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  (Extremely well written online textbook (a little outdated))
- Deep learning by Ian Goodfellow, Yoshua Bengio and Aaron Courville

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

  ("Classical" overview of the theory of neural networks (a little outdated))
- Probabilistic Machine Learning: An Introduction by Kevin Murphy

  https://probml.github.io/pml-book/book1.html

  (Great advanced ML textbook with (almost) up-to-date basic neural networks.)
- Inifinitely many online tutorials on everything (to build intuition)

Suggested: deeplearning.ai courses by Andrew Ng

Course organization

Evaluation:

- Project (Dr. Tomáš Foltýnek)
  - implementation of a selected model + analysis of given data
  - implementation C/C++/Java/Rust **without use of any specialized libraries for data analysis and machine learning**
  - need to get over a given accuracy threshold (a gentle one, just to eliminate non-functional implementations)

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- Oral exam
  - I may ask about anything from the lecture! You will get a detailed manual specifying the mandatory knowledge.

FAQ

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

A: There are at least two reasons:

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

Notable features of the course

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

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

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

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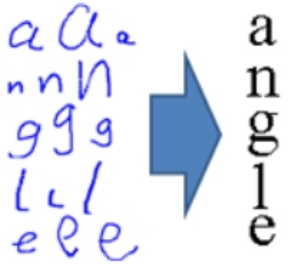

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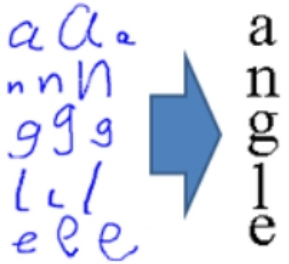

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  - and lots of much much more sophisticated applications ...

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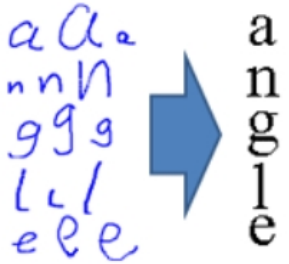

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- Basic attributes of learning algorithms:
  - **representation**: ability to capture the inner structure of training data
  - **generalization**: ability to work properly on new data

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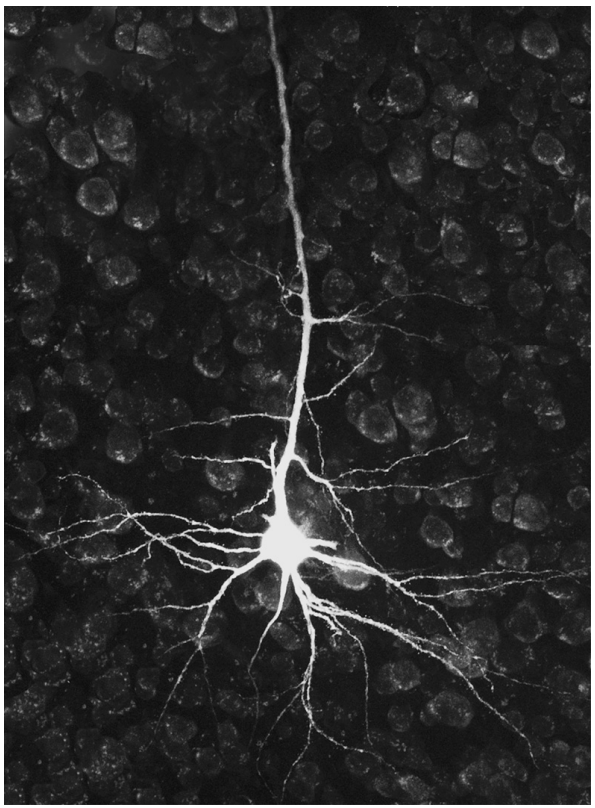
There are many types of models:

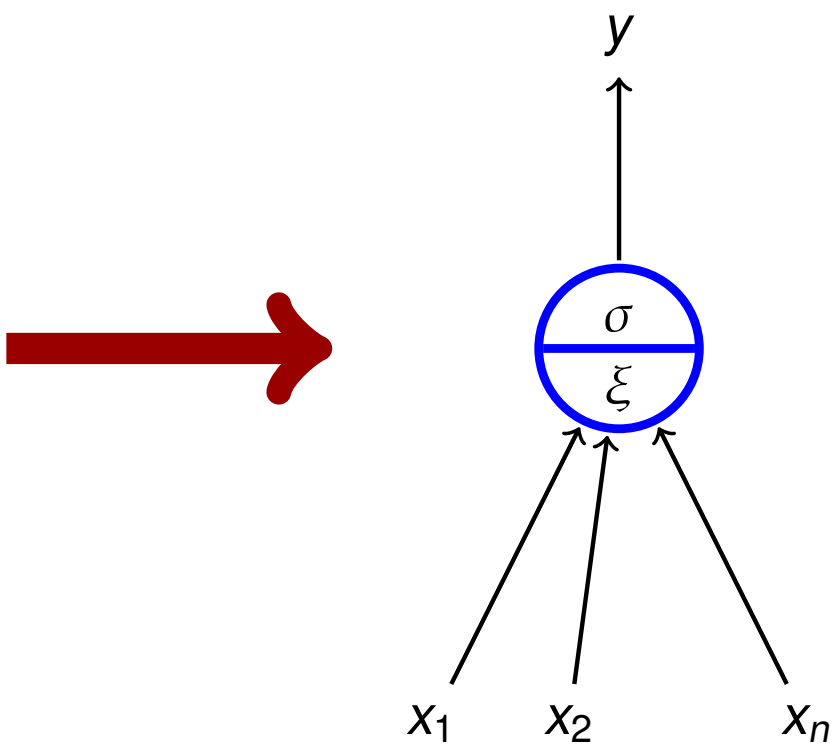
- decision trees
- support vector machines
- hidden Markov models
- Bayes networks and other graphical models
- **neural networks**
- ...

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 the brain receives information?
  - How the information is stored?
  - How the 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, Starcraft, ...
  - finance - stock prices, risk analysis
  - medicine - diagnosis, signal processing (EKG, EEG, ...), image processing (MRI, CT, WSI ...)
  - text and speech processing - machine translation, *text generation*, speech recognition
  - other signal processing - filtering, radar tracking, noise reduction
  - art - music and painting generation, deepfakes
  - ...

I will concentrate on this area!

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

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- We will concentrate on
  - basic techniques and principles of neural networks,
  - fundamental models of neural networks and their applications.
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  - Basic information about current implementations
    (TensorFlow-Keras, Pytorch)

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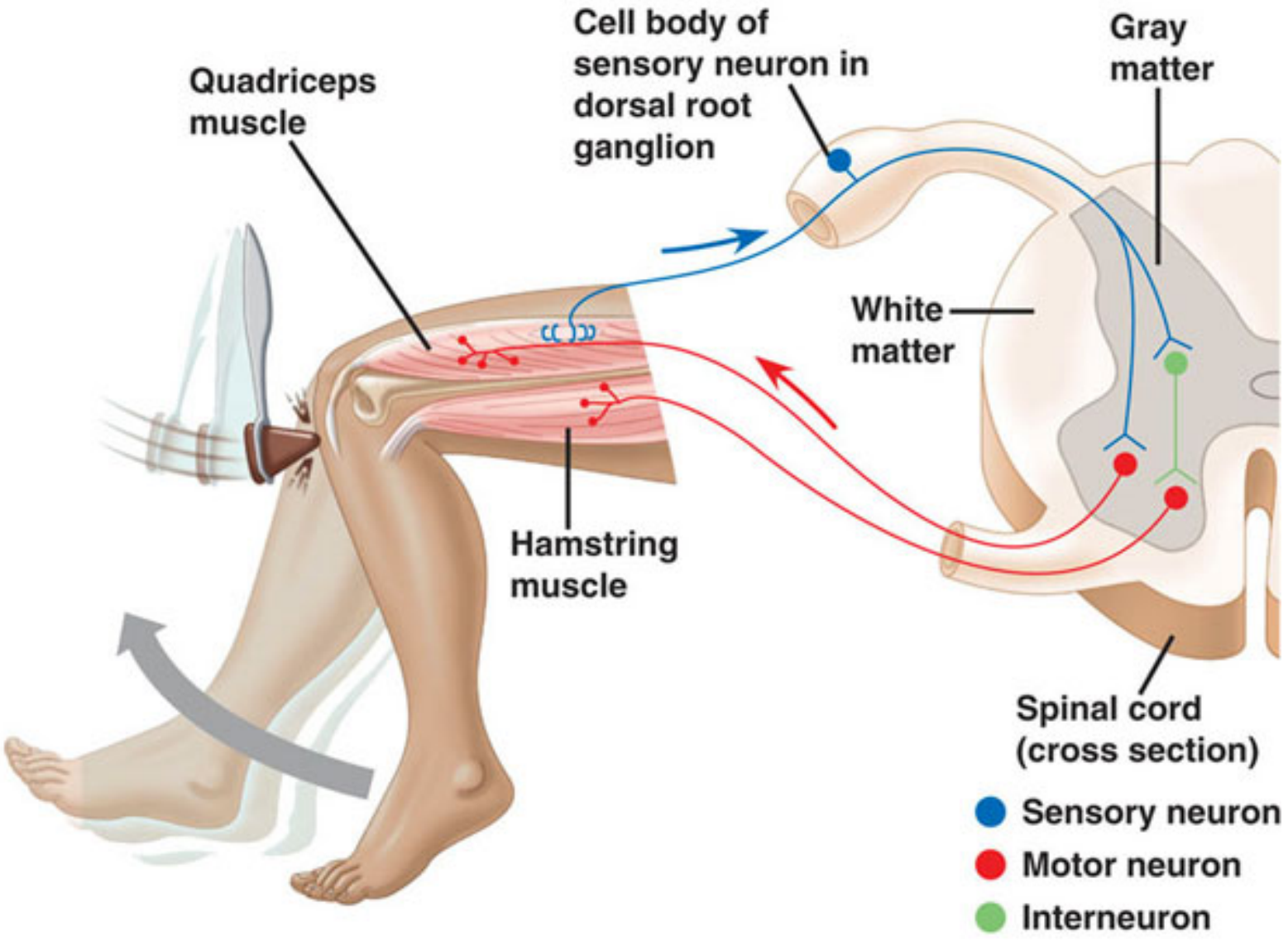
- Afterwards, the output signal is transfered via PNS to *effectors* (e.g. muscle cells).

Biological neural network



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

Summation

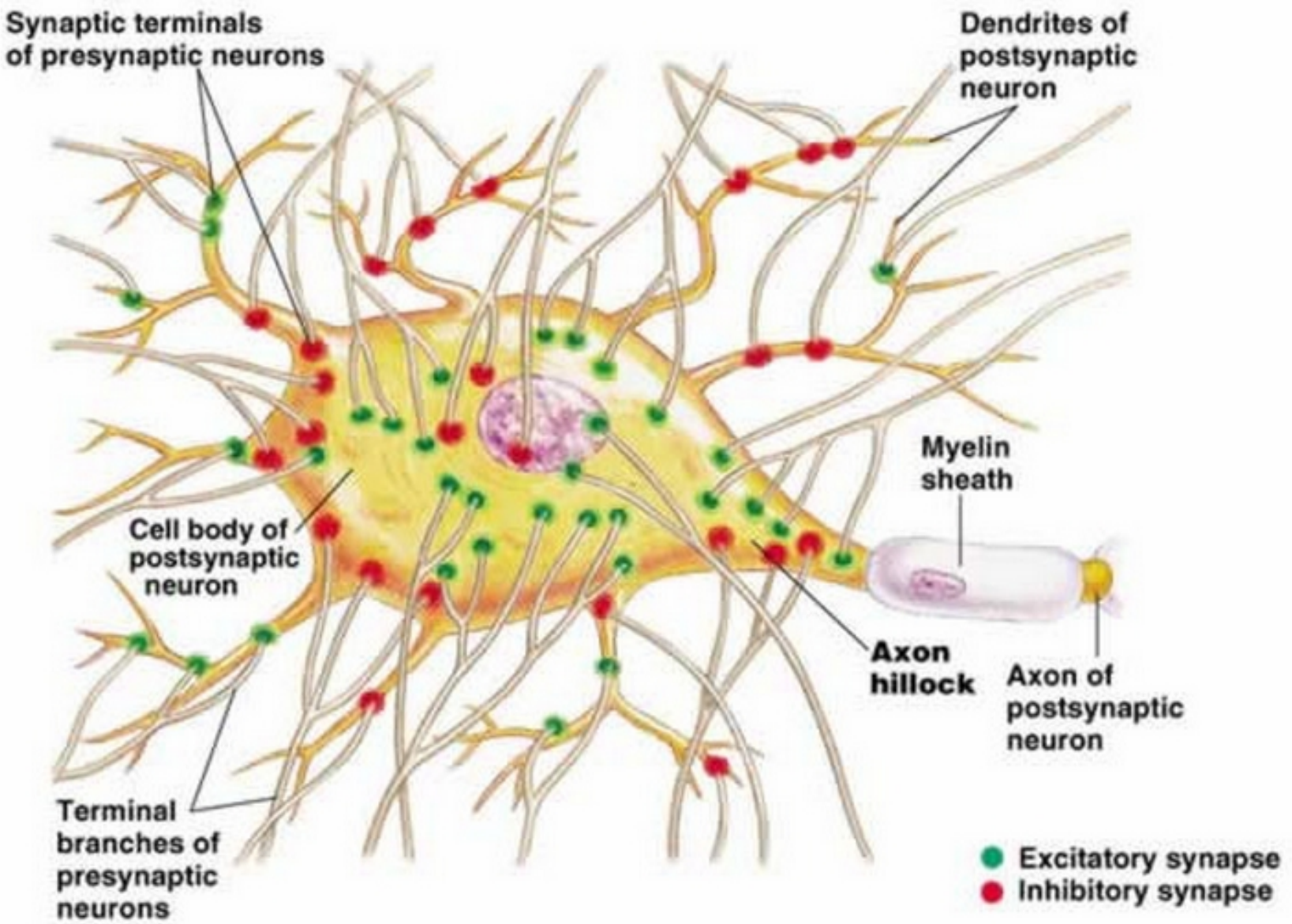
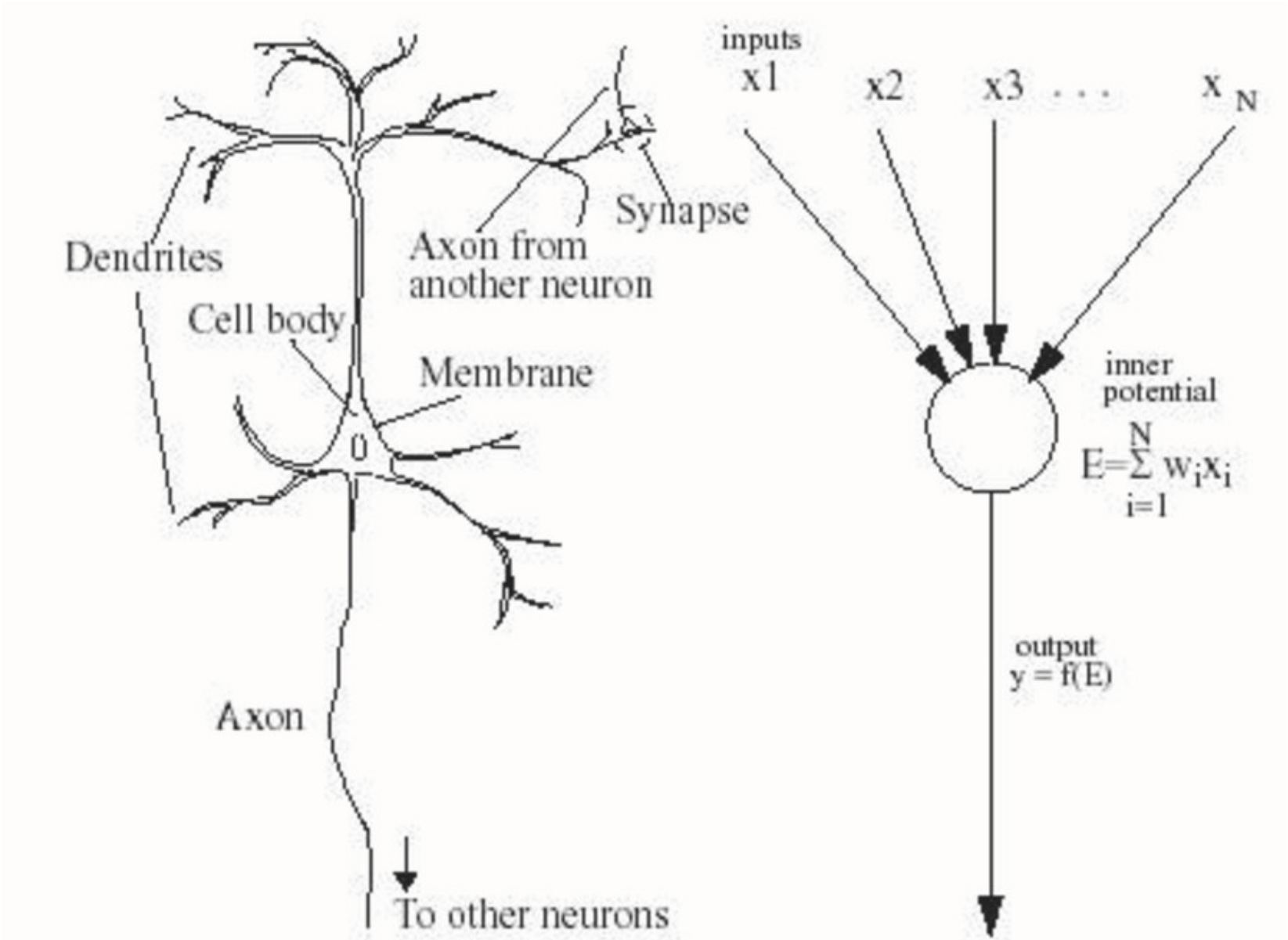
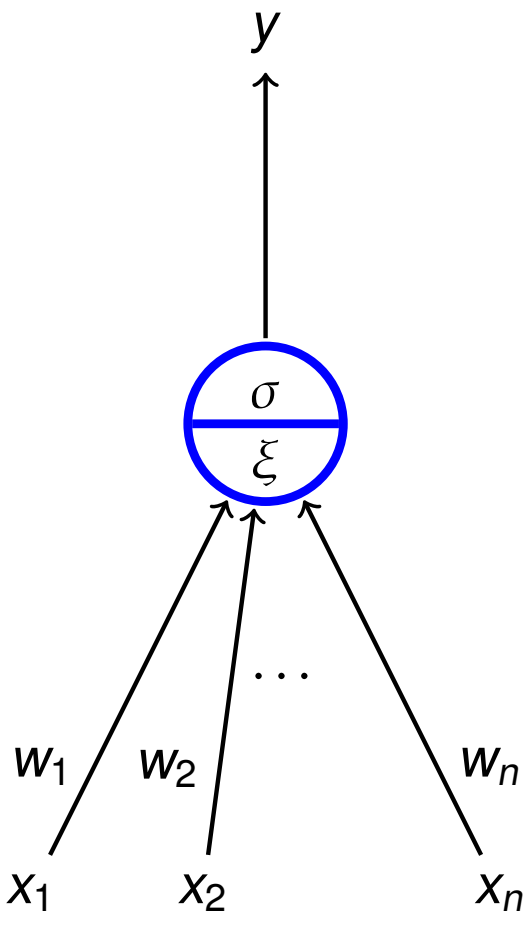


