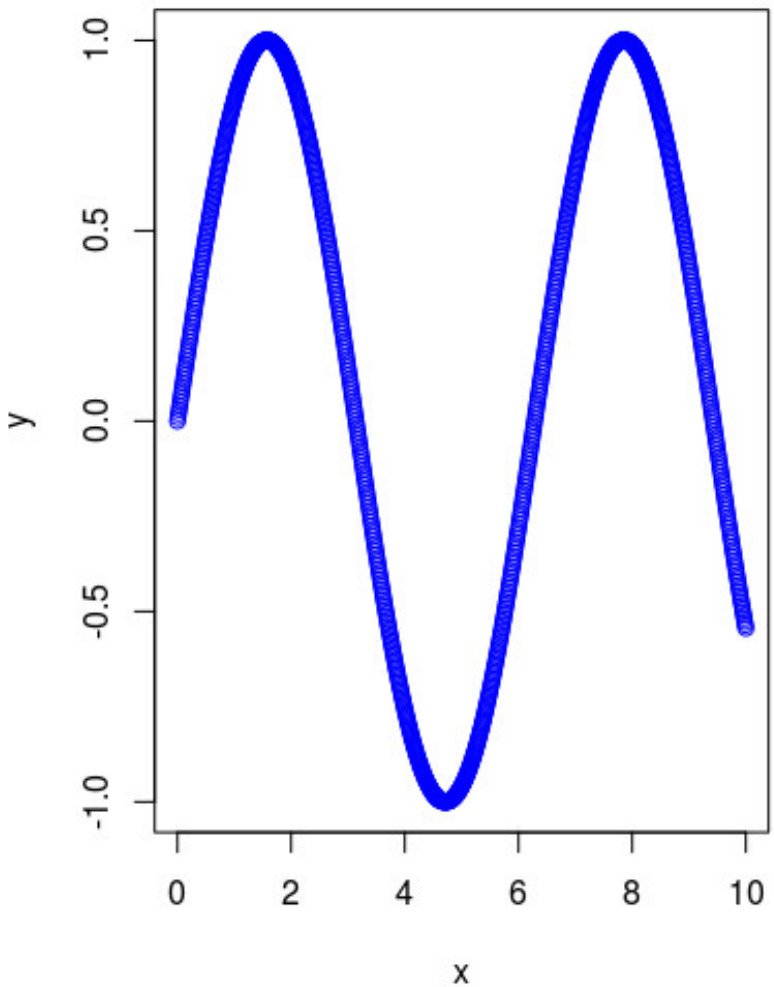
One iteration:

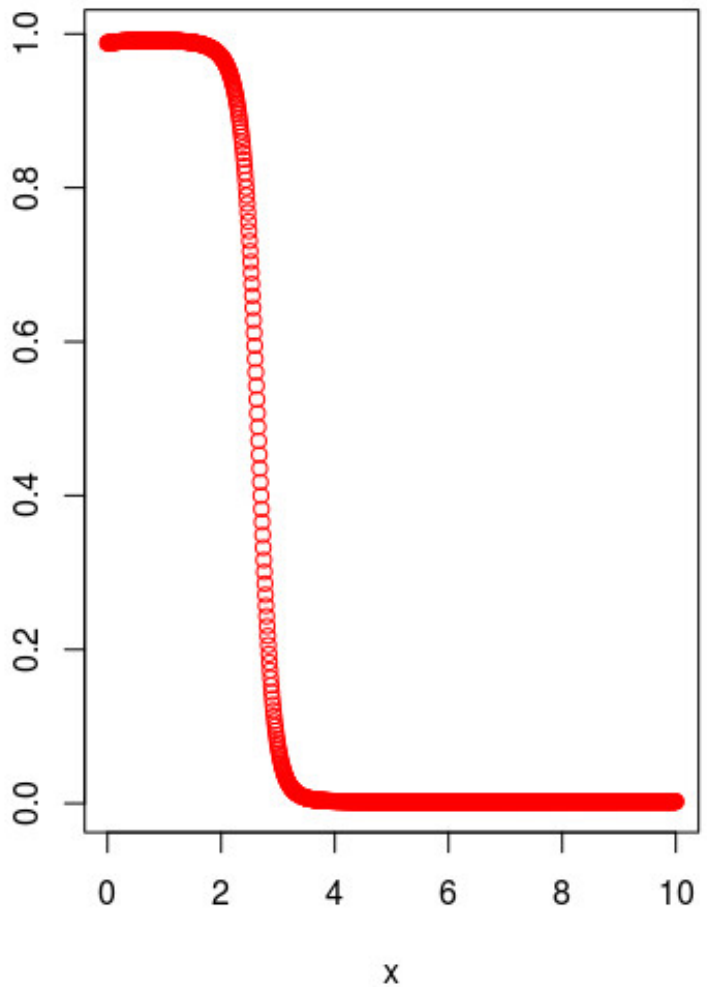




Animation (sin(x)), network 1-5-1)

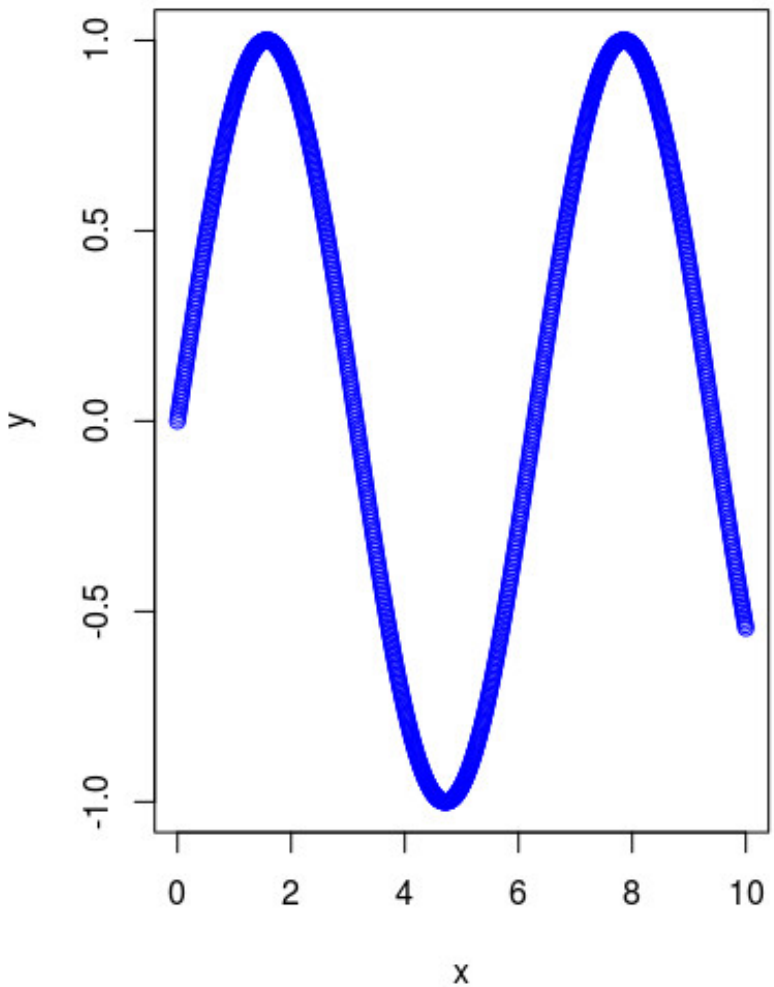
10 iterations:

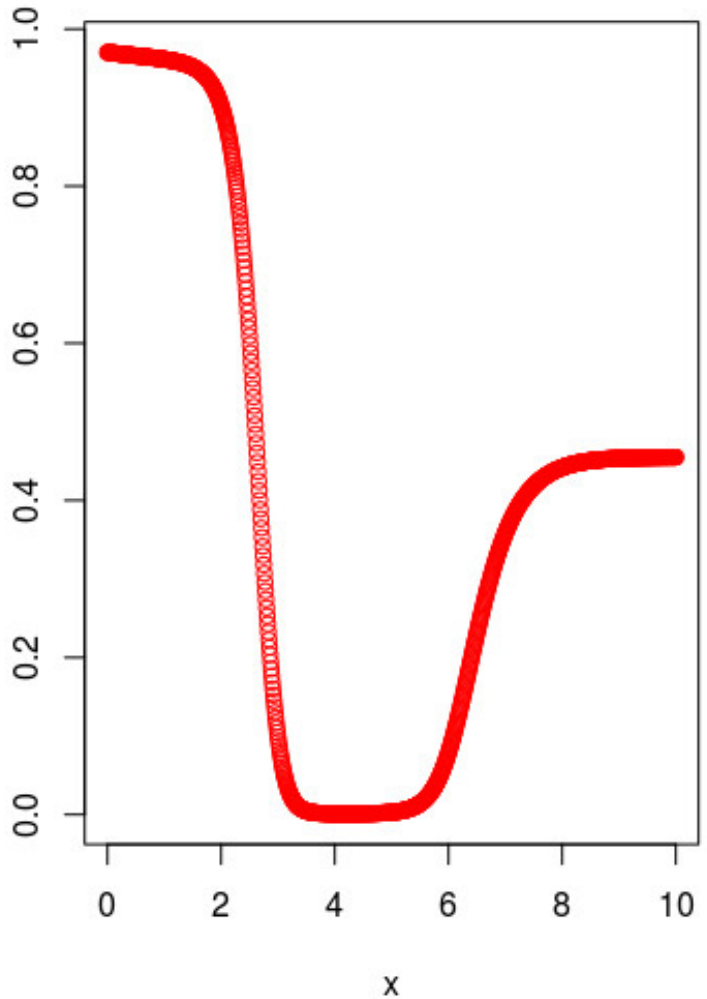




Animation (sin(x)), network 1-5-1)

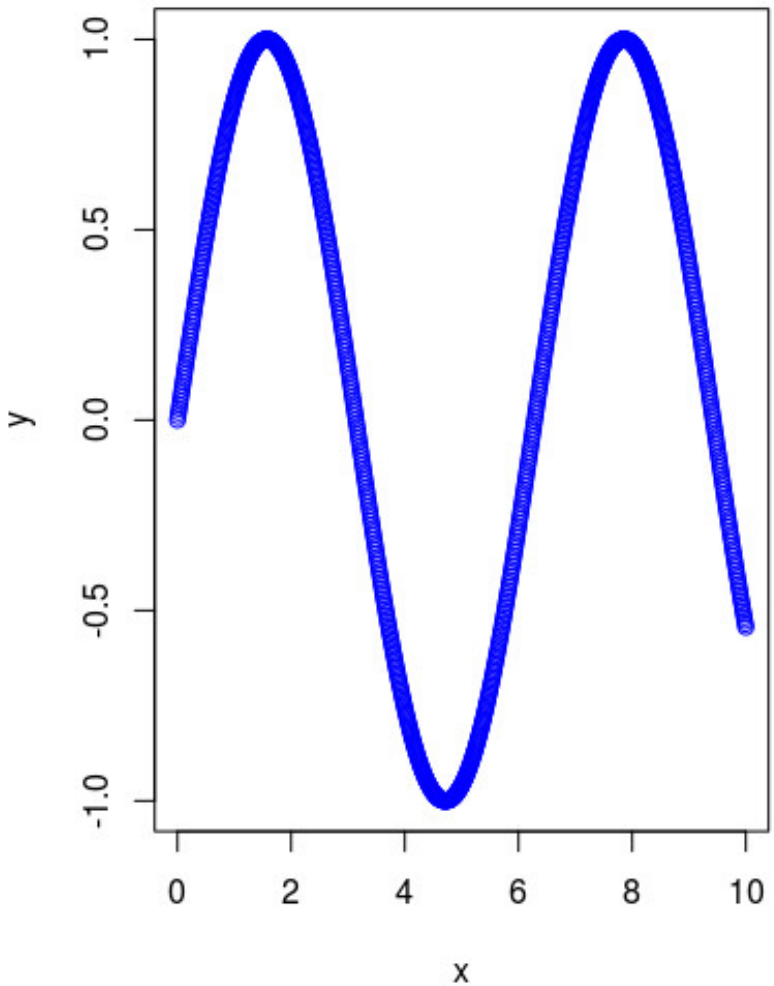
20 iterations:

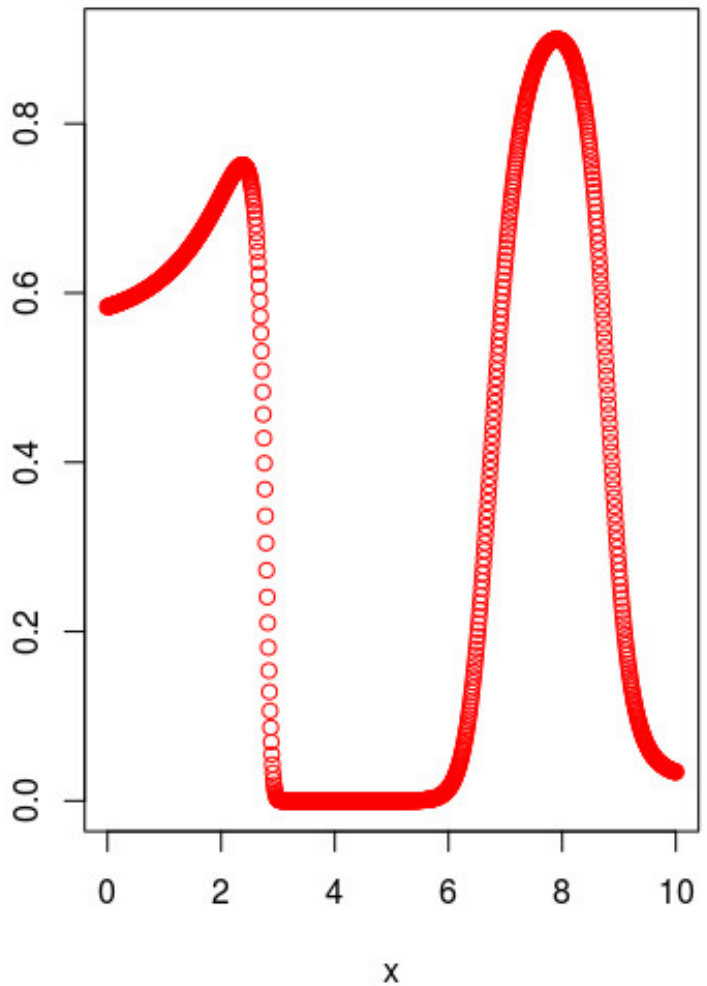




Animation (sin(x)), network 1-5-1)