Figure 48.11(a), page 972, Campbell's *Biology, 5th Edition*

Biological and Mathematical neurons



Formal neuron (without bias)



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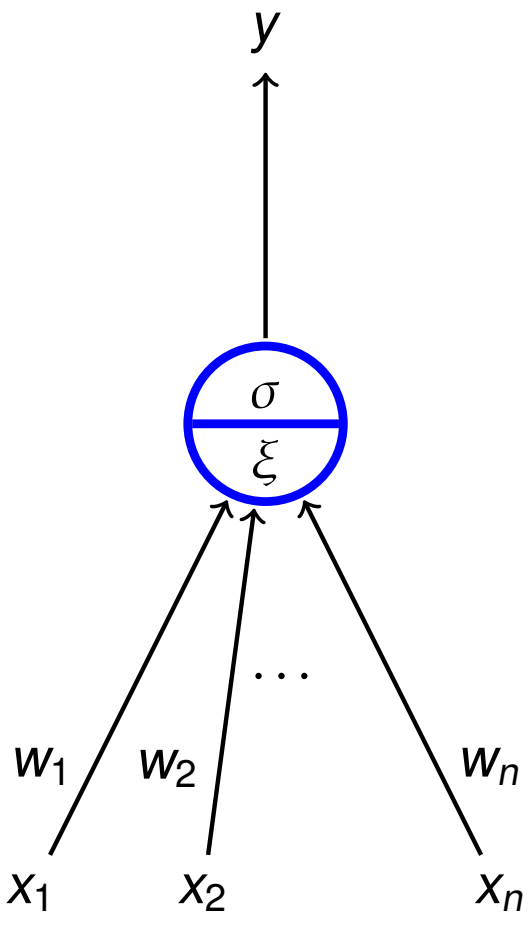

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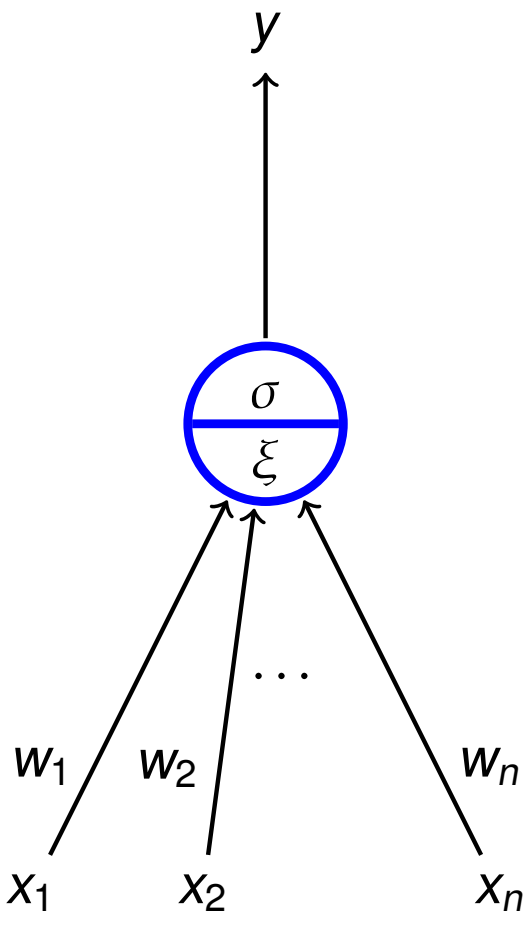

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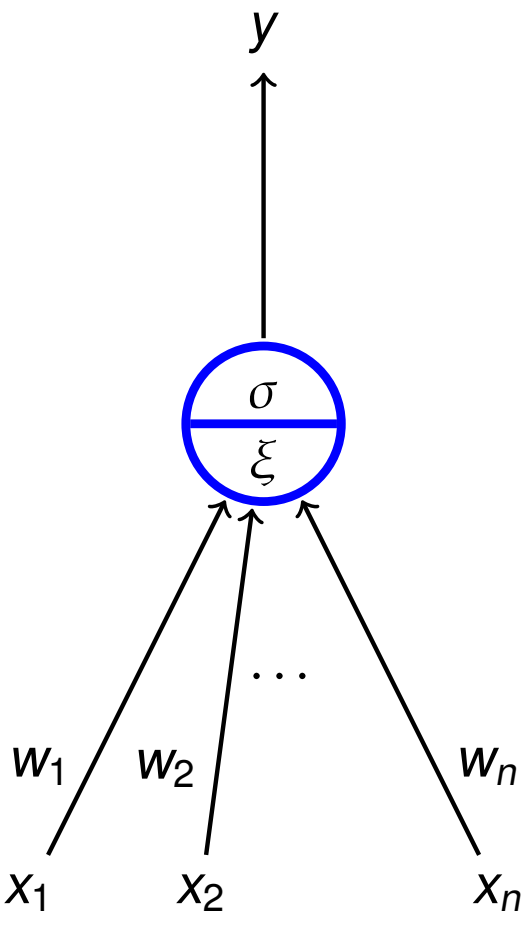

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- y is an **output** given by $y = \sigma(\xi)$
  where σ is an **activation function**;
  e.g. a *unit step function*

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

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

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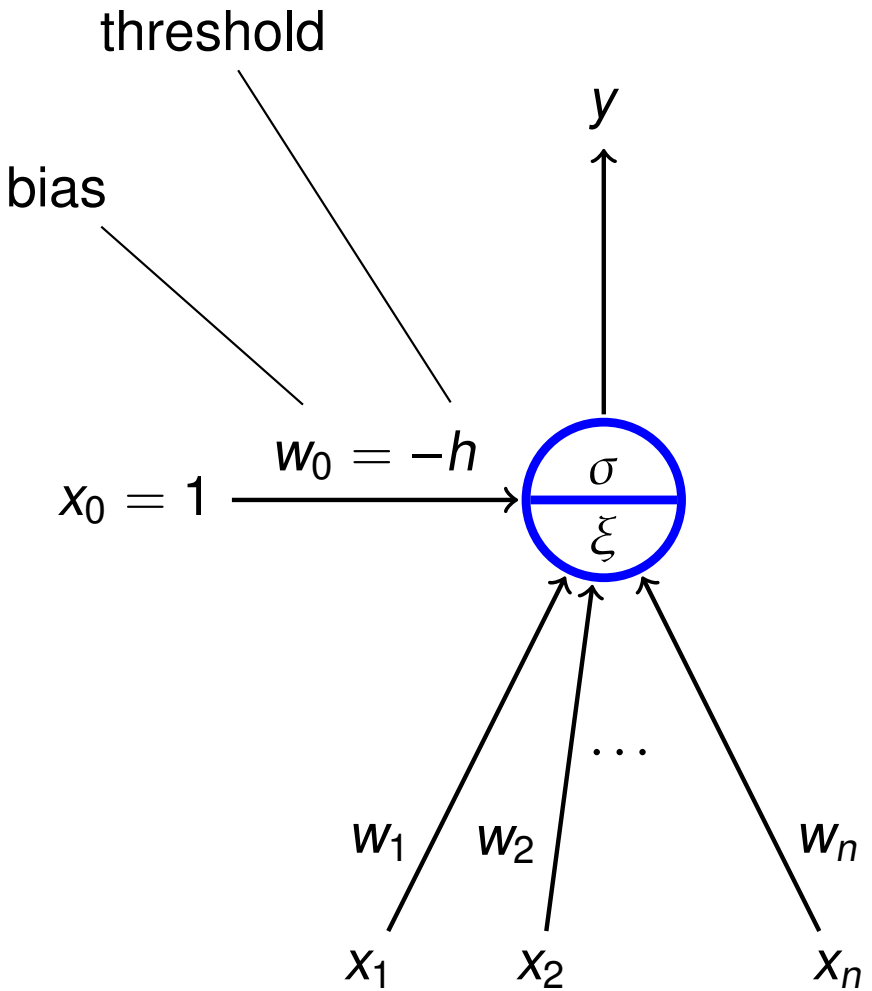

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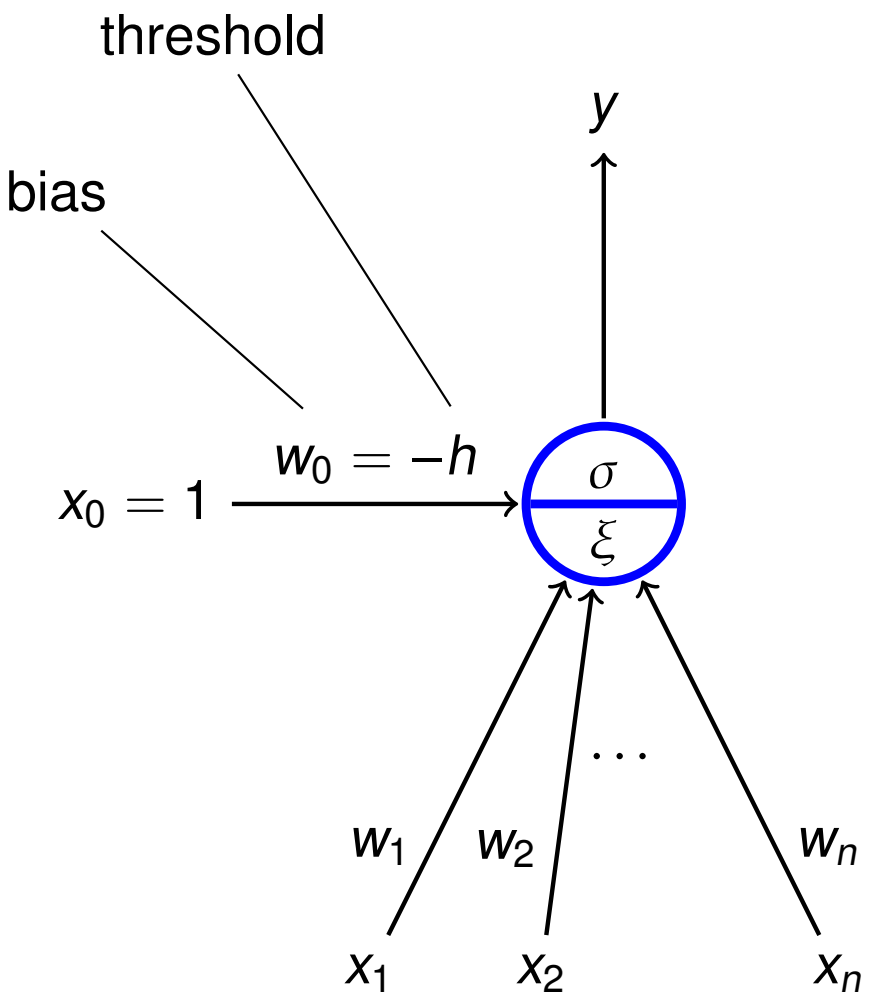

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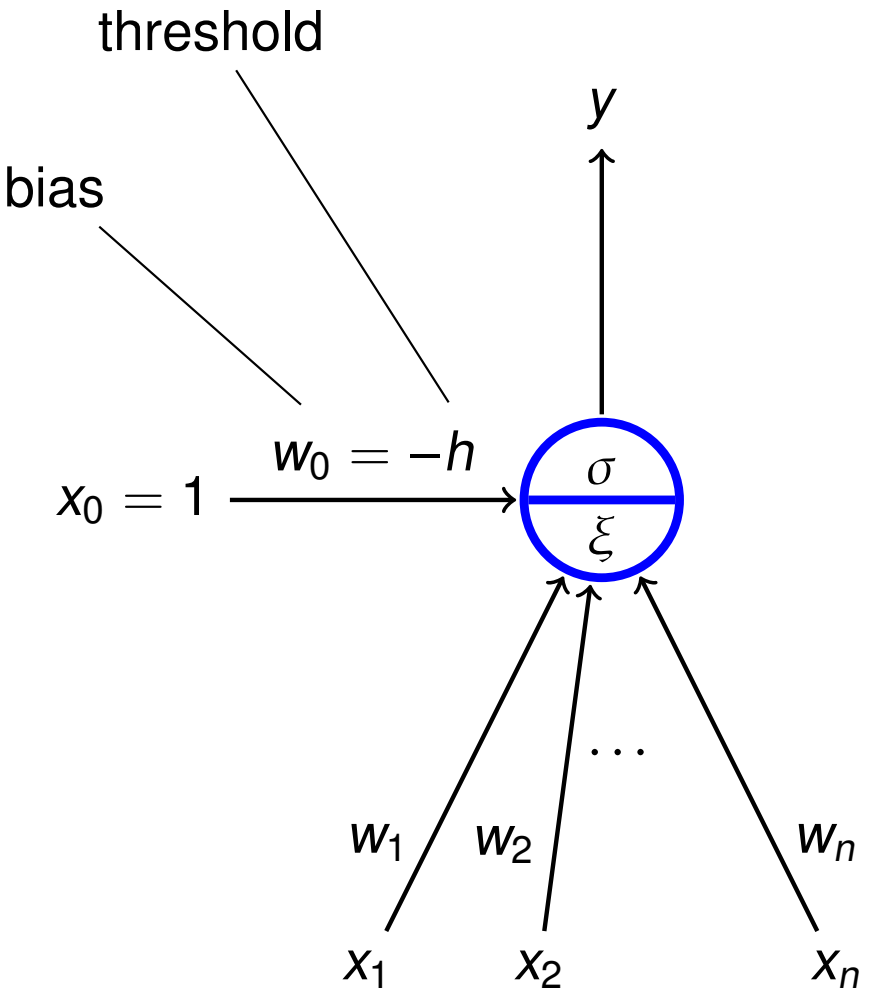

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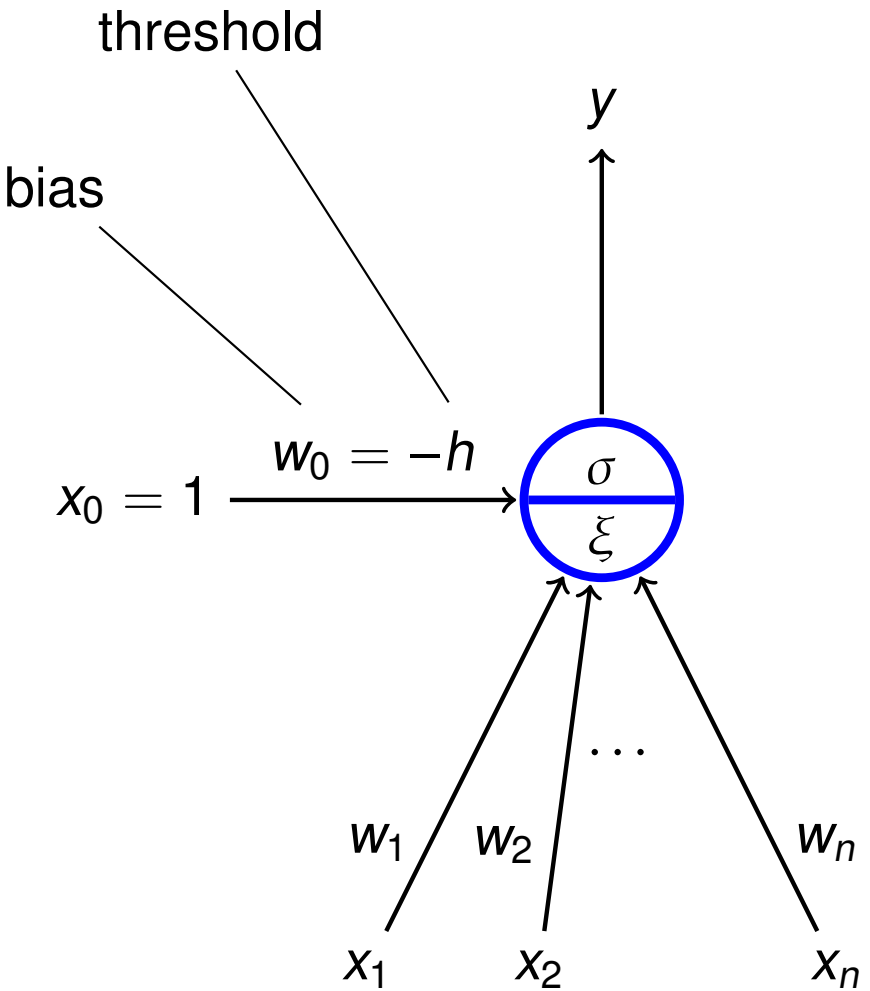

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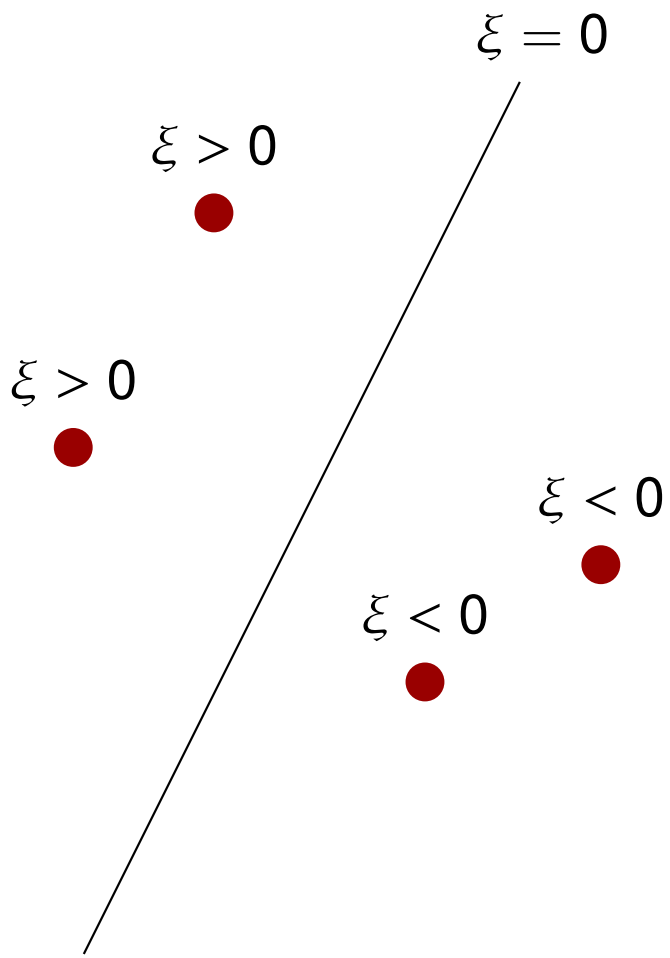
(The threshold h has been substituted with the new input $x_0 = 1$ and the weight $w_0 = -h$.)