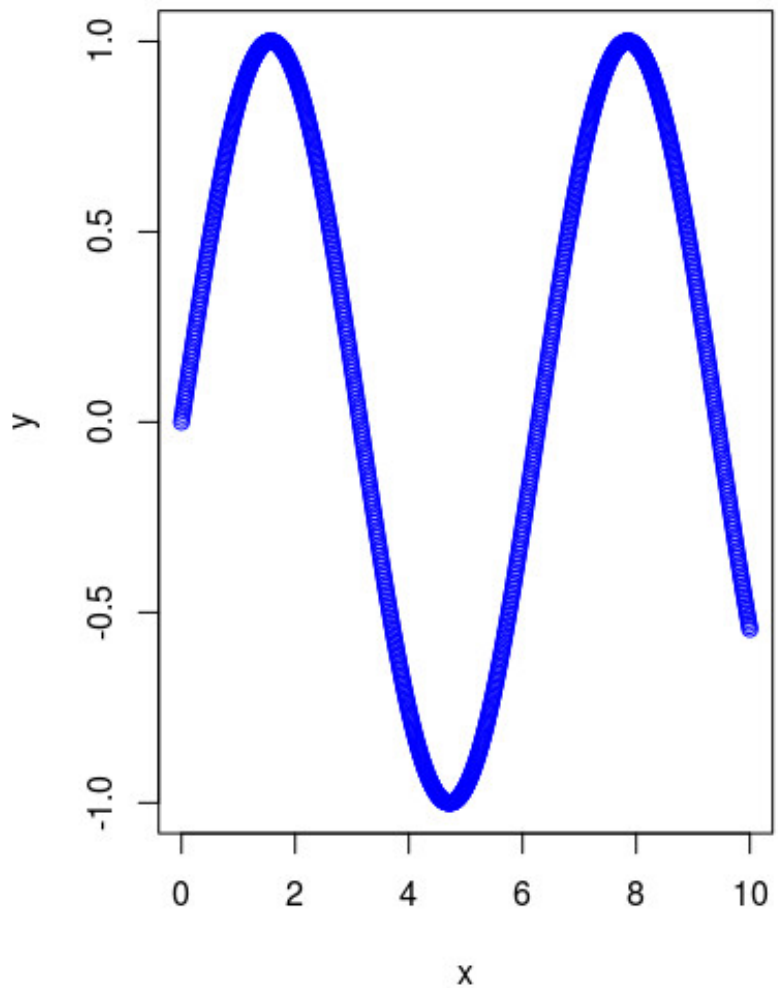
40 iterations:

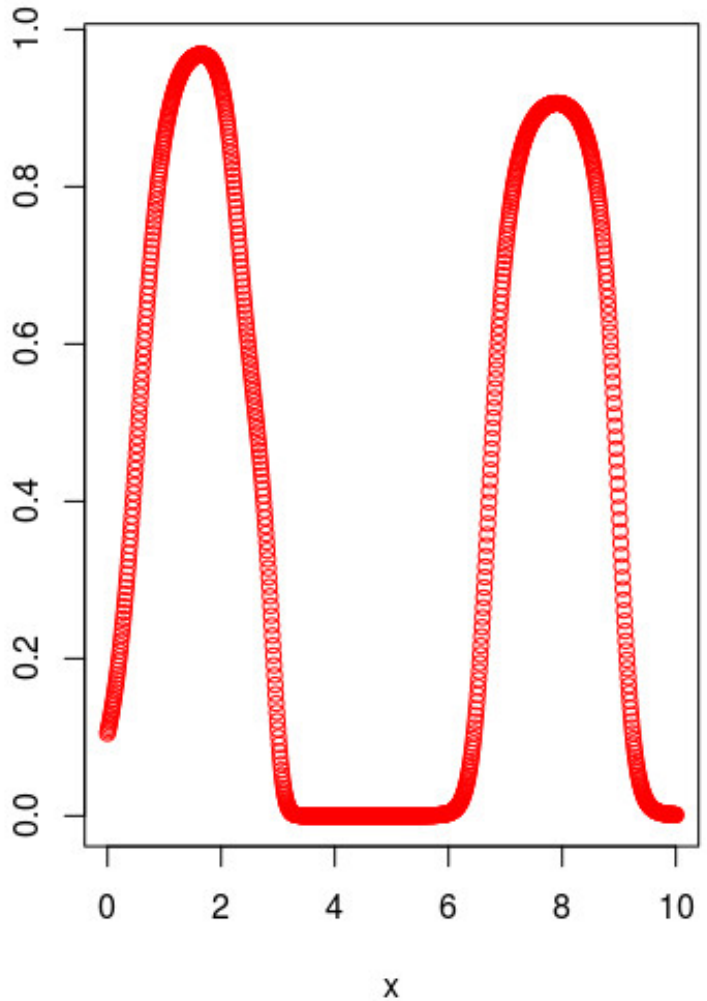




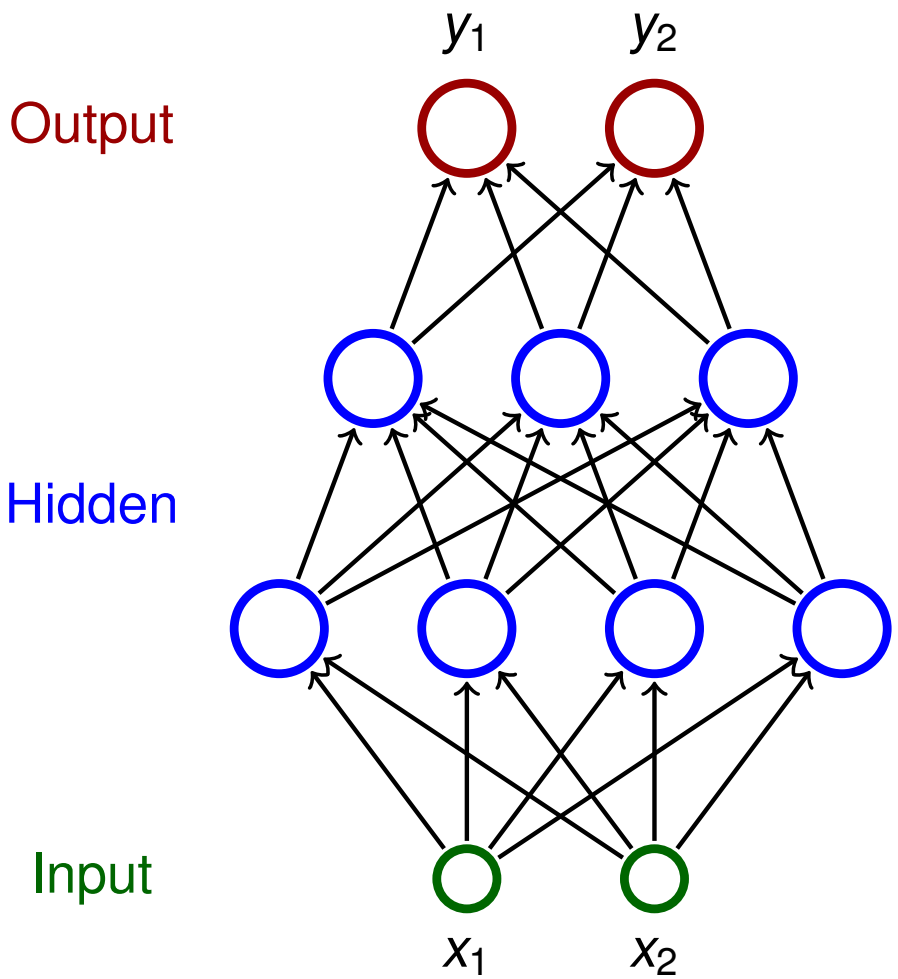
Animation (sin(x)), network 1-5-1)

100 iterations:





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

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

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:**

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

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 – batch learning

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:

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

Here

$$\Delta\vec{w}^{(t)} = -\varepsilon(t) \cdot \nabla E(\vec{w}^{(t)}) = -\varepsilon(t) \cdot \sum_{k=1}^{p} \nabla E_k(\vec{w}^{(t)})$$

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

MLP – error functions

- **square 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 square error (mse):**

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

I will use mse throughout the rest of this lecture.