Neuron and linear separation



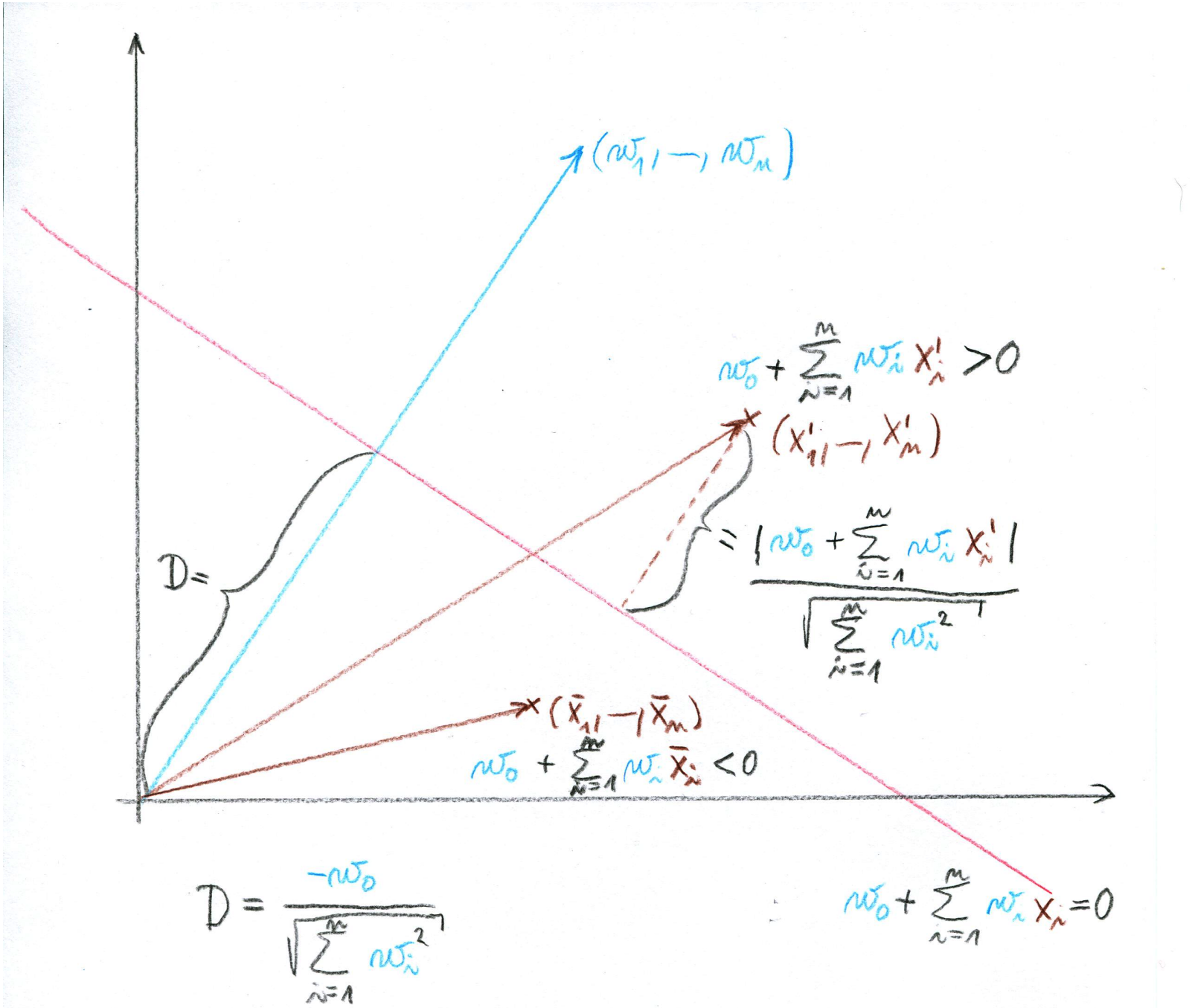
- inner potential

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

determines a separation hyperplane in the n-dimensional **input space**

- in 2d line
- in 3d plane
- ...

Neuron geometry



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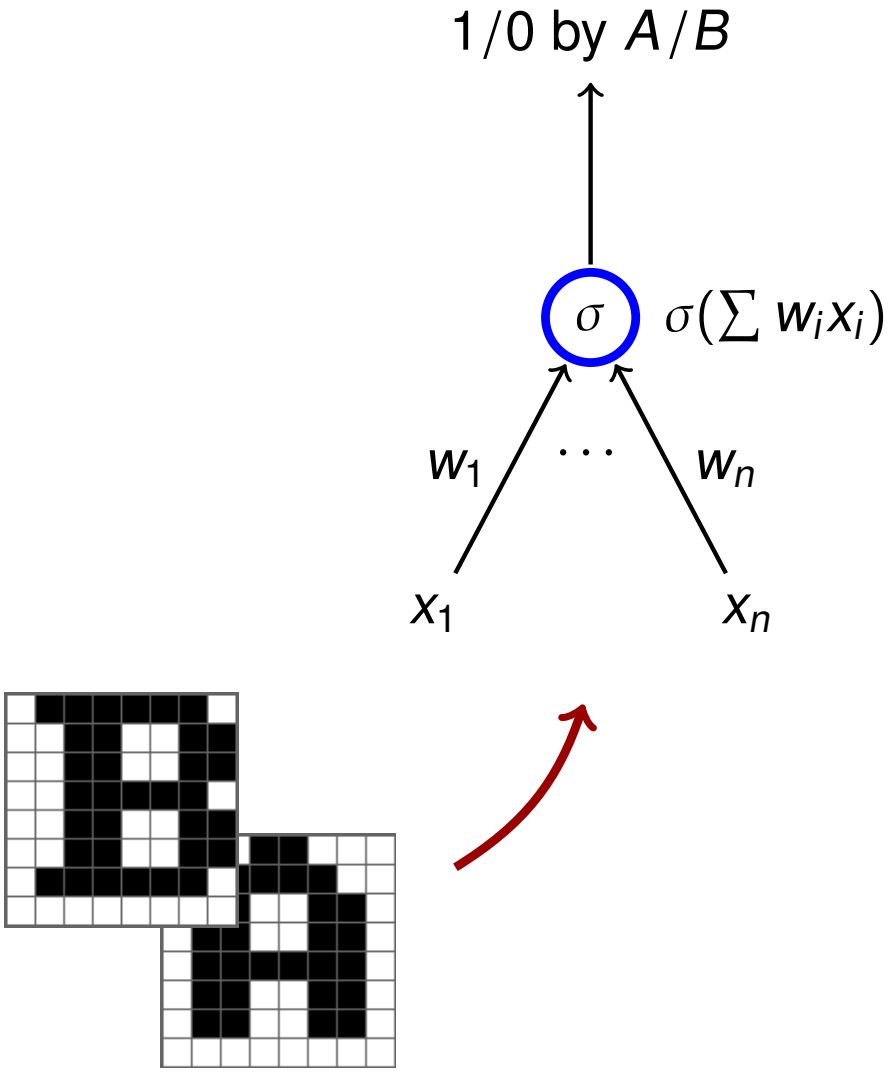

$n = 8 \cdot 8$, i.e. the number of pixels in the images. Inputs are binary vectors of dimension n (black pixel ≈ 1, white pixel ≈ 0).

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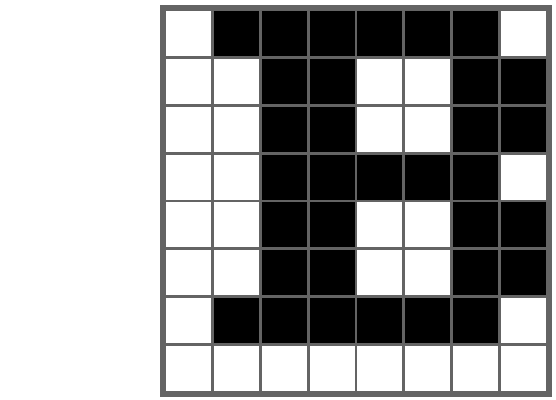

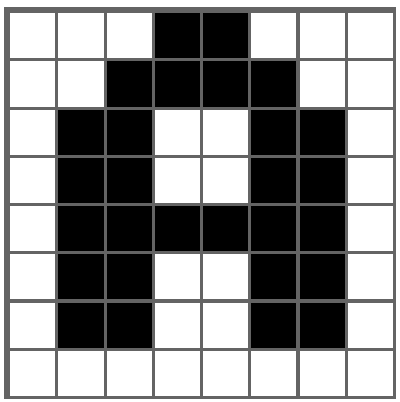

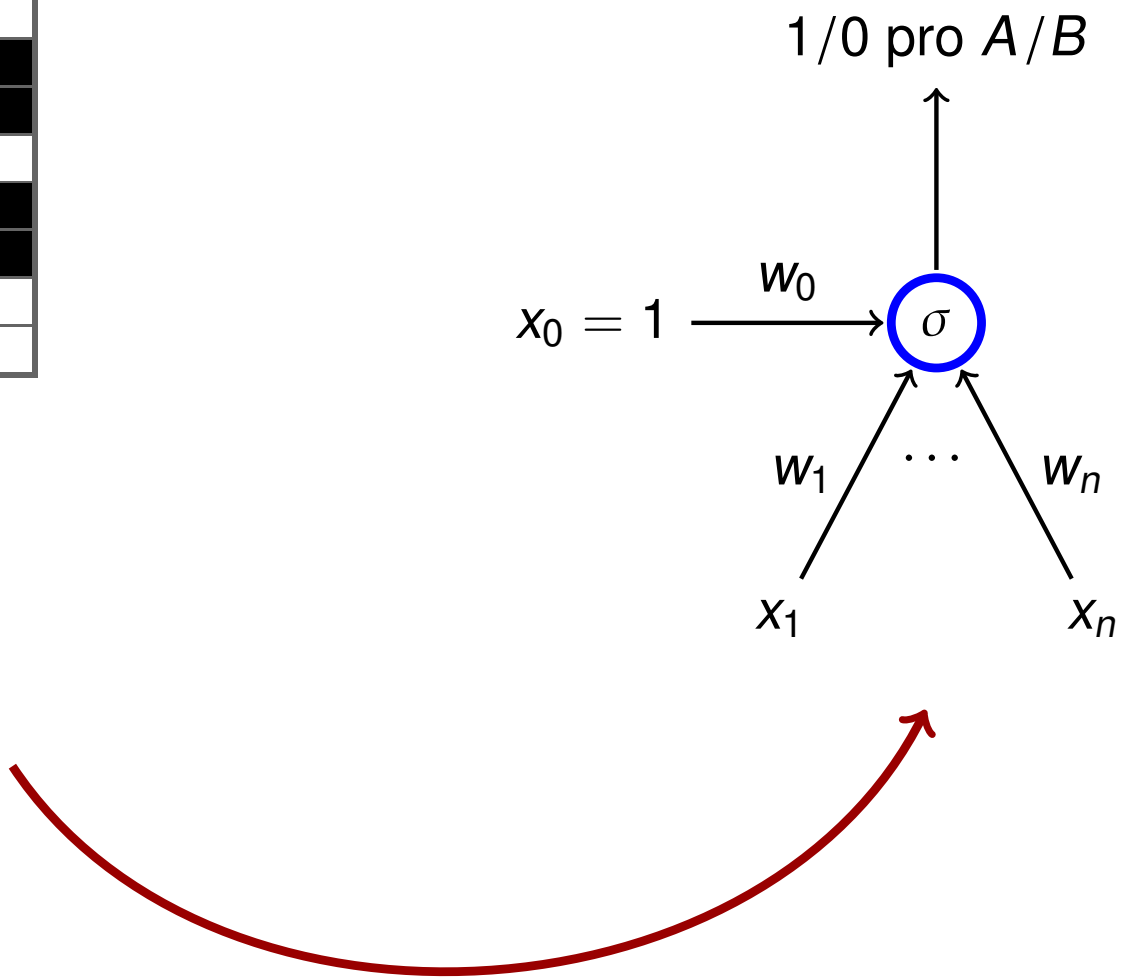

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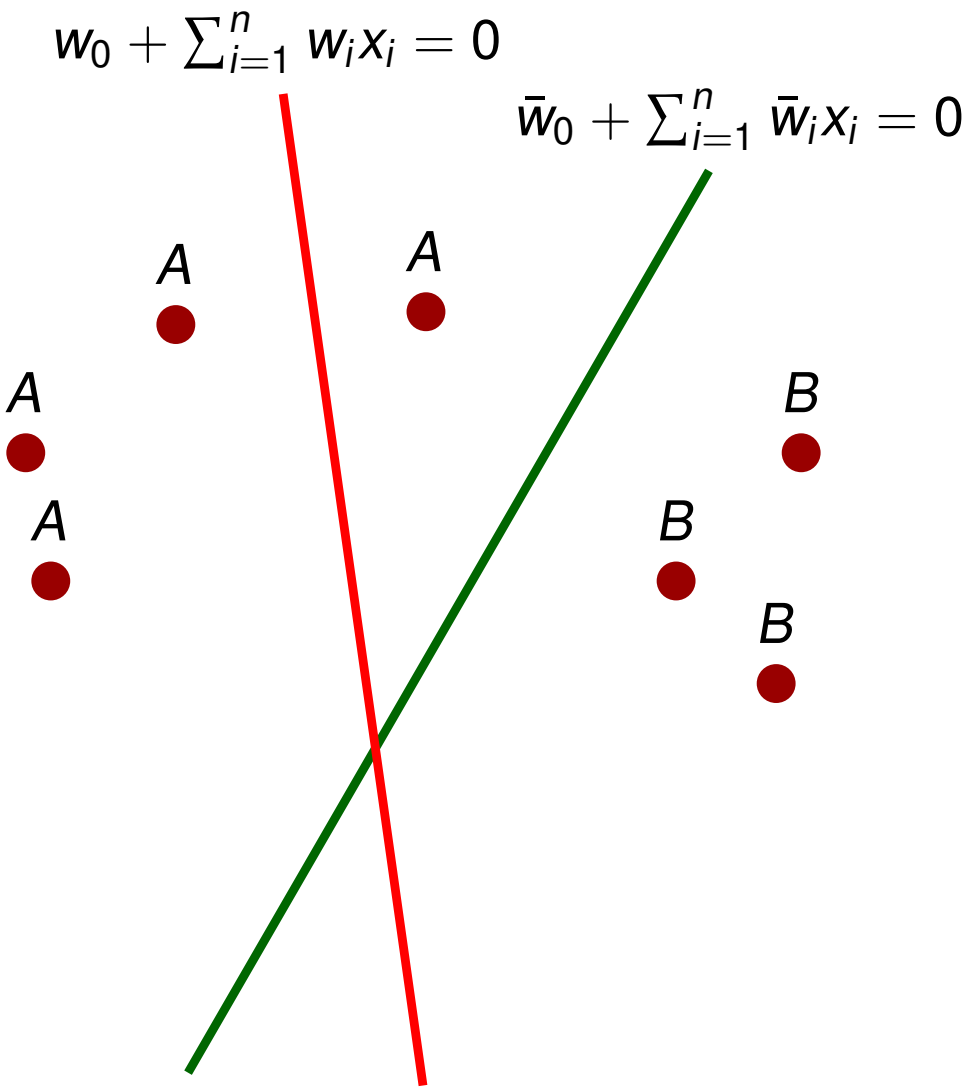
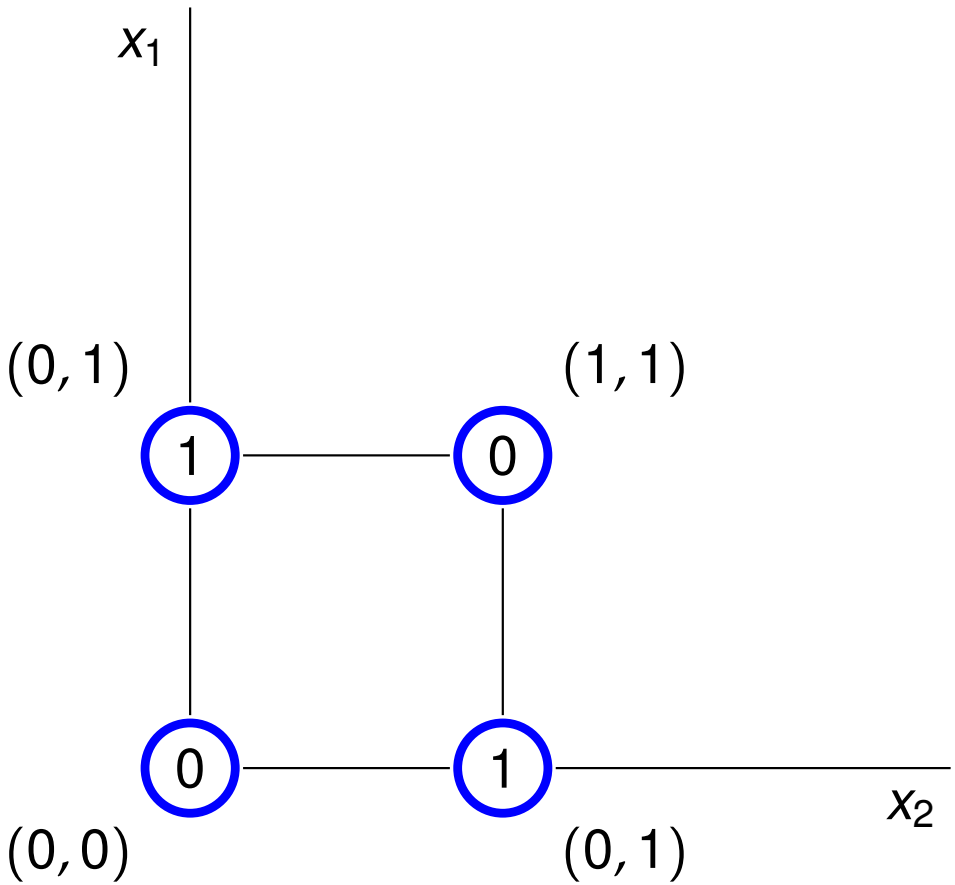


- Red line classifies incorrectly
- Green line classifies correctly (may be a result of a correction by a learning algorithm)

Neuron and linear separation (XOR)



- No line separates ones from zeros.

Neural networks

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

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

- Architecture

  How the neurons are connected.
- Activity

  How the network transforms inputs to outputs.
- Learning

  How the weights are changed during training.

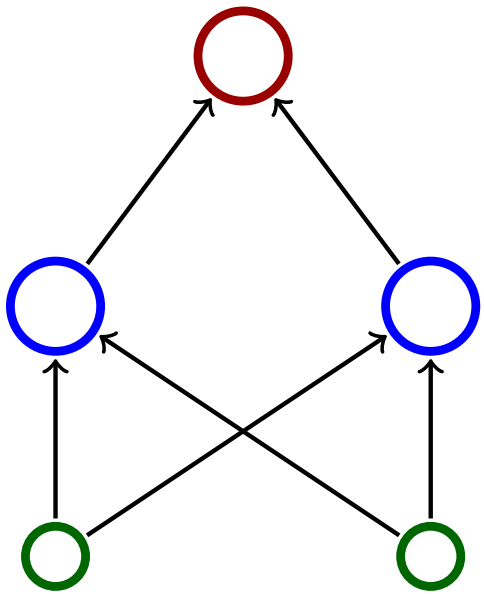
Architecture

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

We distinguish several categories of neurons:

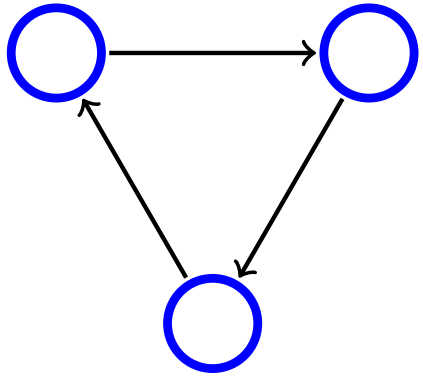
- Output neurons
- Hidden neurons
- Input neurons

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



Architecture – Cycles

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



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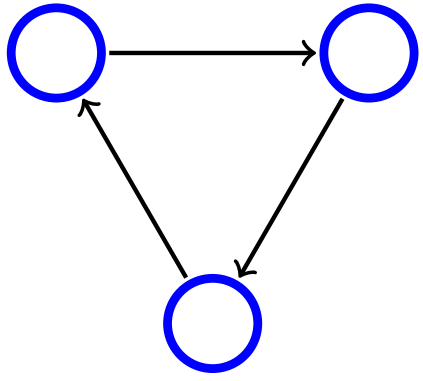
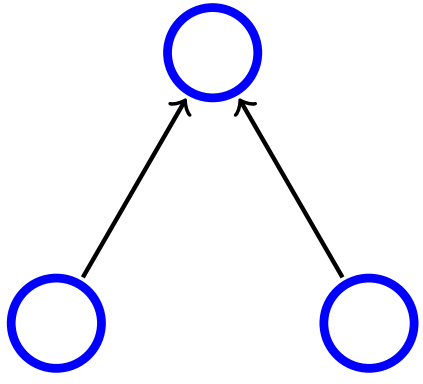
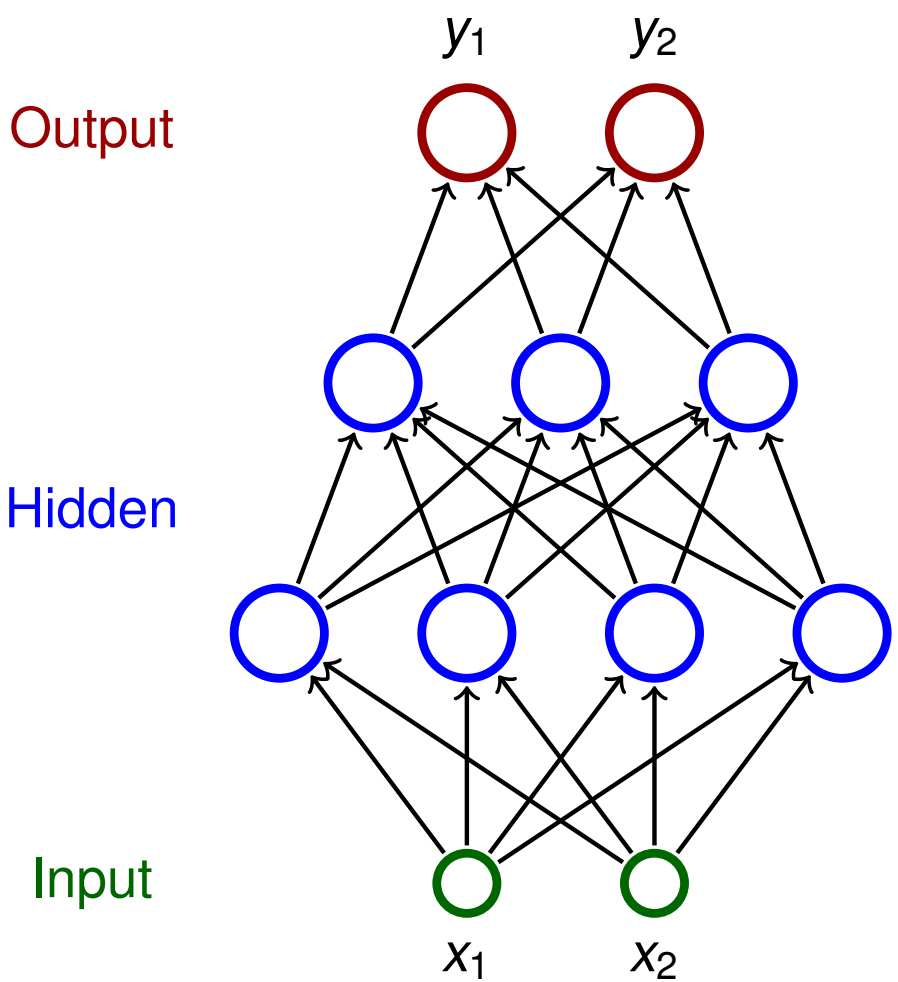


- Otherwise it is **acyclic** (feed-forward)



Architecture – Multilayer Perceptron (MLP)



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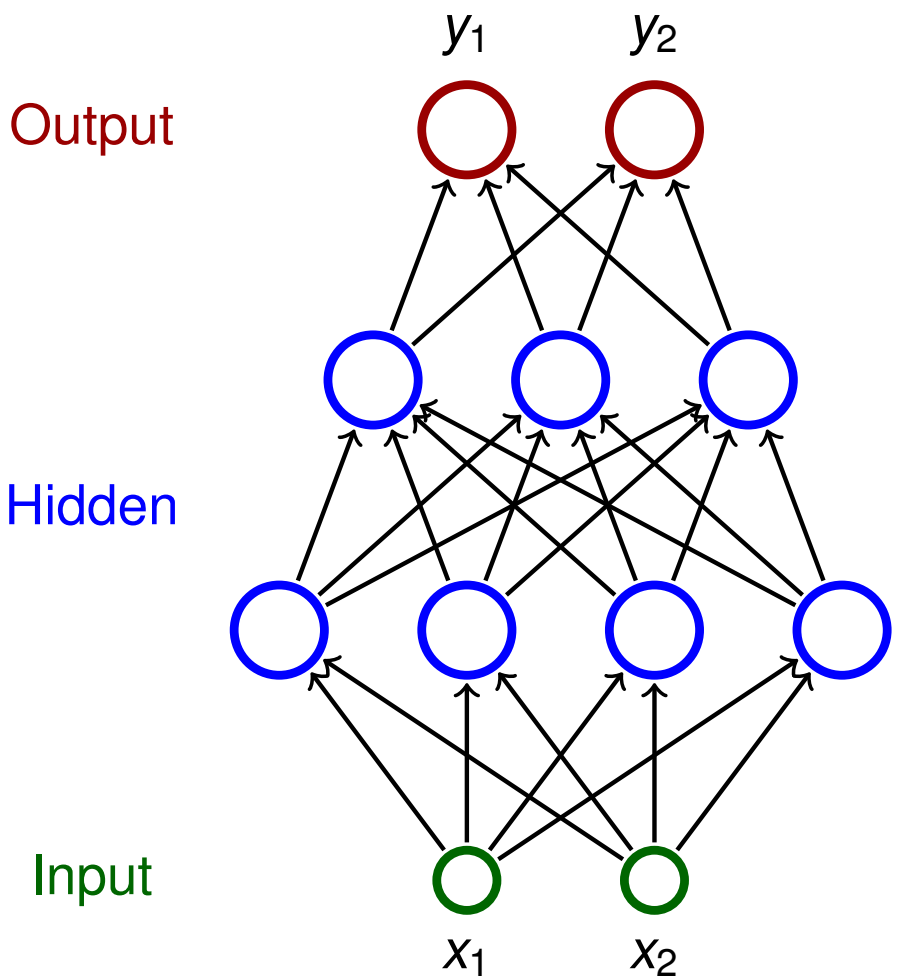

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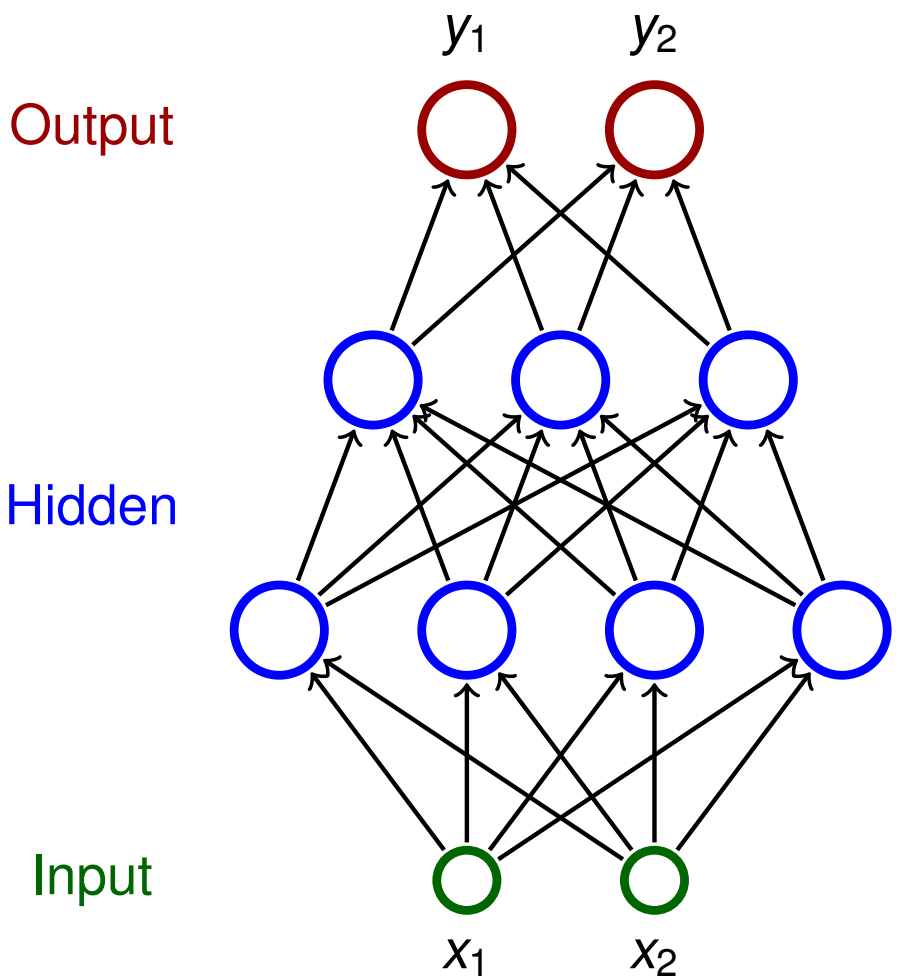

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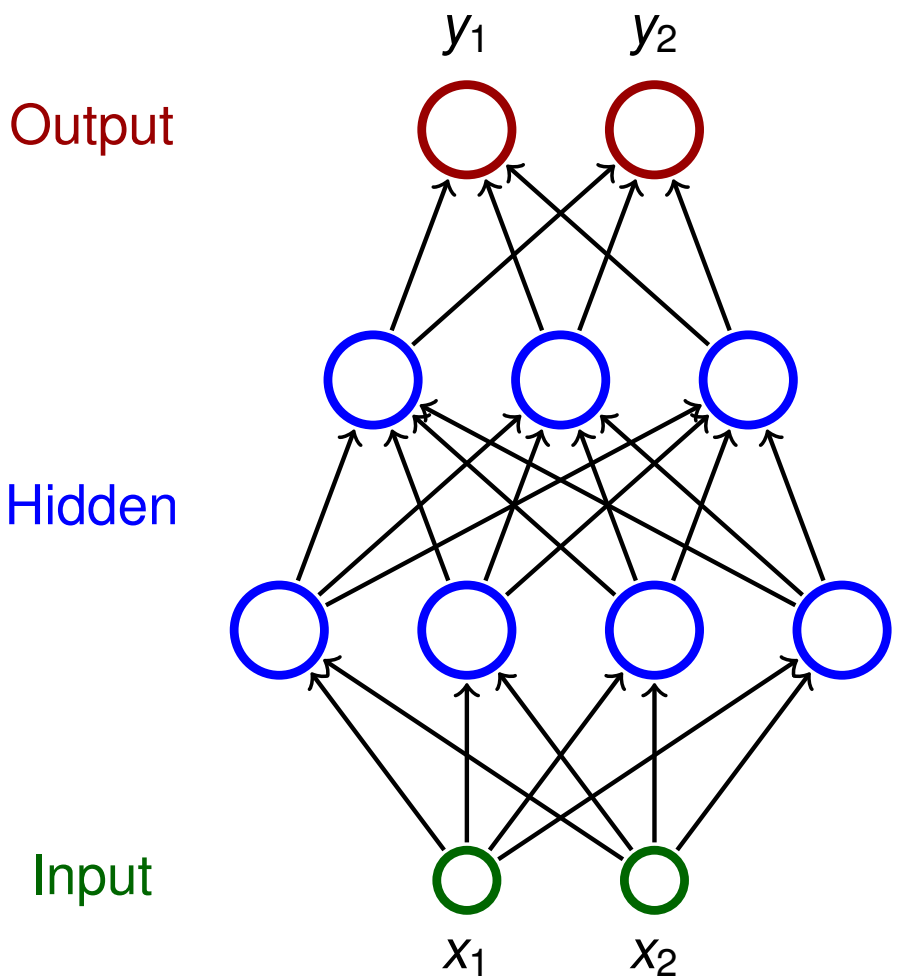

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  - E.g. three-layer network has two hidden layers and one output layer
- Neurons in the i-th layer are connected with all neurons in the $i + 1$-st layer
- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

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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.
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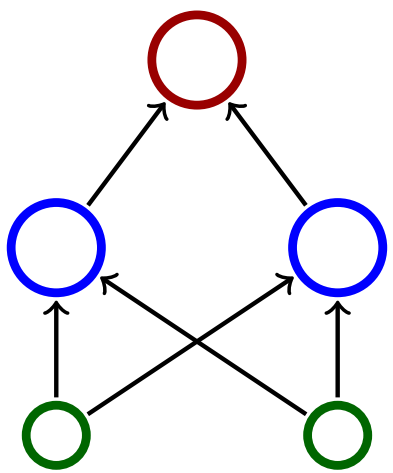
Example 1