MLP – mse gradient

For every w_{ji} we have

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

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where for every $k = 1, \ldots, p$ holds

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

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

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

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

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

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?
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  - 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

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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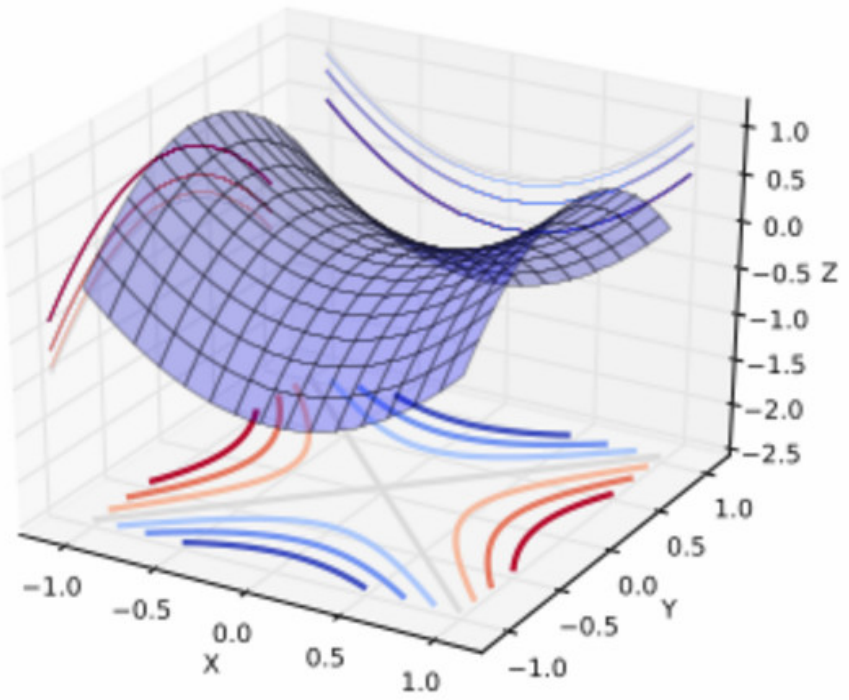
Saddle points

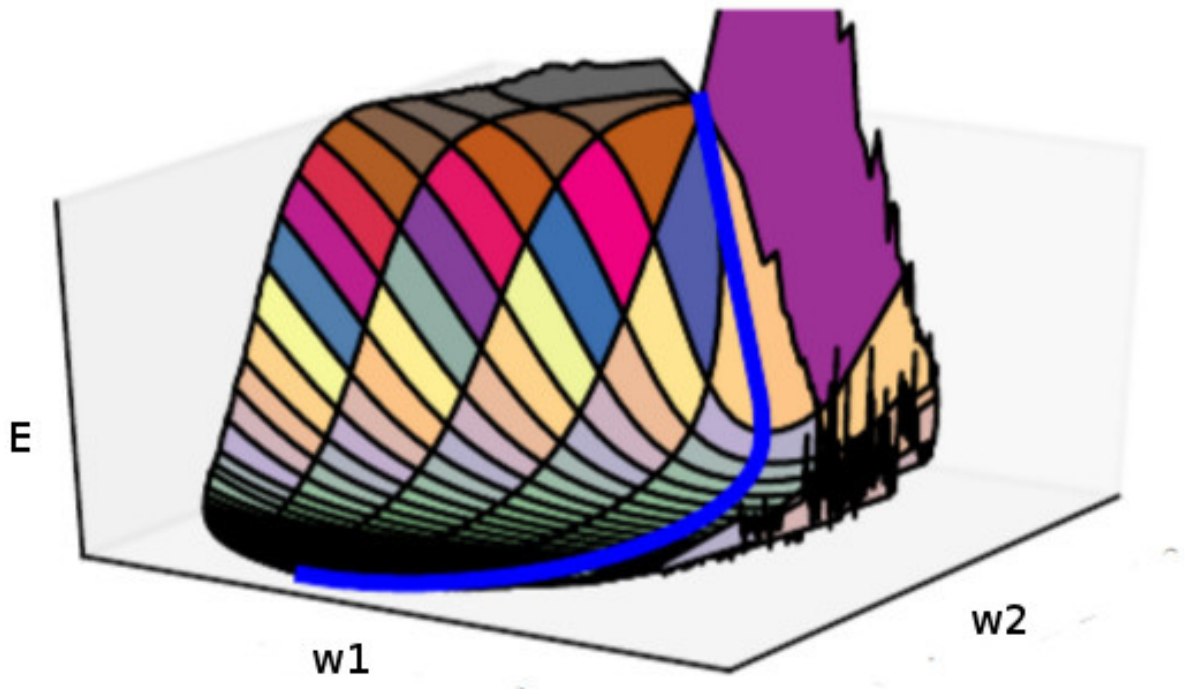
One can show (by a combinatorial argument) that larger networks have exponentially more saddle points than local minima.



Issues in gradient descent – too slow descent

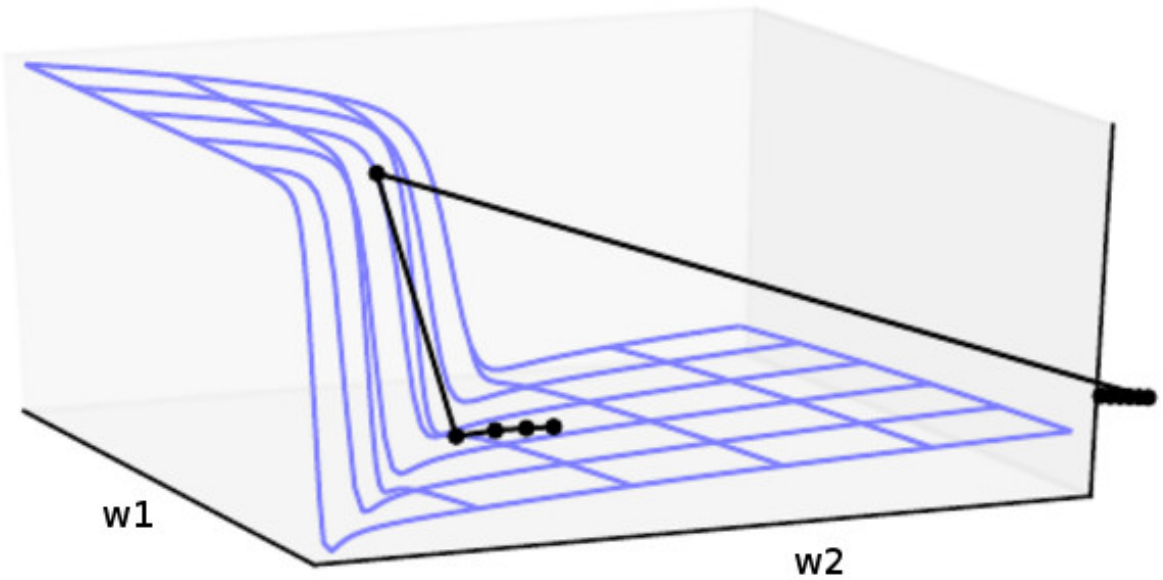
- flat regions

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

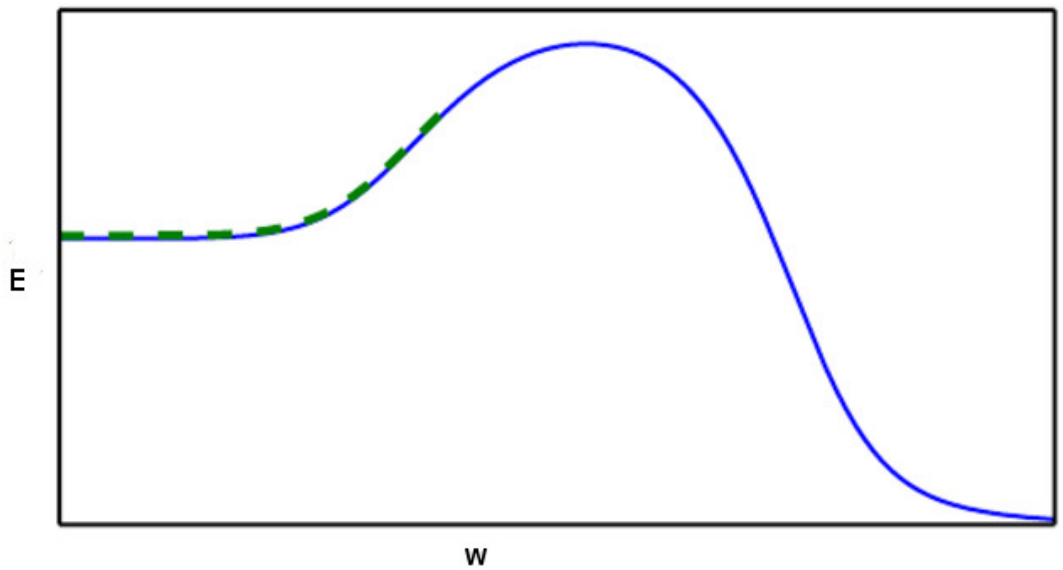


Issues in gradient descent – too fast descent

- 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?