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



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

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

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

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

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- (Logistic) sigmoid

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

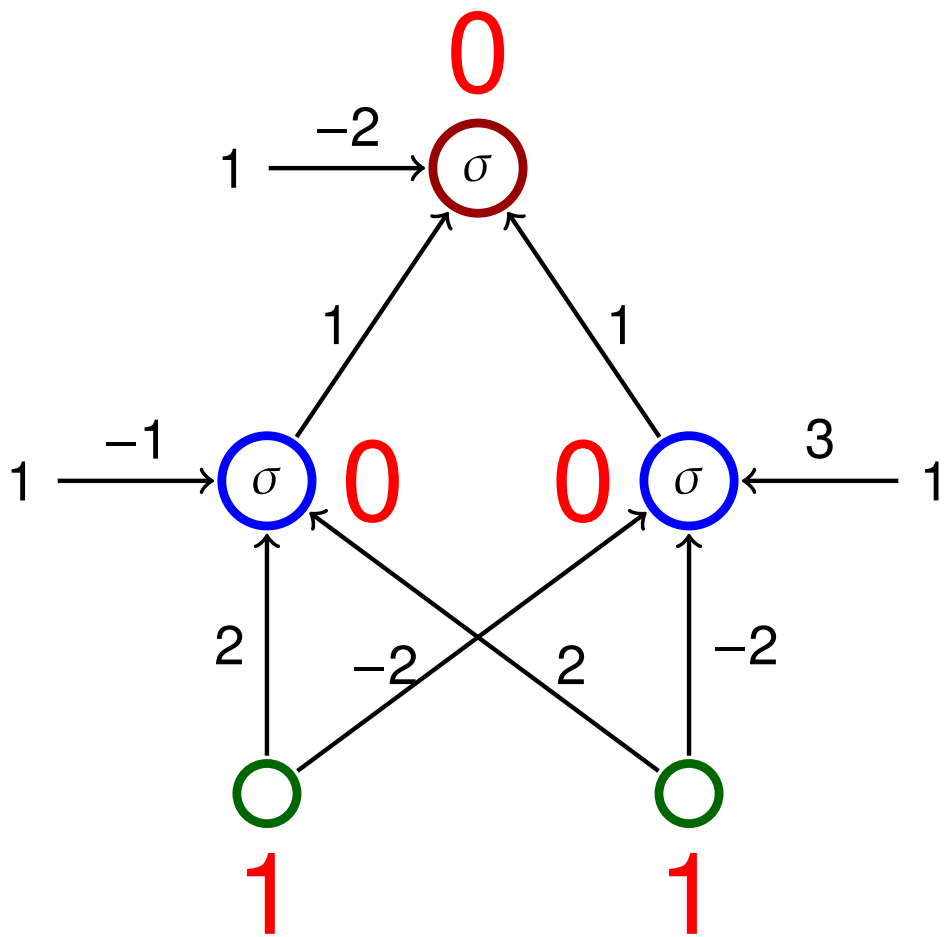
- Hyperbolic tangens

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

- ReLU

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

Activity – XOR



- Activation function is a unit step function

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

x_1	x_2	y
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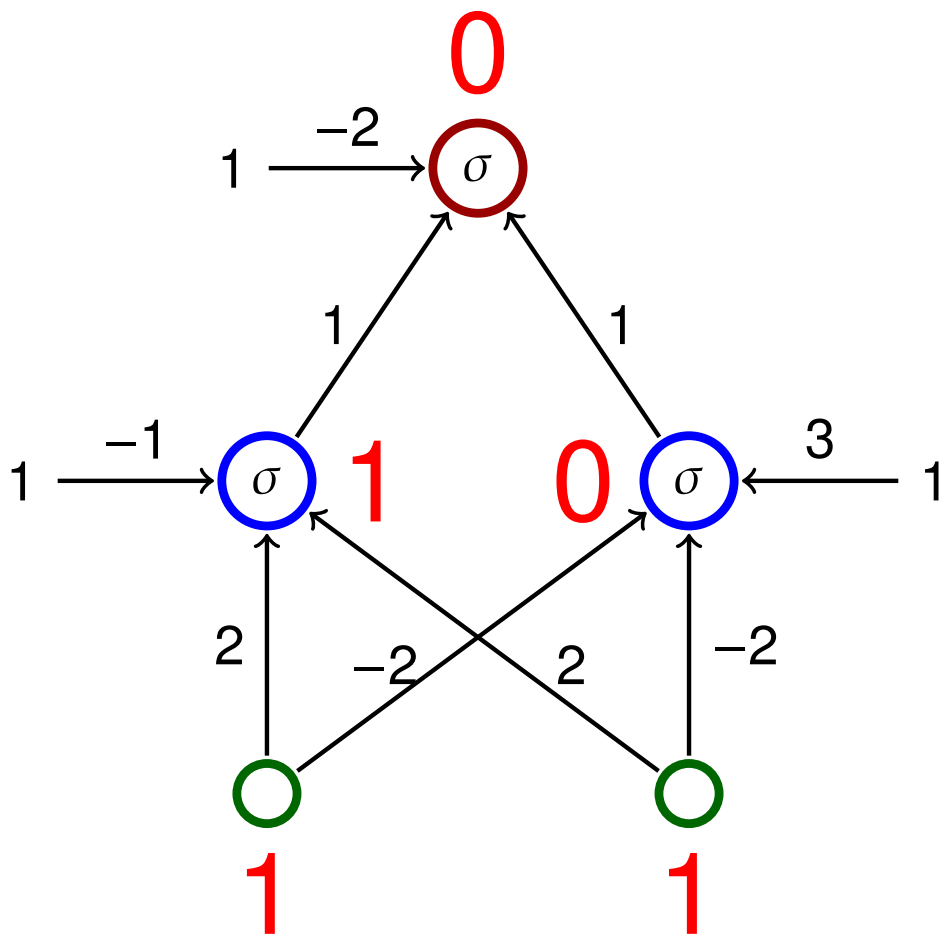

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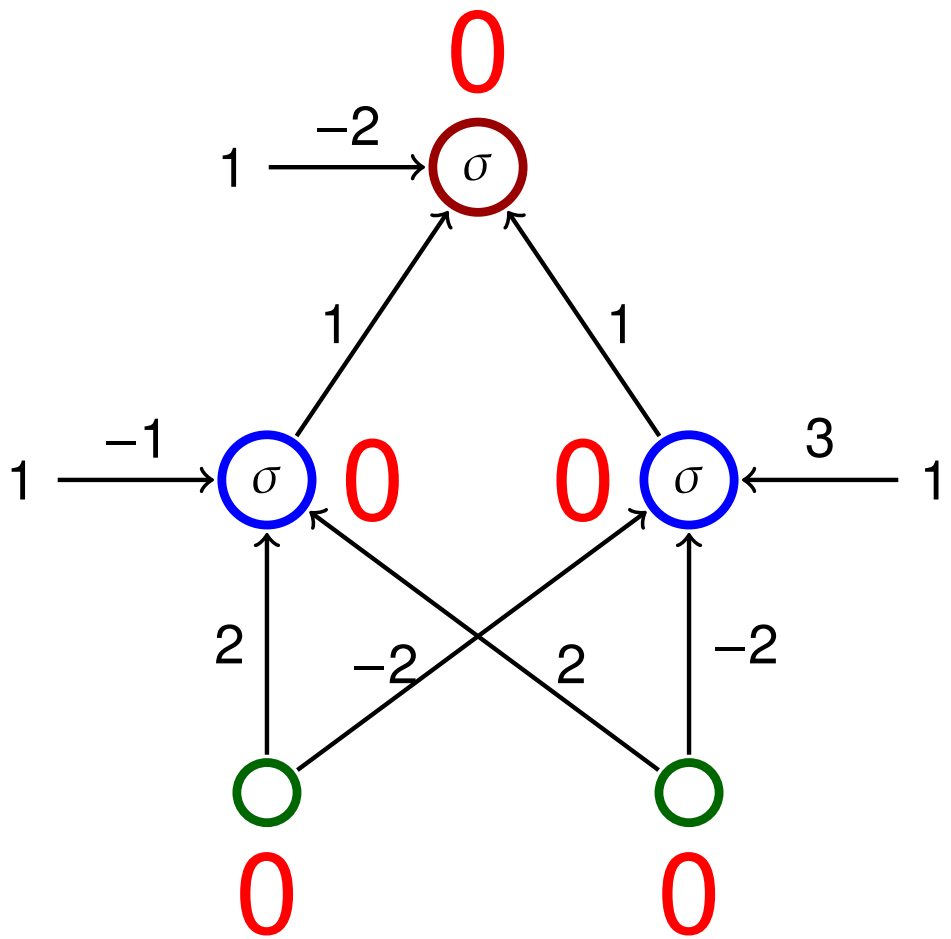

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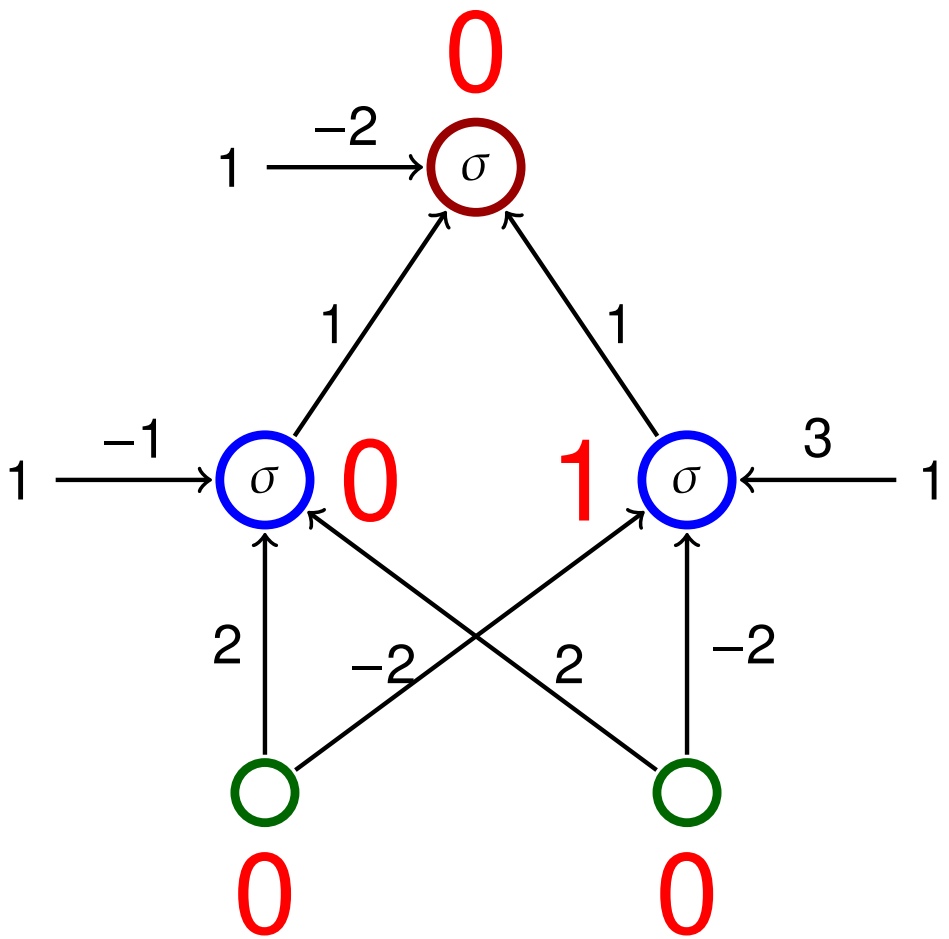

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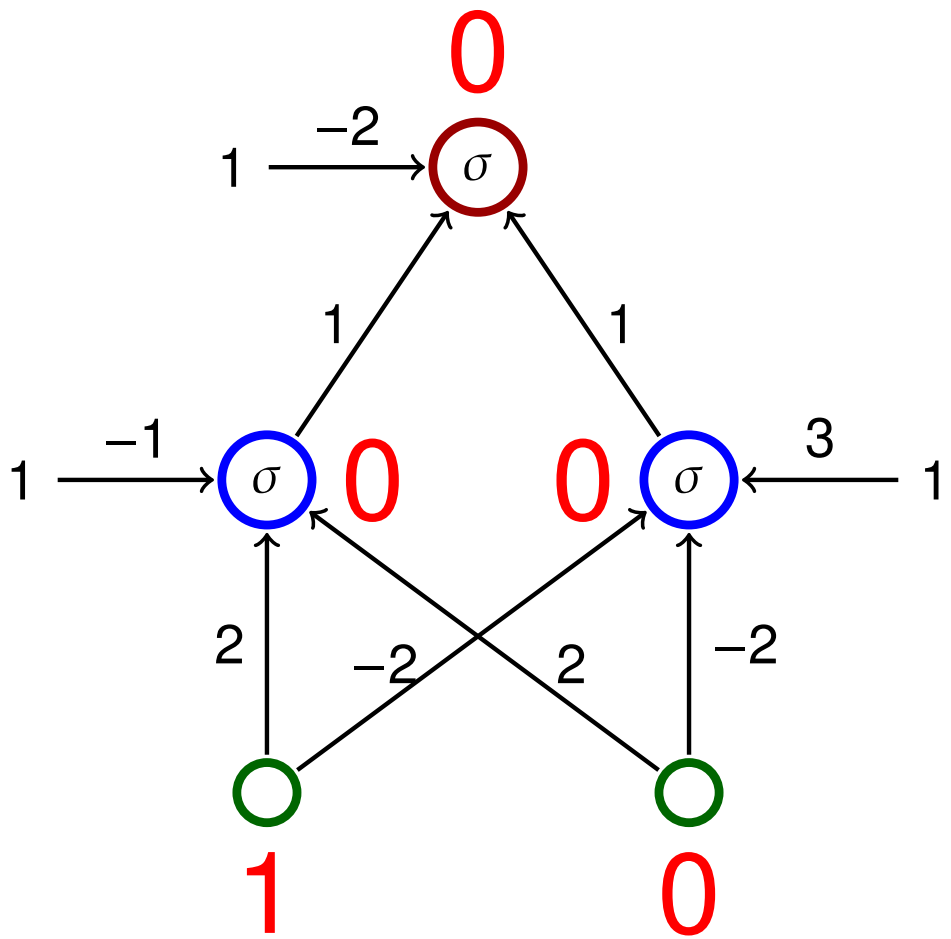

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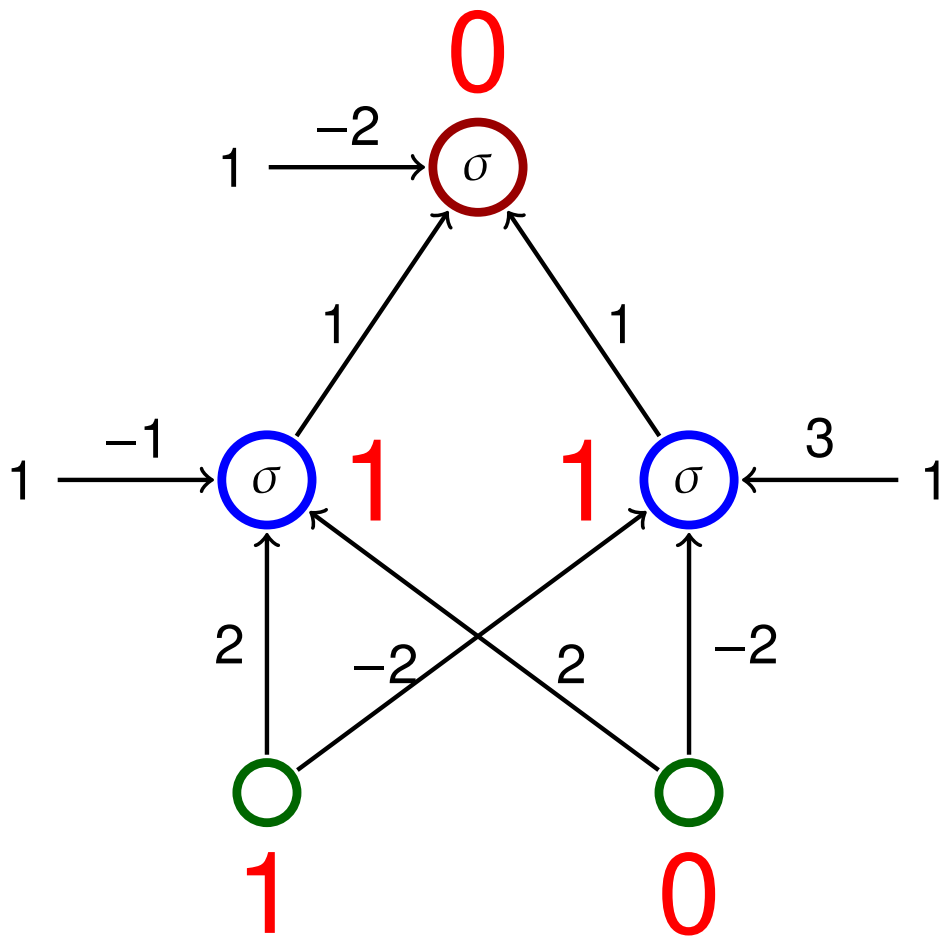

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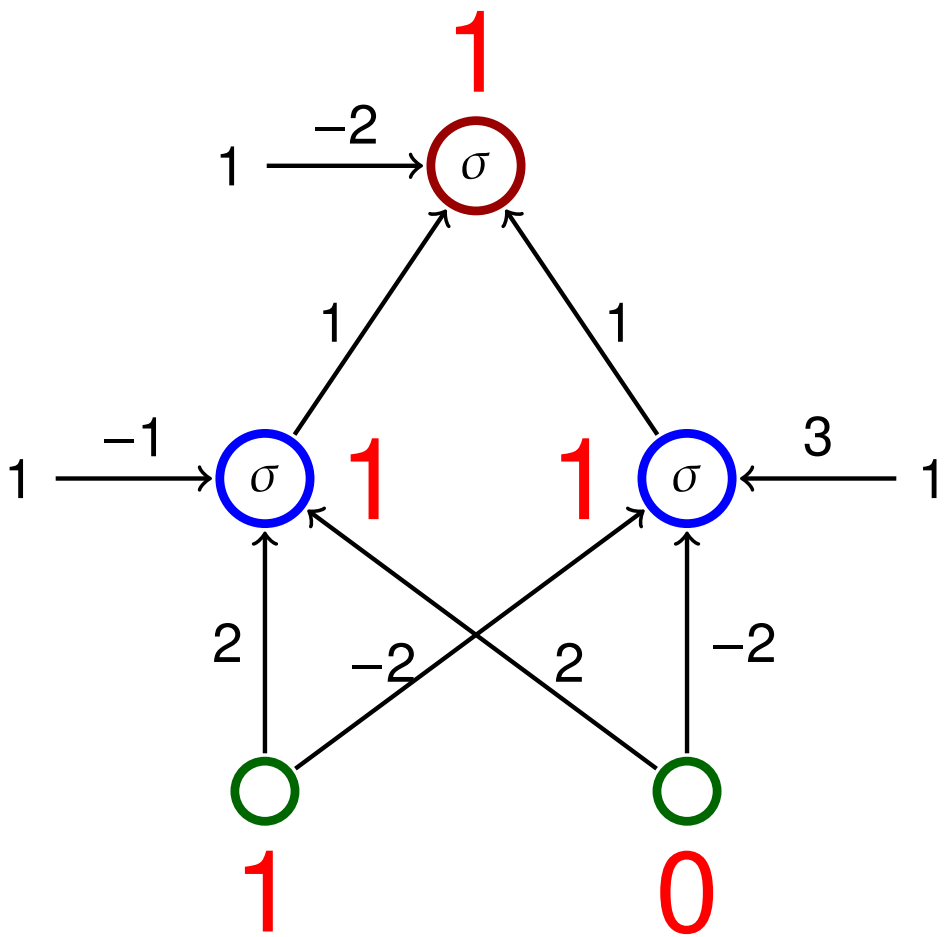

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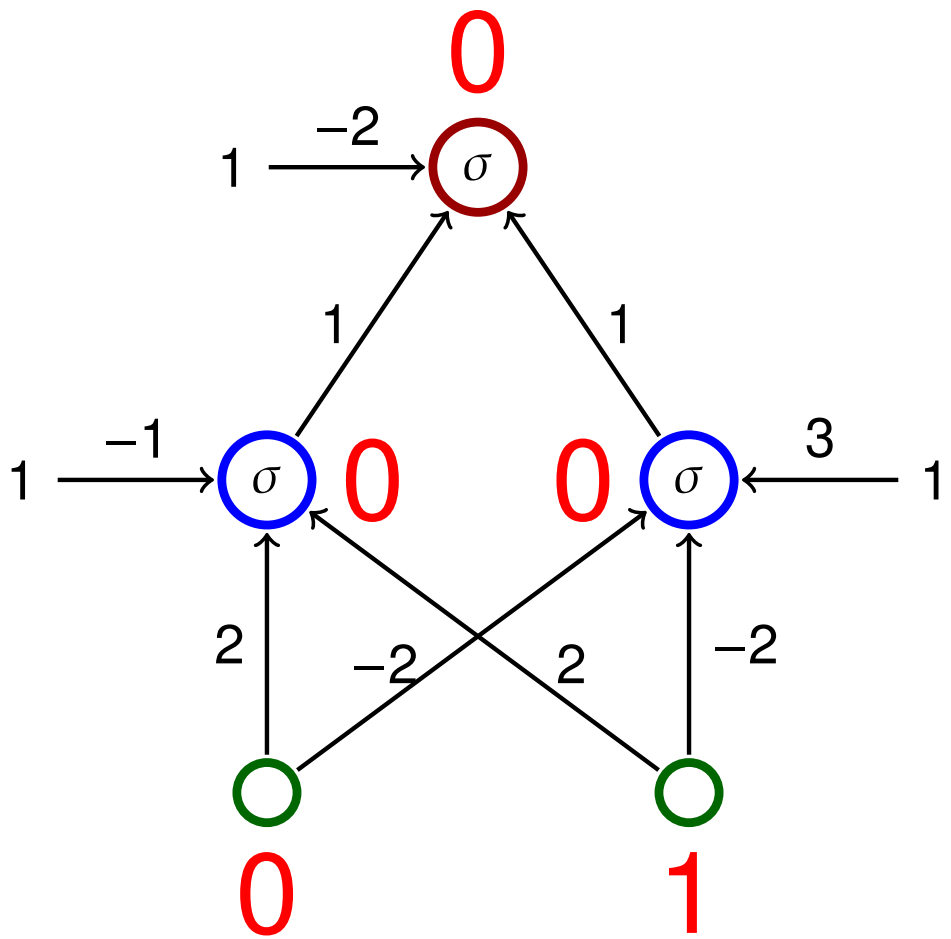

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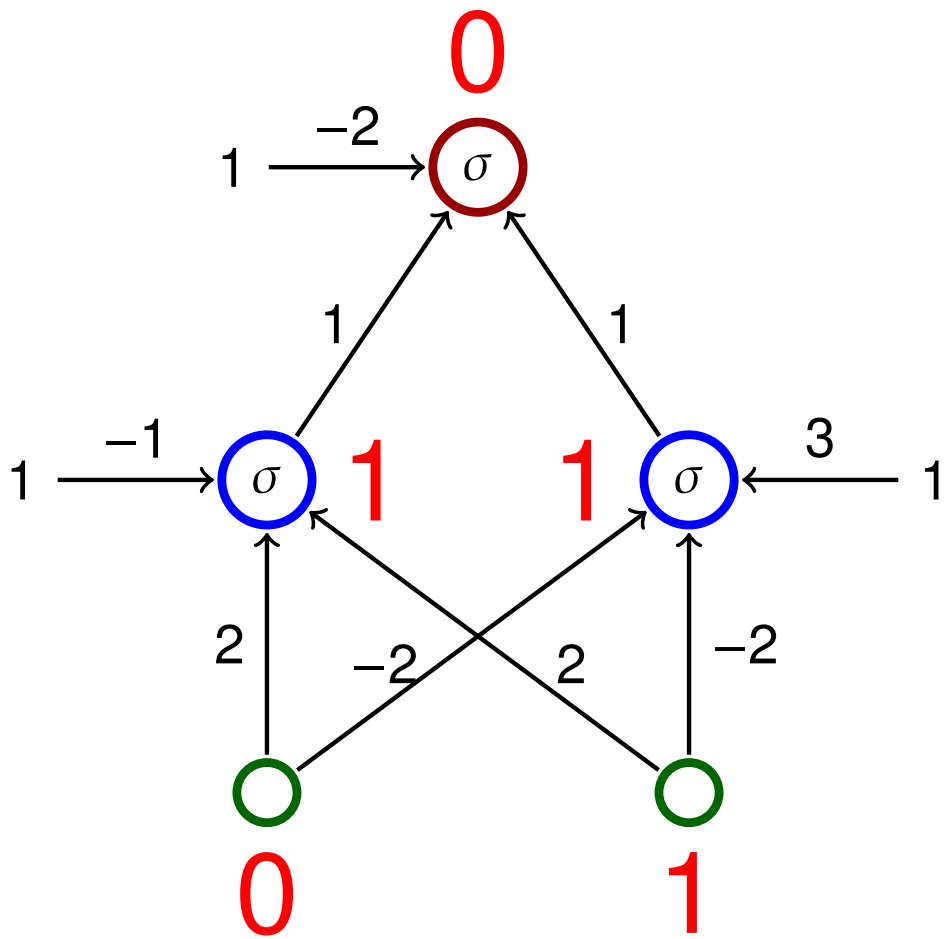

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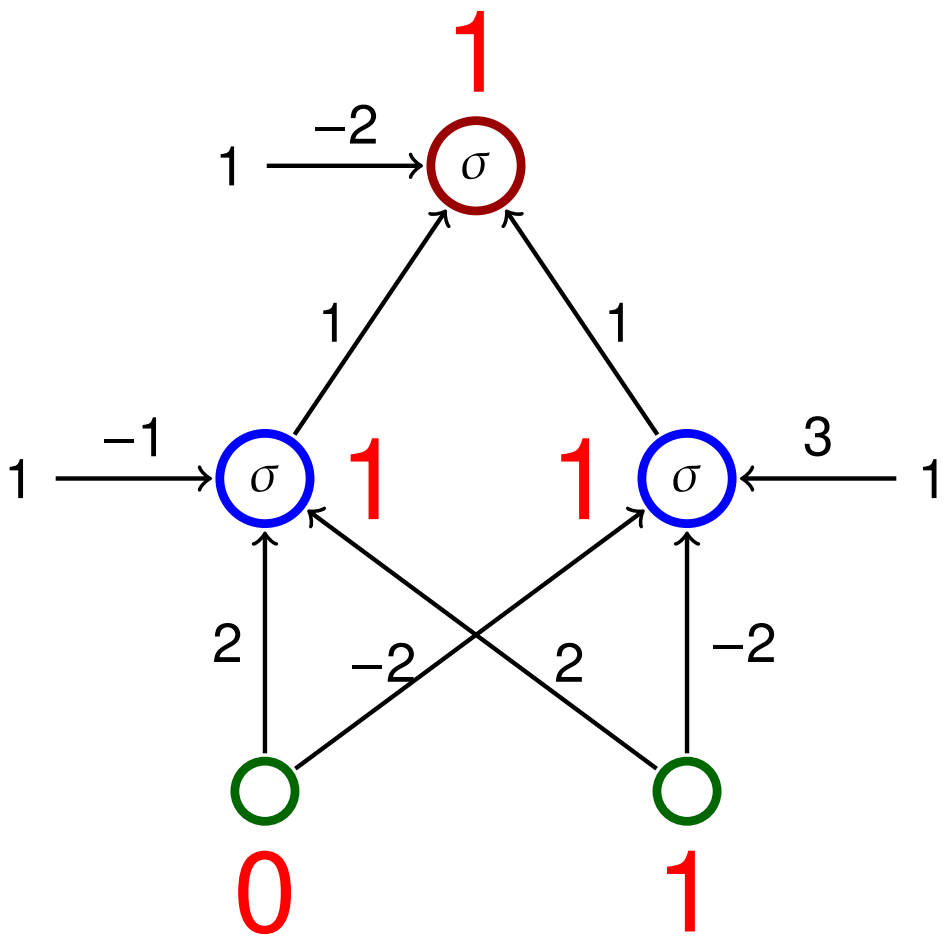

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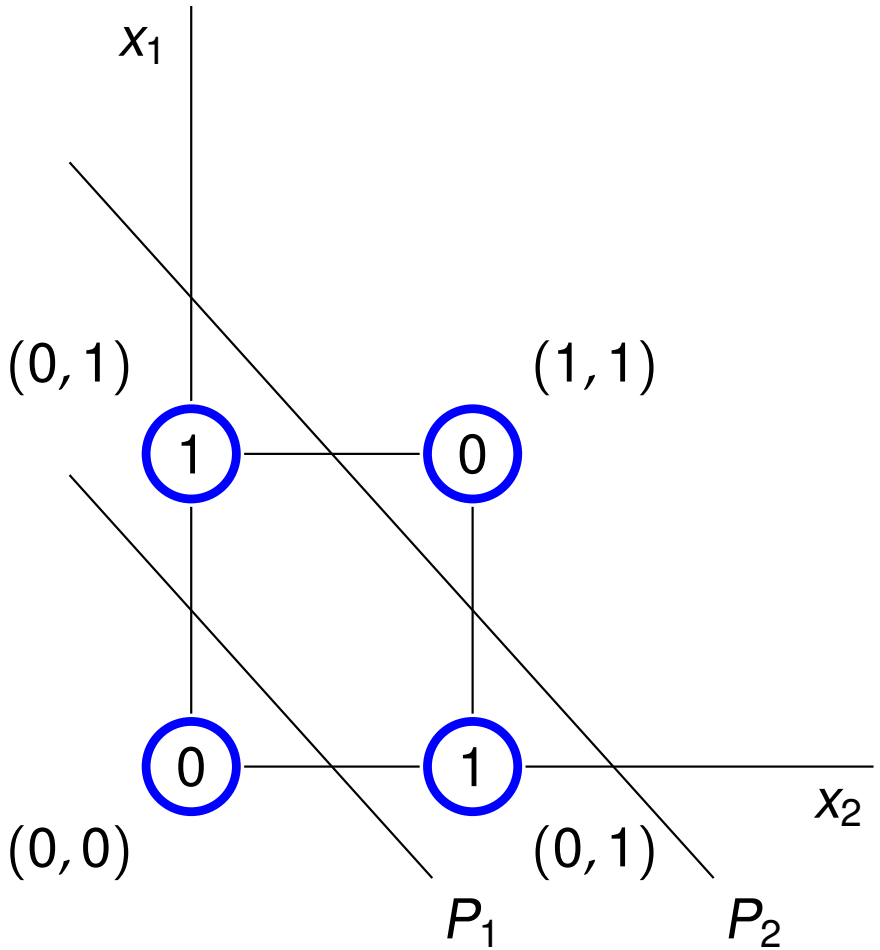
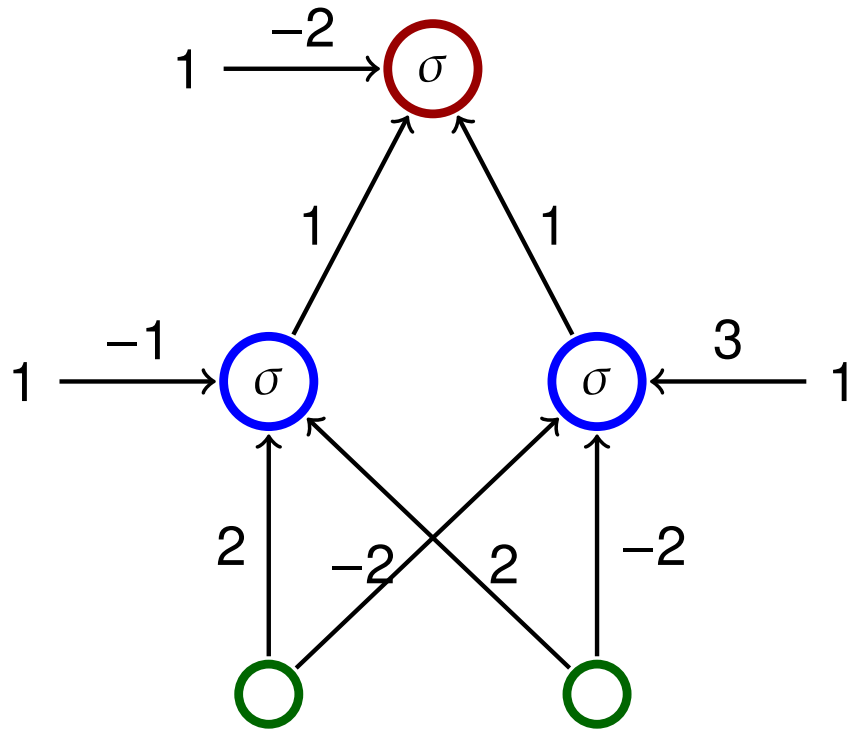
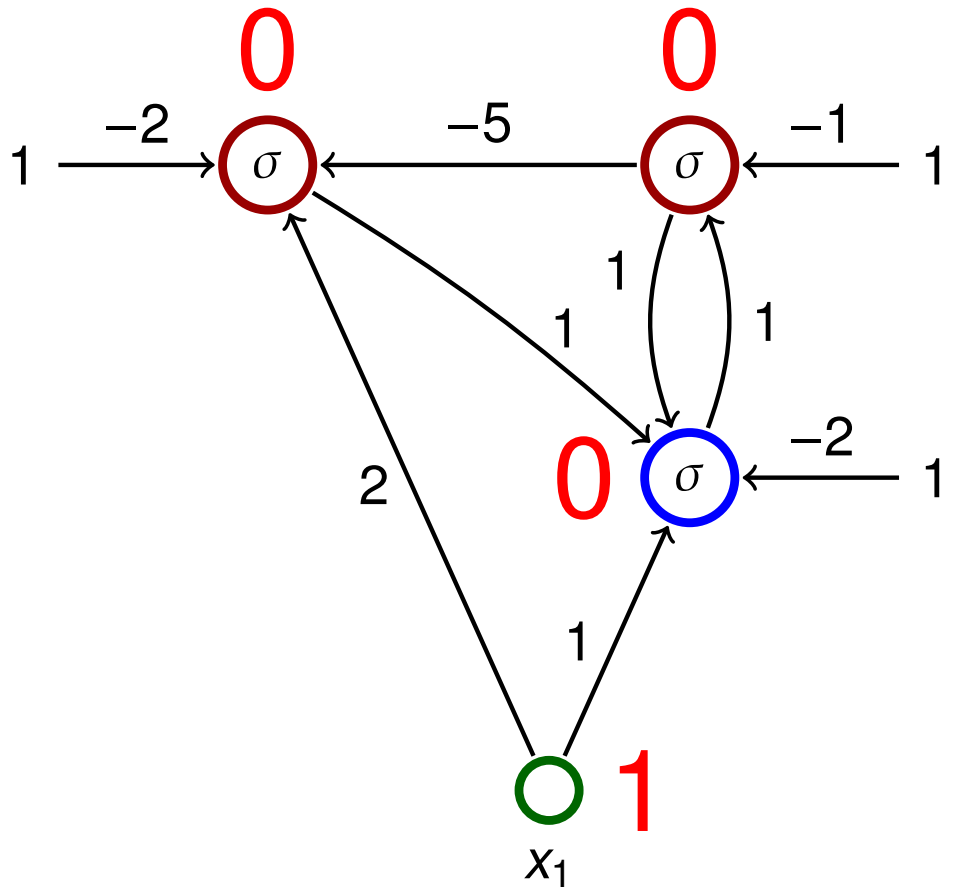




- The line P_1 is given by $-1 + 2x_1 + 2x_2 = 0$
- The line P_2 is given by $3 - 2x_1 - 2x_2 = 0$