Issues in computing the gradient

- vanishing and exploding gradients

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

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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.)

Minibatch size

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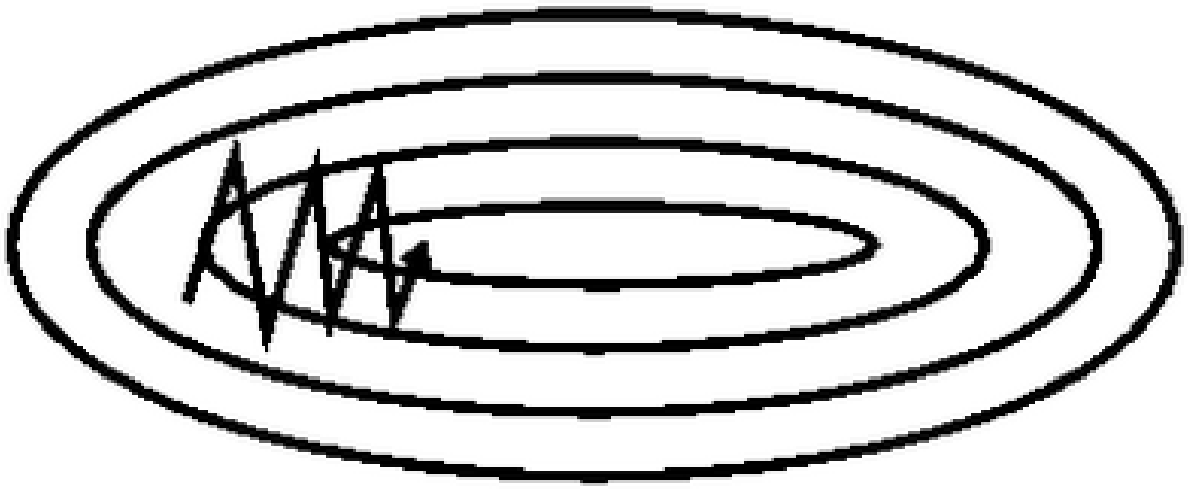
- Some kinds of hardware achieve better runtime with specific sizes of arrays. Especially when using GPUs, it is common for power of 2 batch sizes to offer better runtime. Typical power of 2 batch sizes range from 32 to 256, with 16 sometimes being attempted for large models.
- Small batches can offer a regularizing effect, perhaps due to the noise they add to the learning process.

Moment

Issue in the gradient descent:

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



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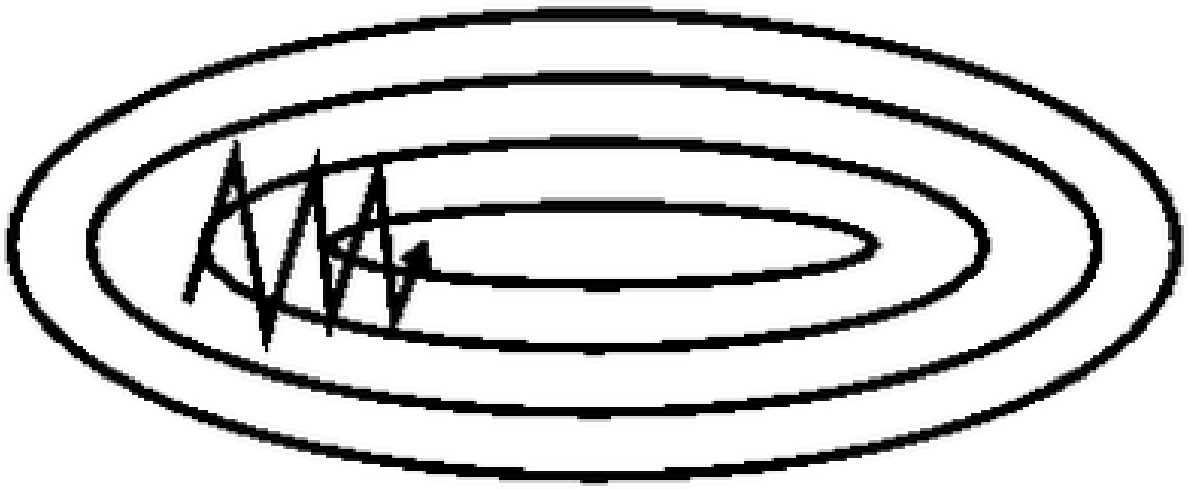
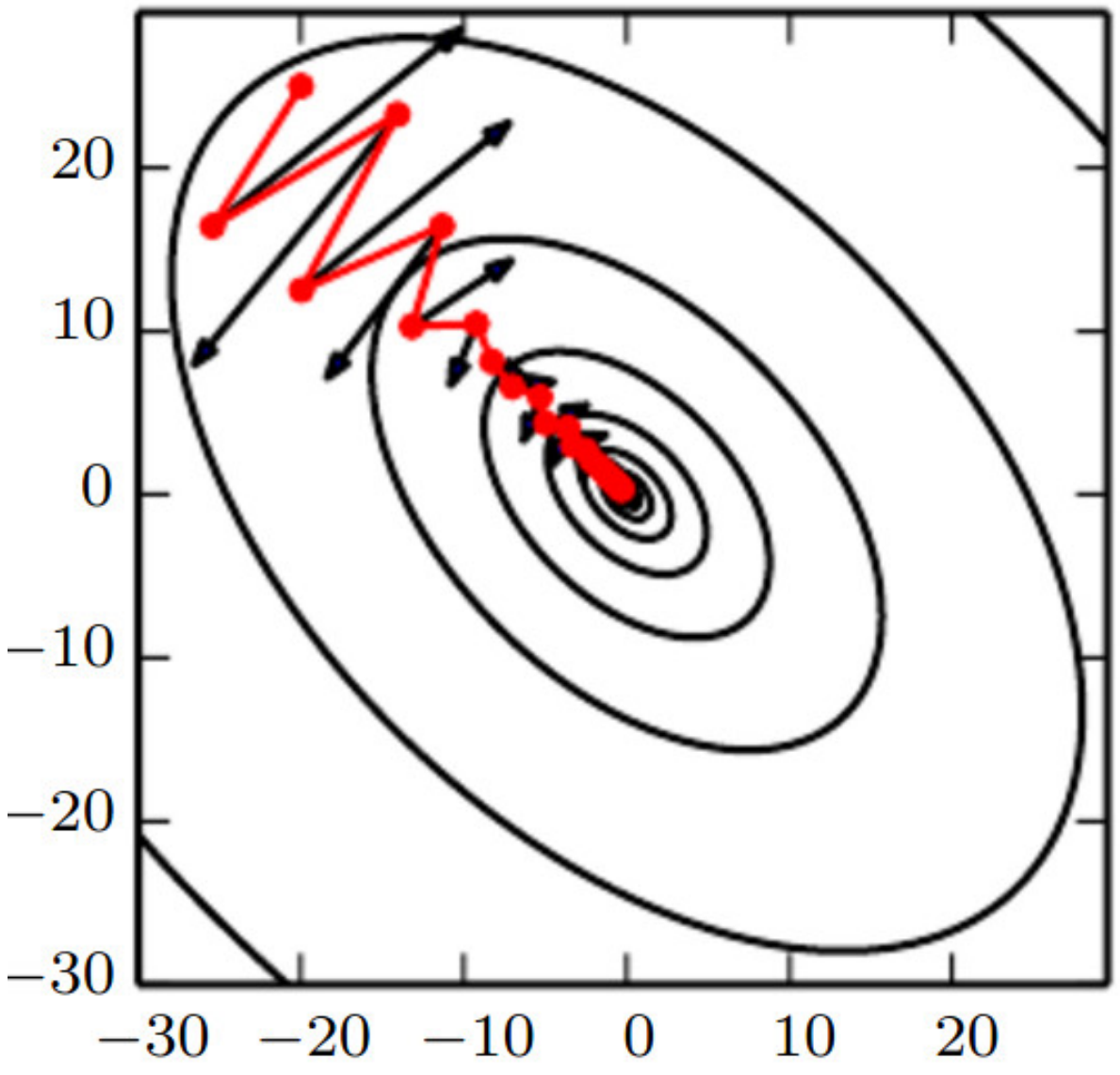


Solution: In every step add the change made in the previous step (weighted by a factor α):

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

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 moment
- $\nabla E_k(\vec{w}^{(t)})$ 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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Generic rules for adaptation of $\varepsilon(t)$

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- Start with a larger learning rate (e.g. $\varepsilon = 0.1$).