Activity – example



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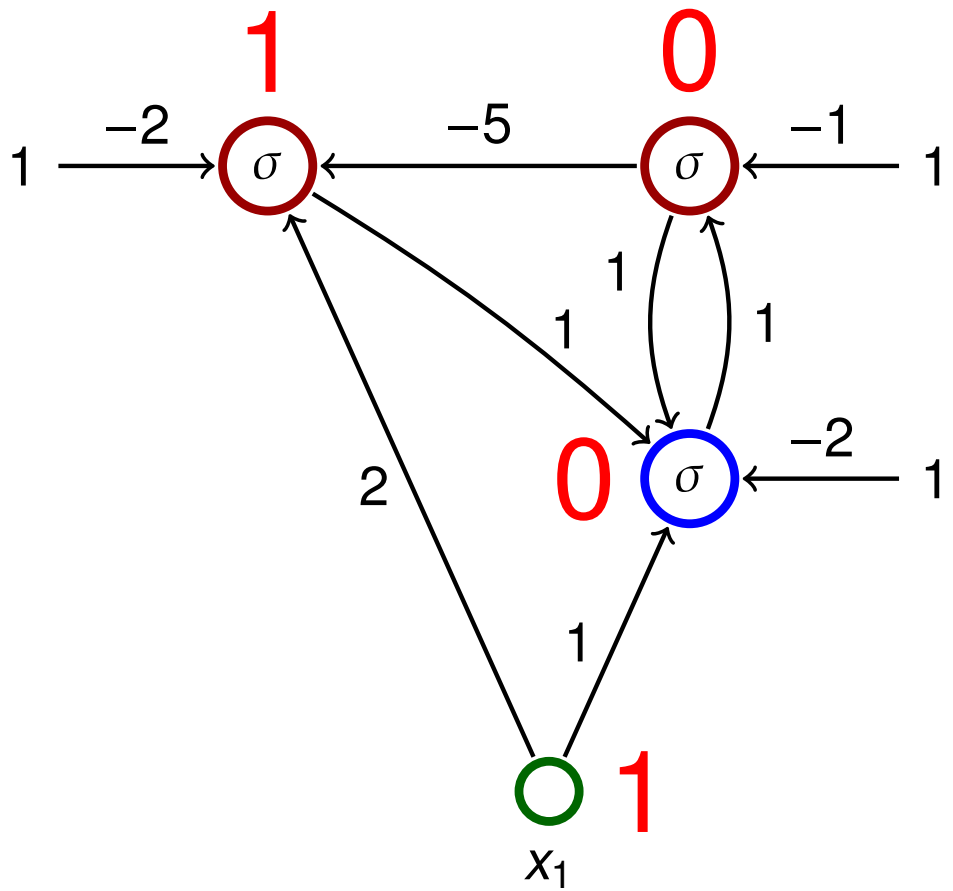

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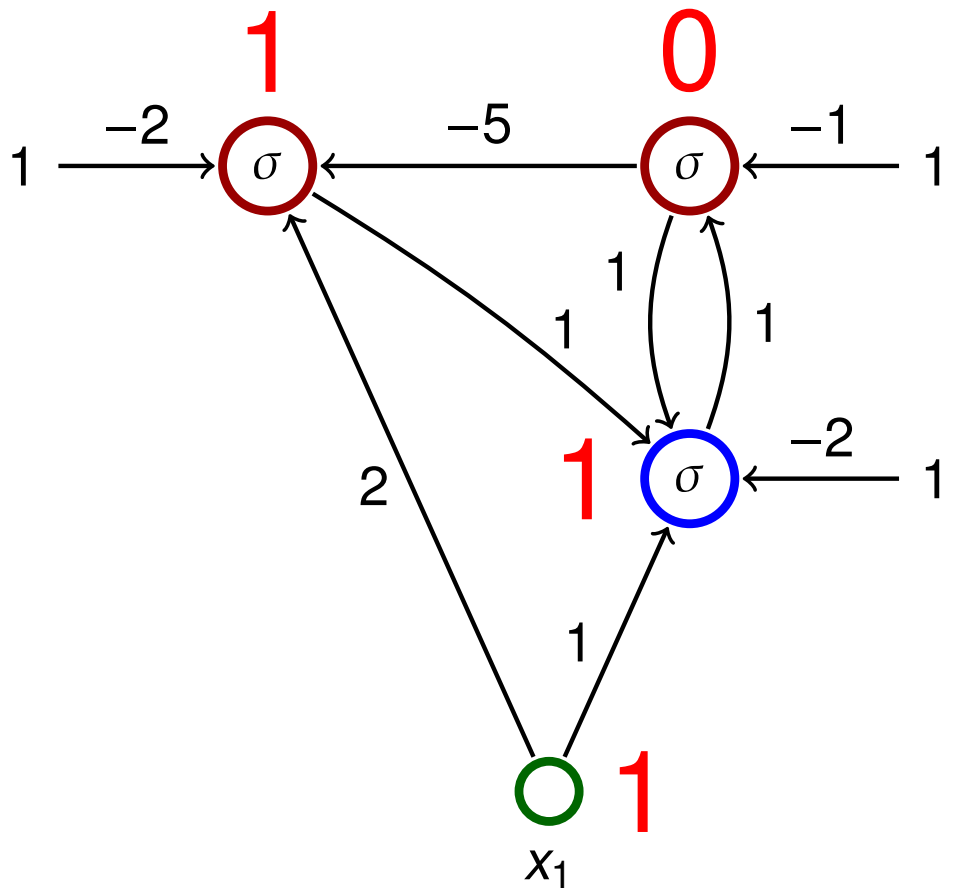

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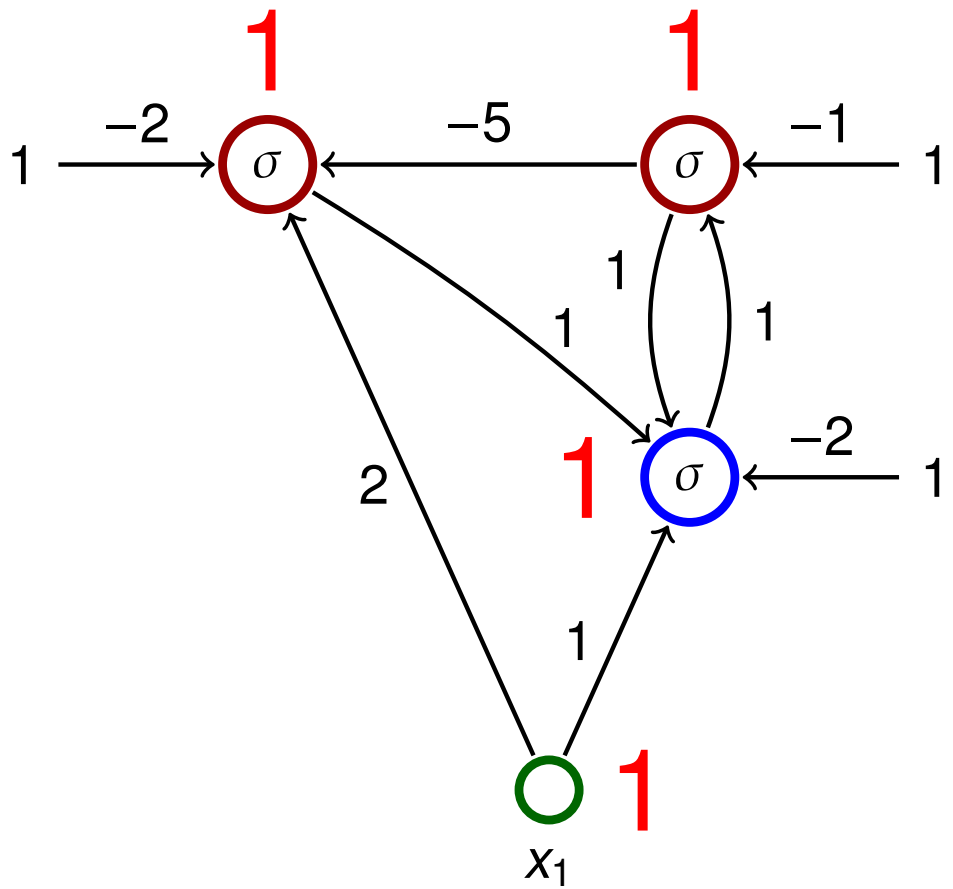

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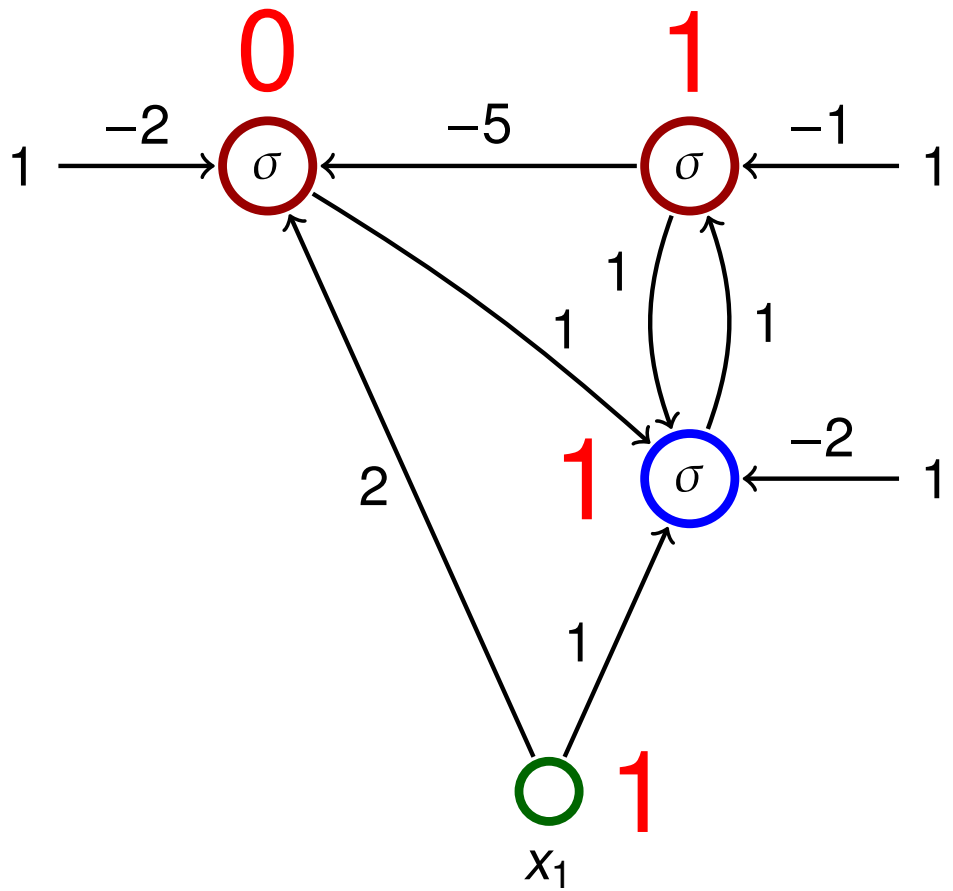

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- **initial configuration**
  weights can be initialized randomly or using some sophisticated algorithm

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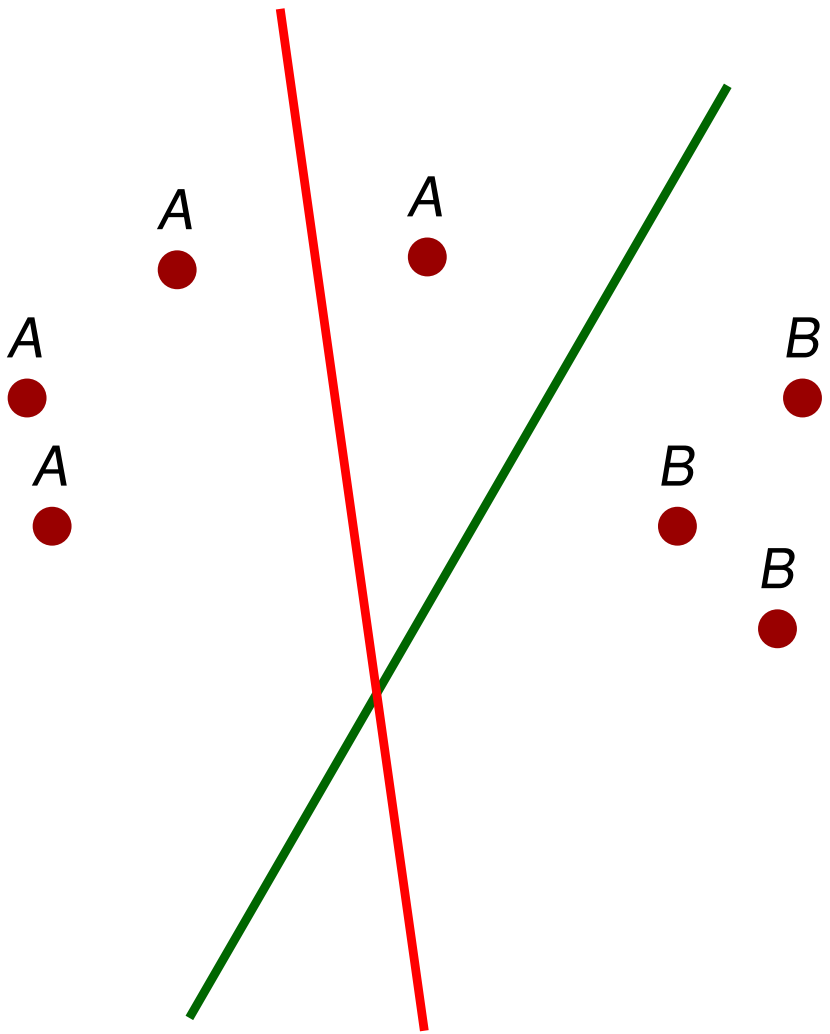
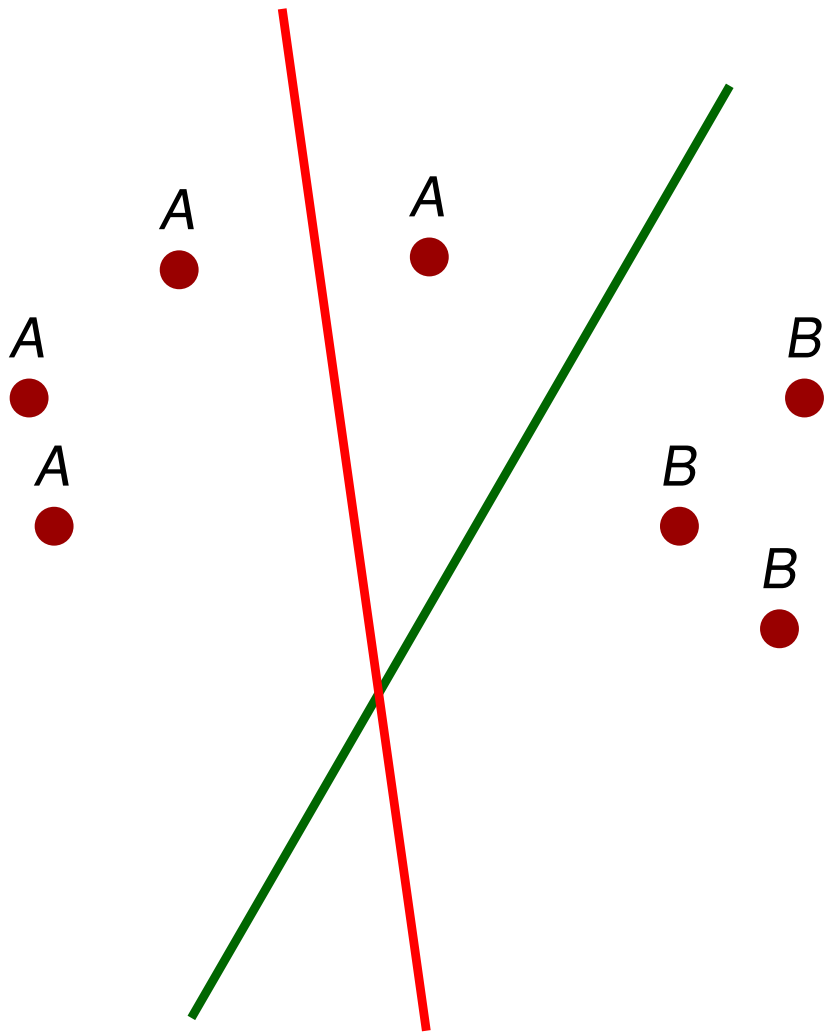
- Unsupervised learning
  - The training set contains only inputs.
  - The goal is to determine distribution of the inputs (clustering, deep belief networks, etc.)