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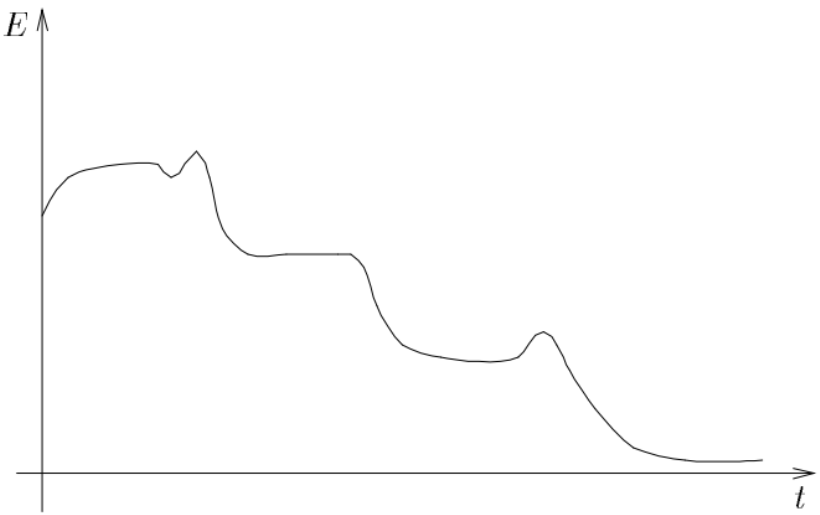
  Later decrease as the descent is supposed to settle in a minimum of E.

  Some tools allow to set a list of learning rates, each rate for one epoch of the descent.

In case you may observe the error evolving:

- If the error decreases, increase slightly the rate.
- If the error increases, decrease the rate.
- Note that the error may increase for the short period without any harm to convergence of the learning process.



AdaGrad

So far we have considered a uniform learning rate.

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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where

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

and

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

- 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

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and

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

- 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

There are more methods such as AdaDelta, Adam (roughly RMSProp combined with momentum), etc.

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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

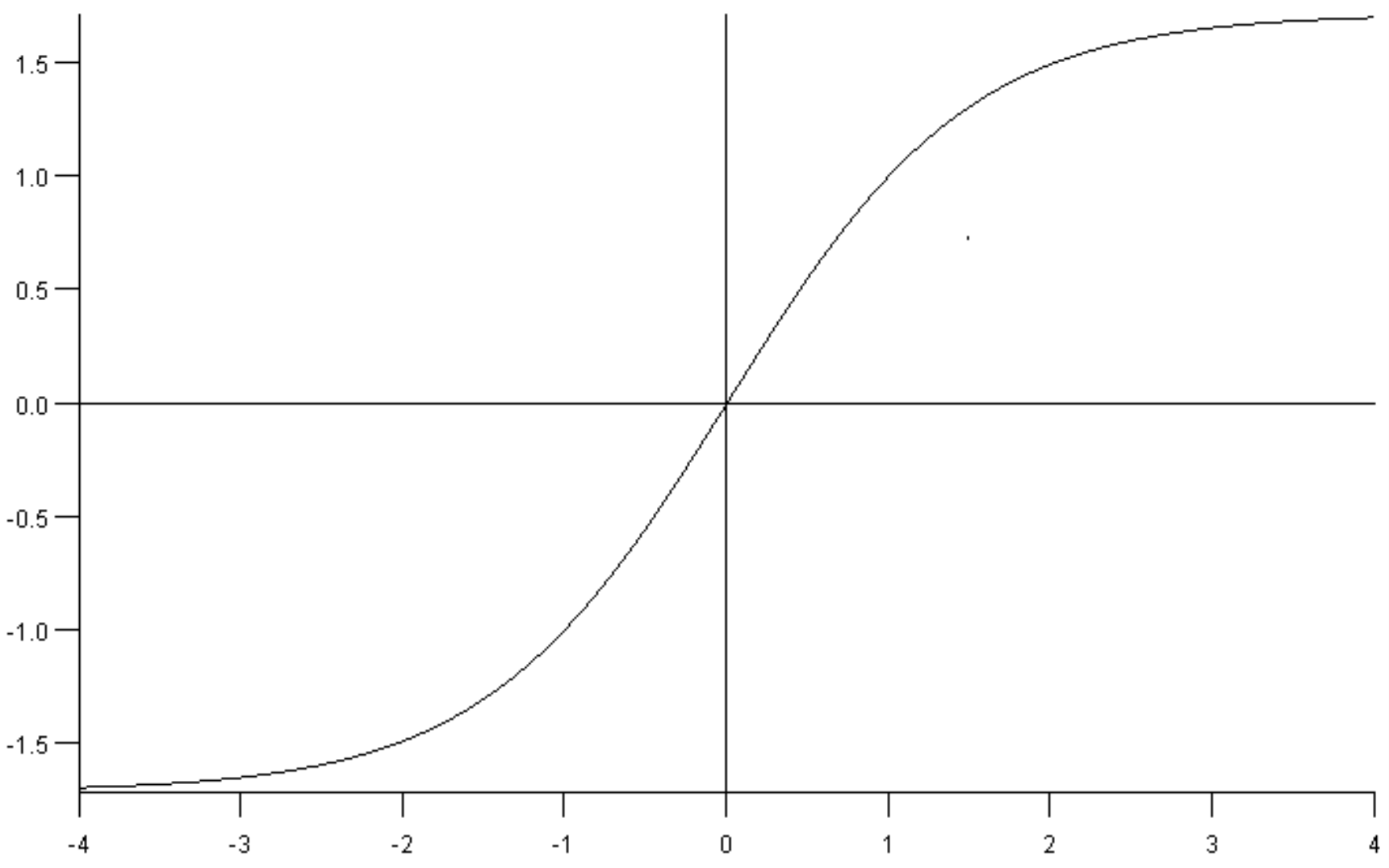
   (local extrema of activation functions induce local extrema of the error function)

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)

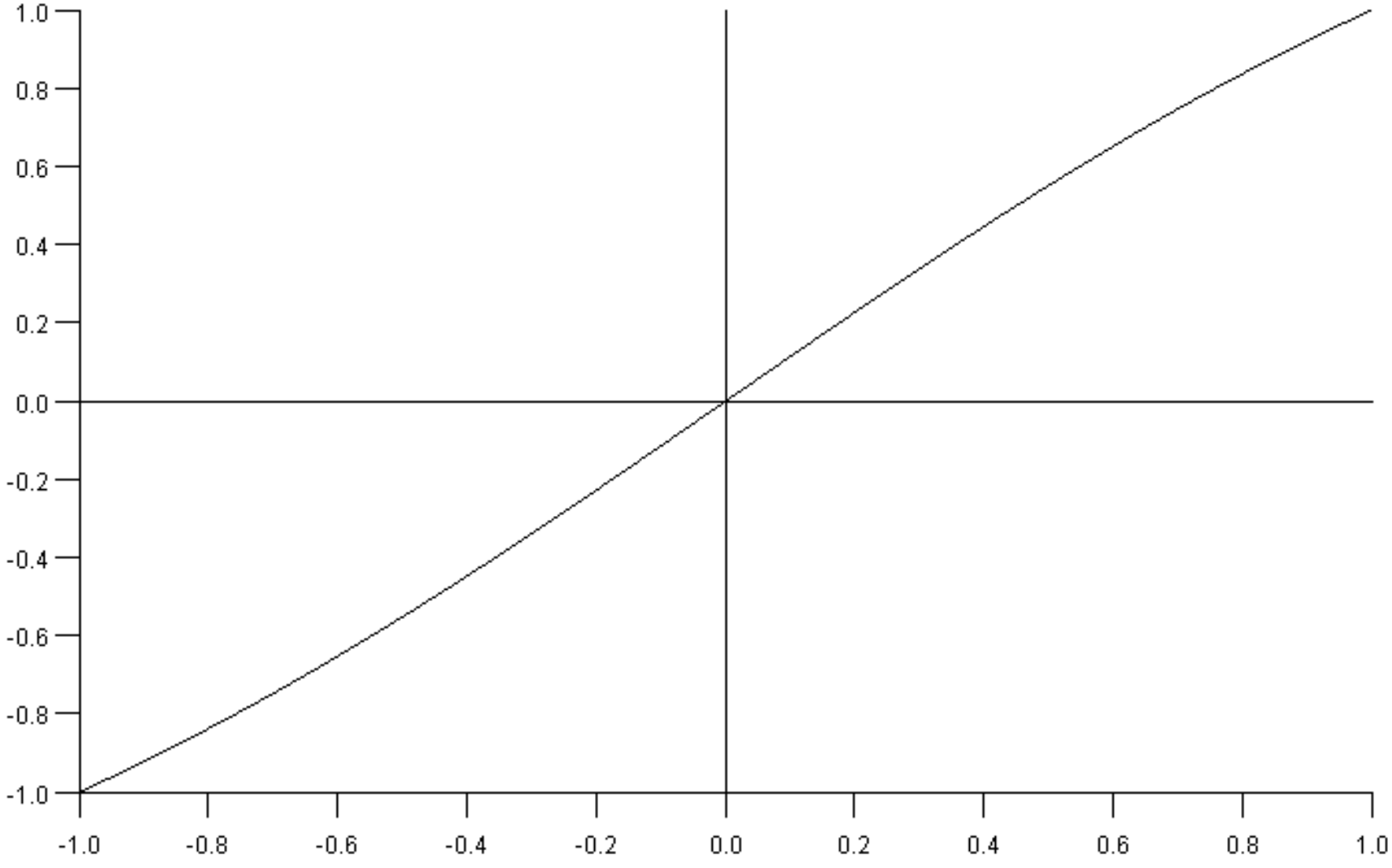
The choice of activation functions is closely related to input preprocessing and the initial choice of weights. I will illustrate the reasoning on sigmoidal functions; say few words about other activation functions later.

Activation functions – tanh



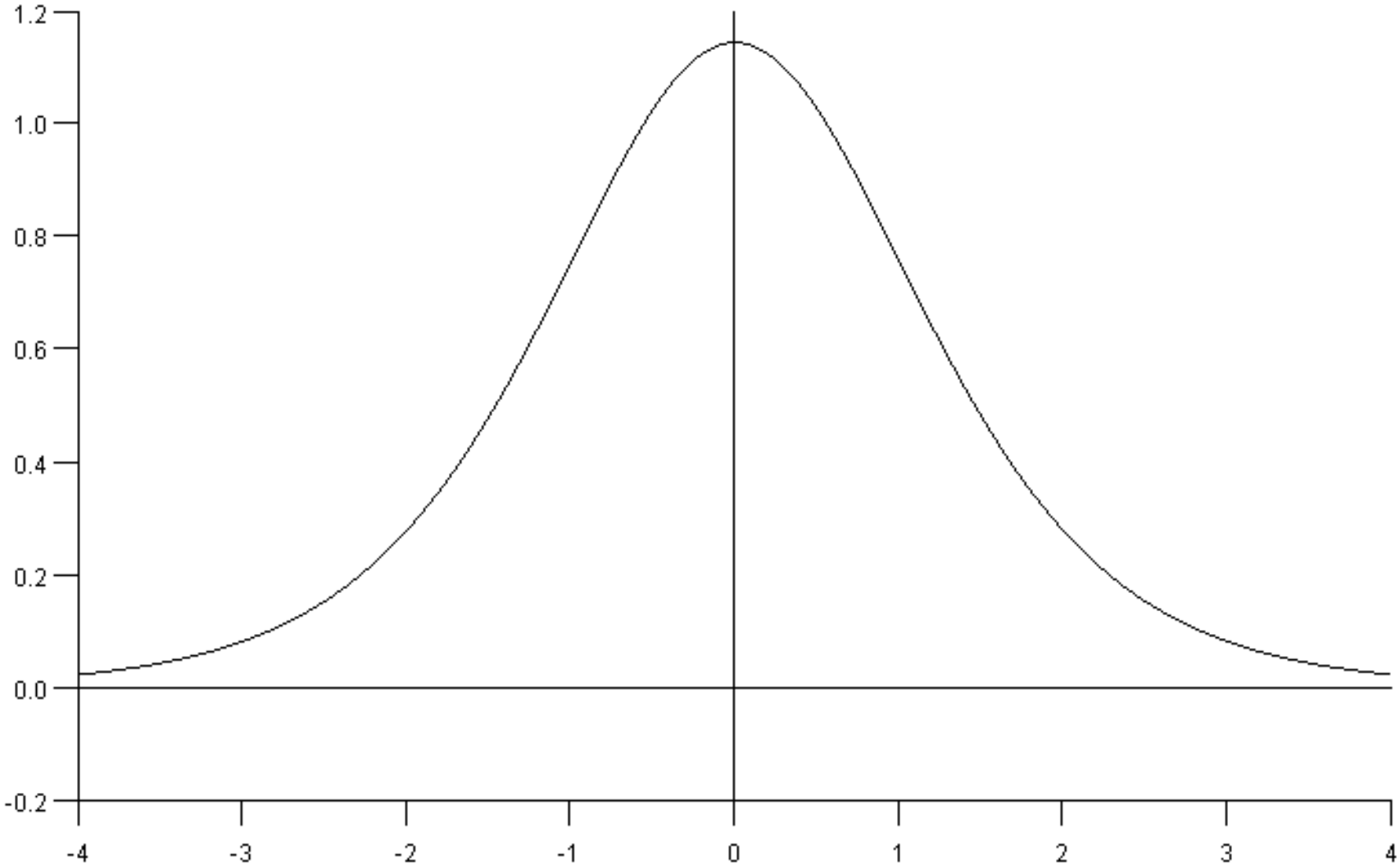
$\sigma(\xi) = 1.7159 \cdot \tanh(\frac{2}{3} \cdot \xi)$, we have $\lim_{\xi \to \infty} \sigma(\xi) = 1.7159$ and $\lim_{\xi \to -\infty} \sigma(\xi) = -1.7159$

Activation functions – tanh



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

Activation functions – tanh



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

Input preprocessing

- Some inputs may be much larger than others.

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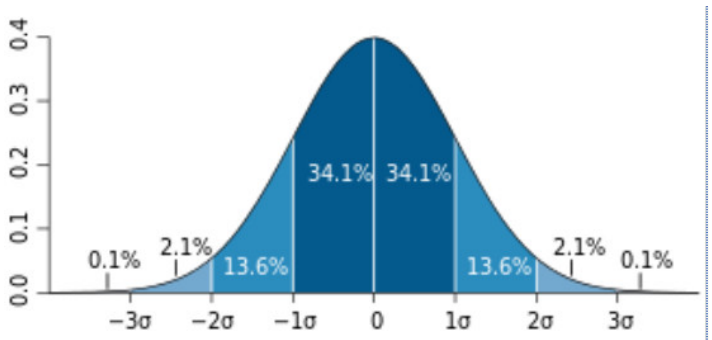
- Large inputs have greater influence on the training than the small ones. In addition, too large inputs may slow down learning (saturation of activation functions).
- Typical standardization:
  - average $= 0$ (subtract the mean)
  - variance $= 1$ (divide by the standard deviation)

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

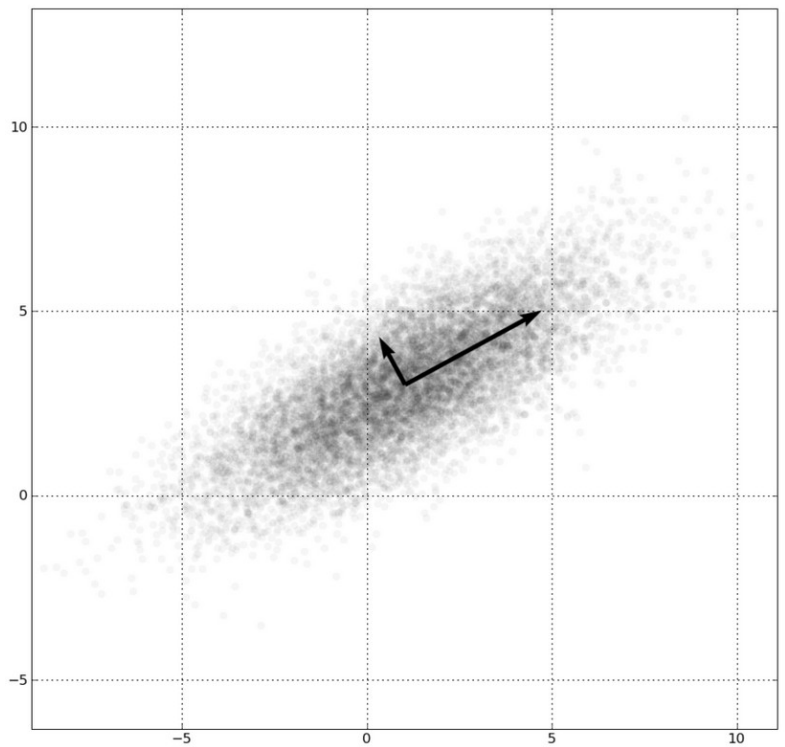


(illustration of standard deviation)

Input preprocessing

- Individual inputs should not be correlated.
- Correlated inputs can be removed as a part of *dimensionality reduction*.

  (Dimensionality reduction and decorrelation can be implemented using neural networks. There are also standard methods such as PCA.)



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  - σ is almost linear on $[-1, 1]$,
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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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  Thus we put $w = \frac{\sqrt{3}}{\sqrt{d}}$.
- The same works for higher layers, d corresponds to the number of neurons in the layer one level lower.

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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.

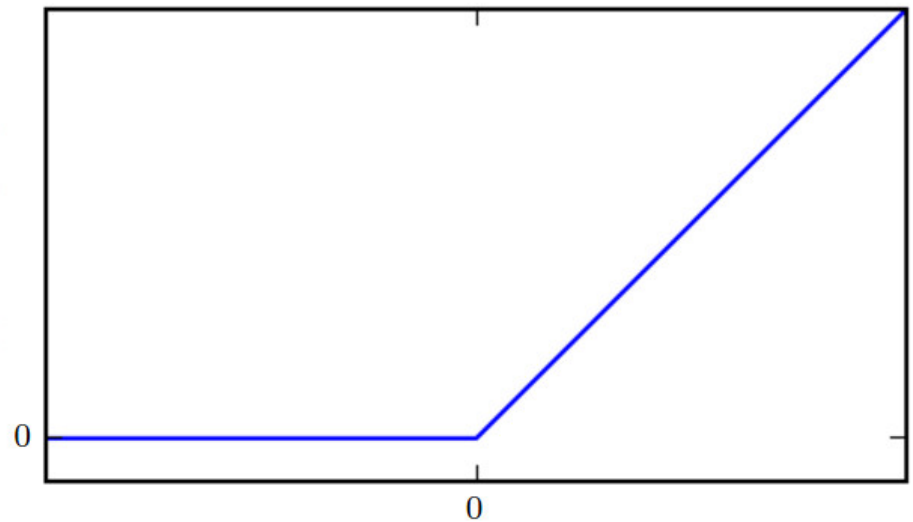
Target values (tanh)

- Target values d_{kj} should be chosen in the range of the output activation functions, in our case $[-1.716, 1.716]$.
- Target values too close to extrema of the output activations, in our case ± 1.716, may cause that the weights will grow indefinitely (slows down learning).
- Thus it is good to choose target values from the interval $[-1.716 + \delta, 1.716 - \delta]$.

  As before, ideally $[-1.716 + \delta, 1.716 - \delta]$ should span the interval on which the activation function is linear, i.e. d_{kj} should be taken from $[-1, 1]$.

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.

Output neurons

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

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

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For classification, the current activation functions of choice are

- logistic sigmoid or tanh – binary classification
- softmax:

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for multi-class classification.

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

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

... 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

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

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

- For a training set

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

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

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

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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In case of function approximation, the network should not return exact results as in the training set.

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

Regularization is a big issue in neural networks, as they typically use a huge amount of parameters and thus are very susceptible to overfitting.

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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 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.
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Solution: Optimal number of neurons :-)

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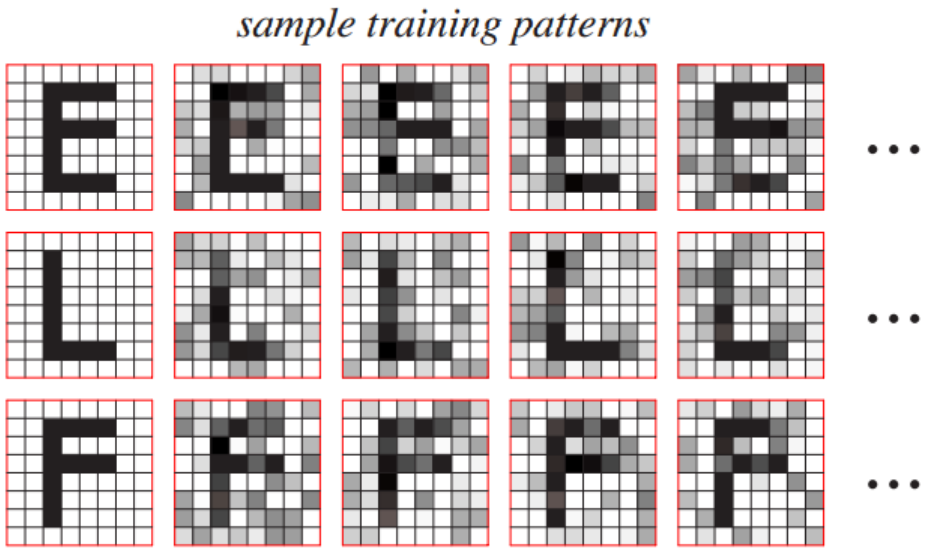
Solution: Optimal number of neurons :-)

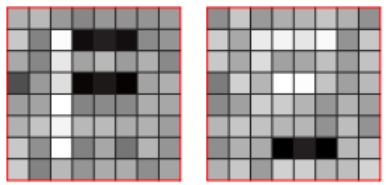
- there are some (useless) theoretical bounds
- there are algorithms dynamically adding/removing neurons (not much use nowadays)
- In practice:
  - start using a rule of thumb: the number of neurons $\approx$ ten times less than the number of training instances.
  - experiment, experiment, experiment.

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:





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.

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Bagging:

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

  If $|T_i| = |\mathcal{T}|$, 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).
- update weights of neurons in N (in a standard way), leave weights of the other neurons unchanged.

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- update weights of neurons in N (in a standard way), leave weights of the other neurons unchanged.

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

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

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

Here $\frac{2\zeta}{\varepsilon}(\vec{w} \cdot \vec{w})$ 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.