Supervised learning – illustration



- classification in the plane using a single neuron

Supervised learning – illustration



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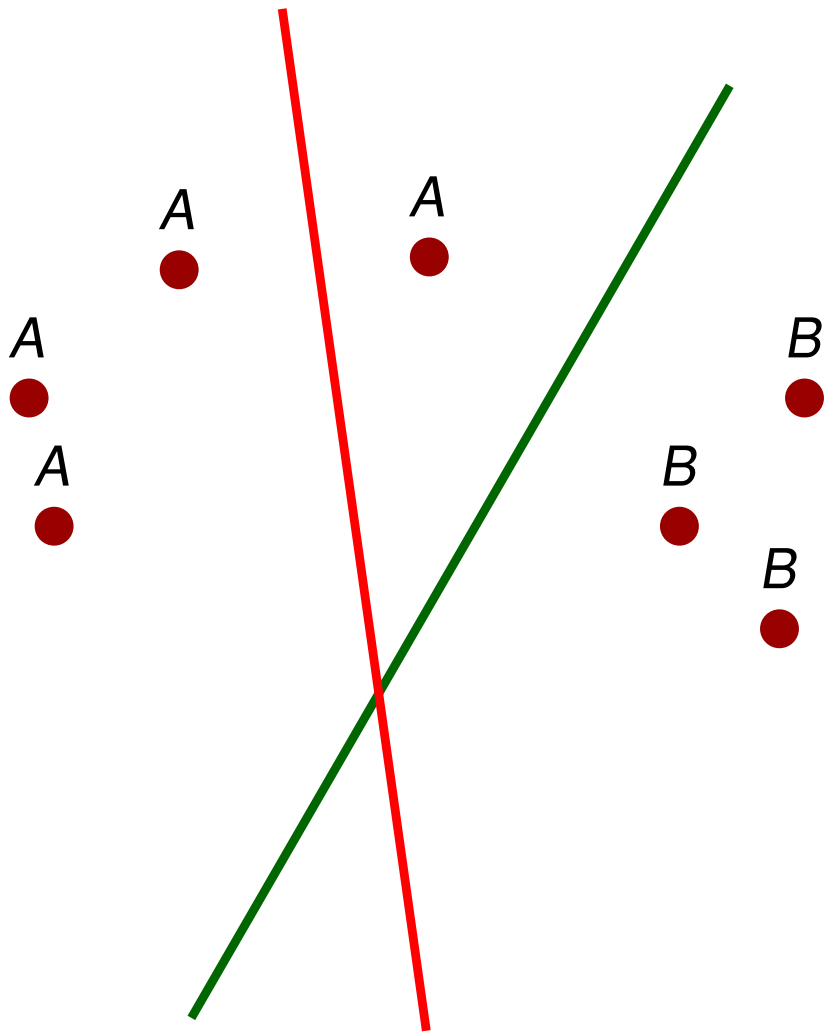

- classification in the plane using a single neuron
- training examples are of the form (point, value) where the value is either 1, or 0 depending on whether the point is either *A*, or *B*
- the algorithm considers examples one after another
- whenever an incorrectly classified point is considered, the learning algorithm turns the line in the direction of the point

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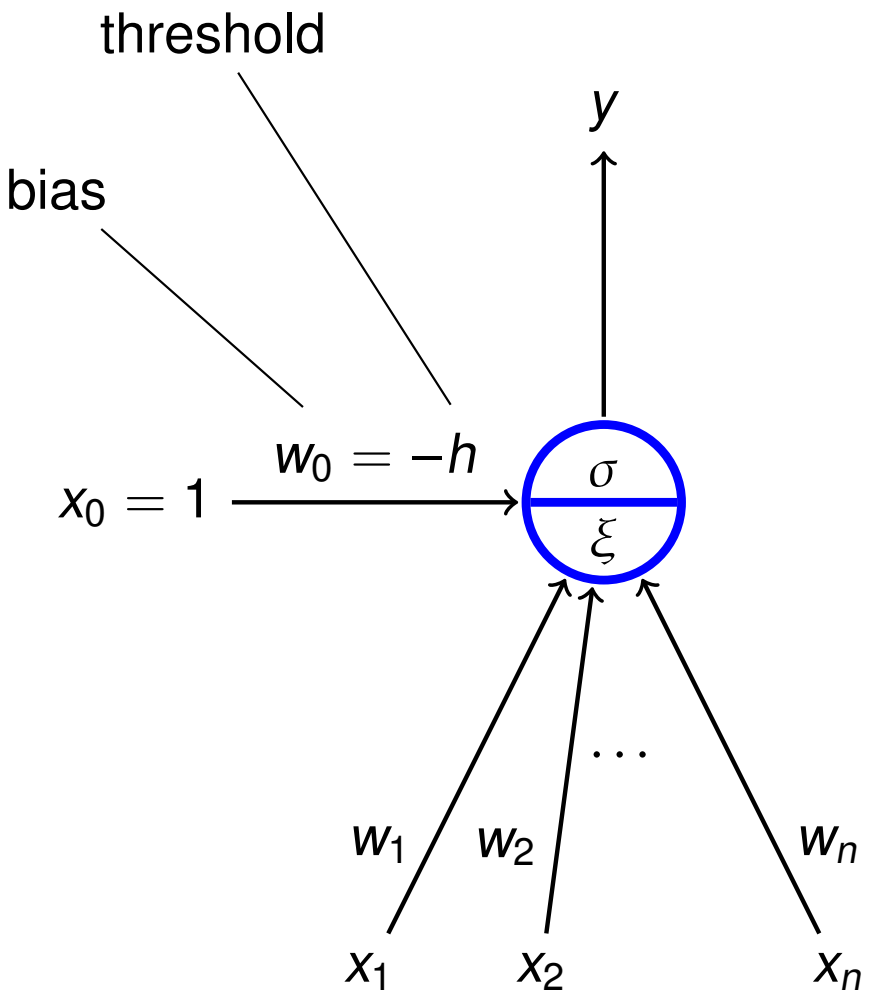
  - "close" inputs typicaly get similar values
- Graceful degradation
  - damage typically causes only a decrease in precision of results

Expressive power of neural networks

Formal neuron (with bias)



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

  e.g. a *unit step function*

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

Boolean functions

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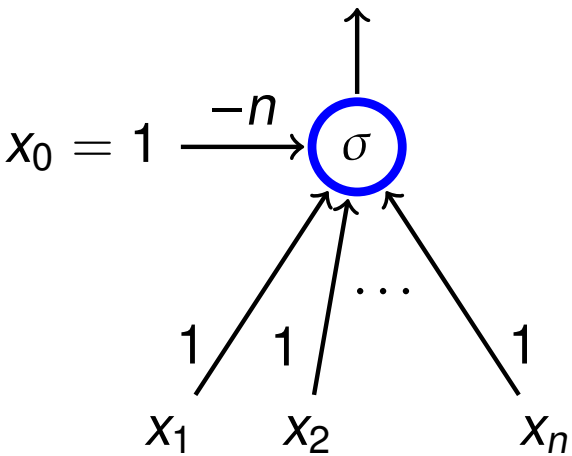
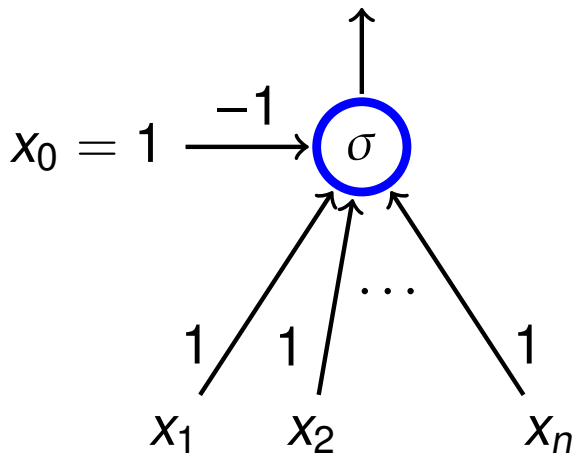
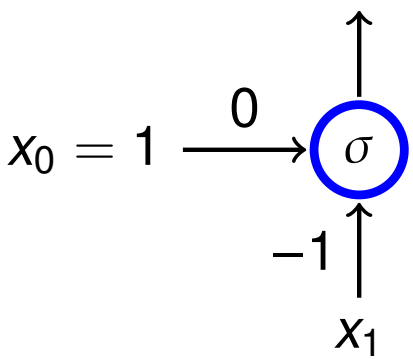
$y = AND(x_1, \ldots, x_n)$



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



$y = NOT(x_1)$



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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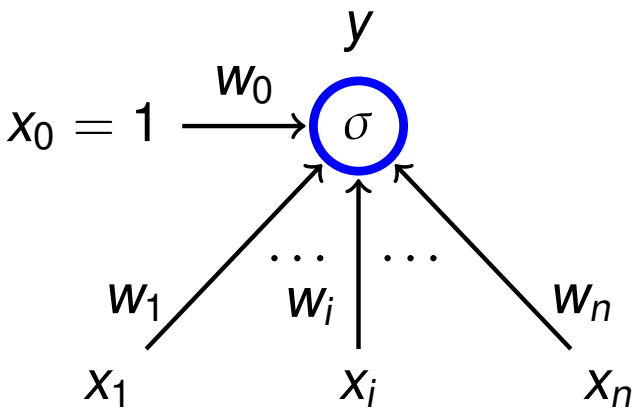
Proof.

- 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 $\vec{v}$:

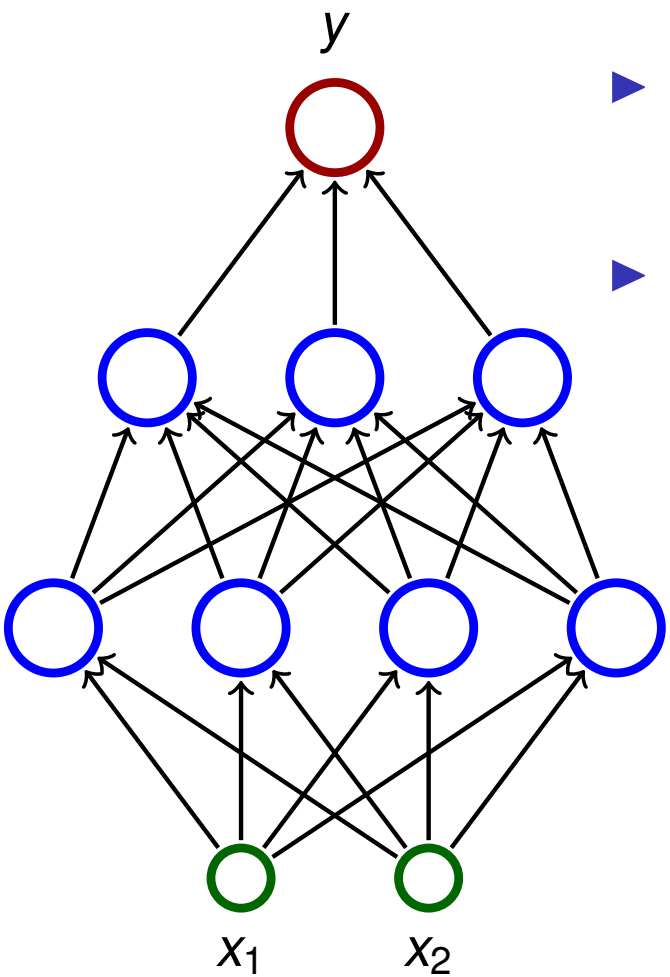


$$w_0 = -\sum_{i=1}^{n} v_i$$

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

- 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



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

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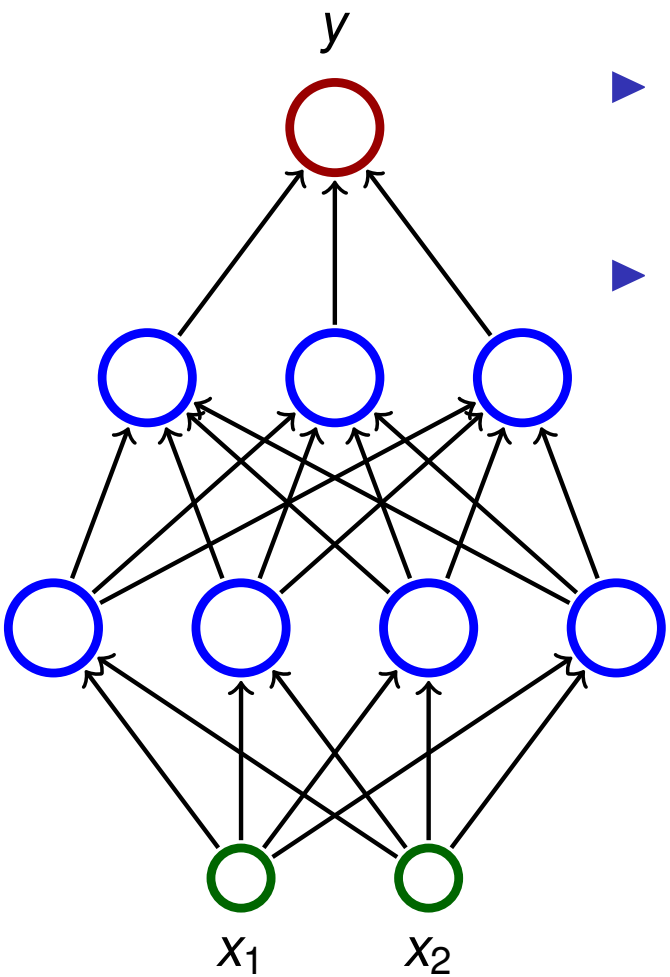

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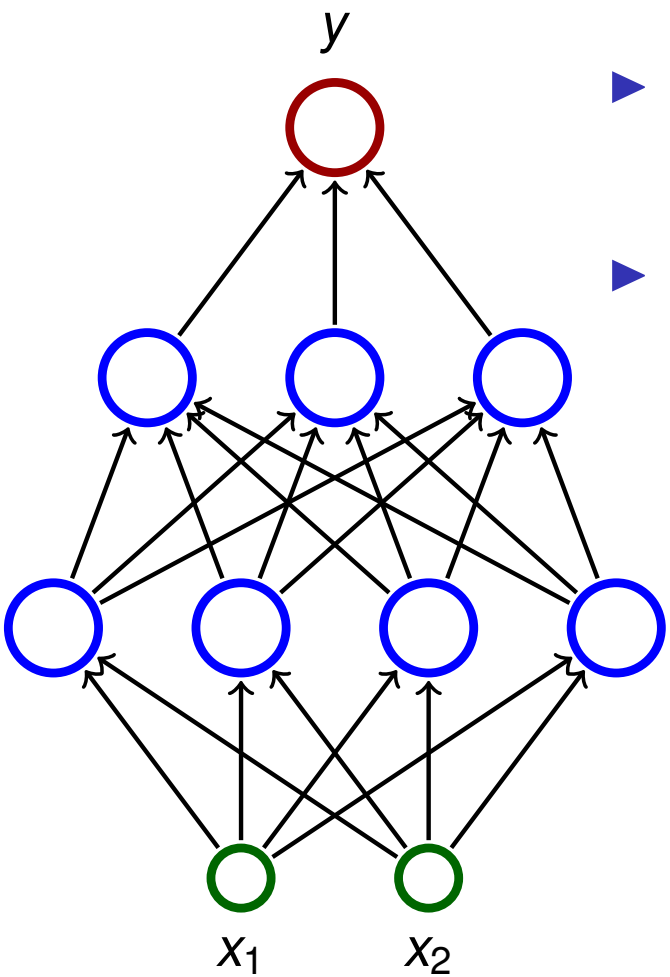

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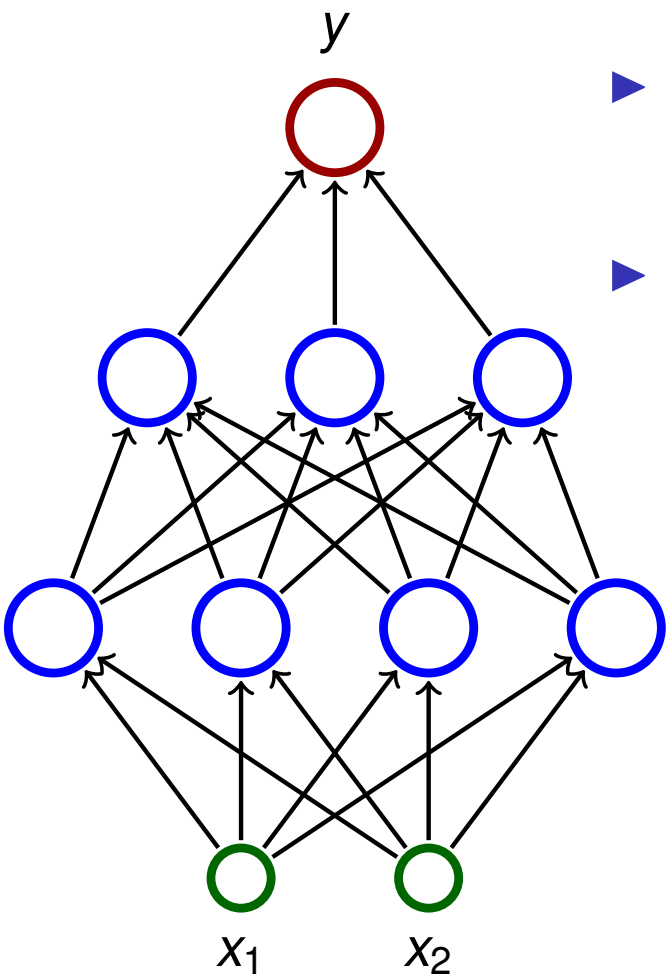

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  - The third layer may e.g. make unions of some convex sets.

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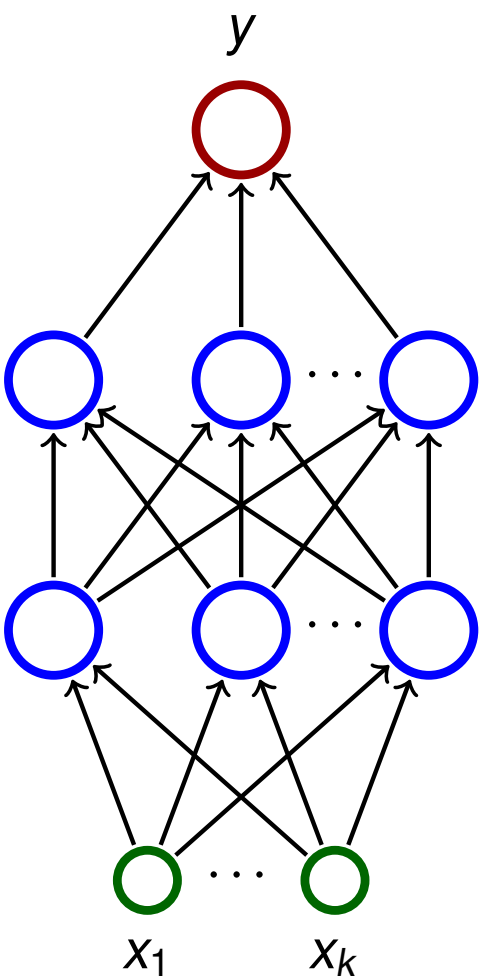

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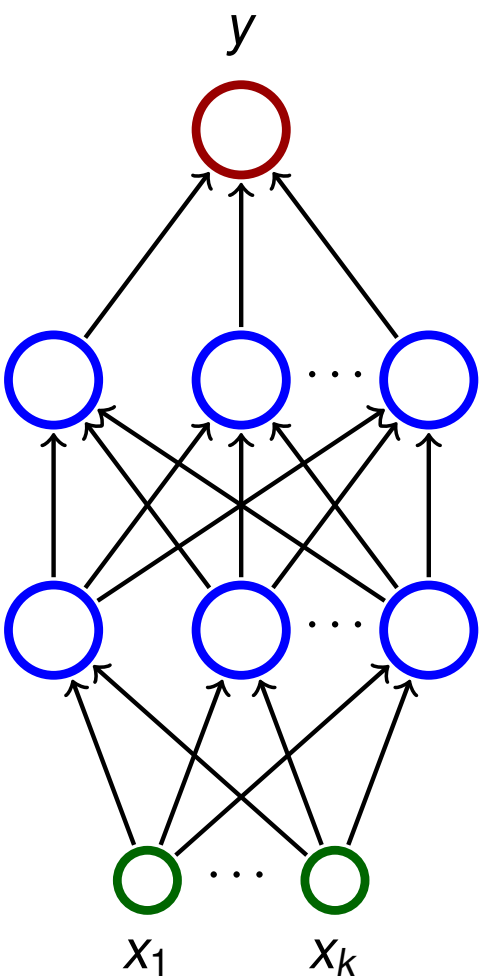

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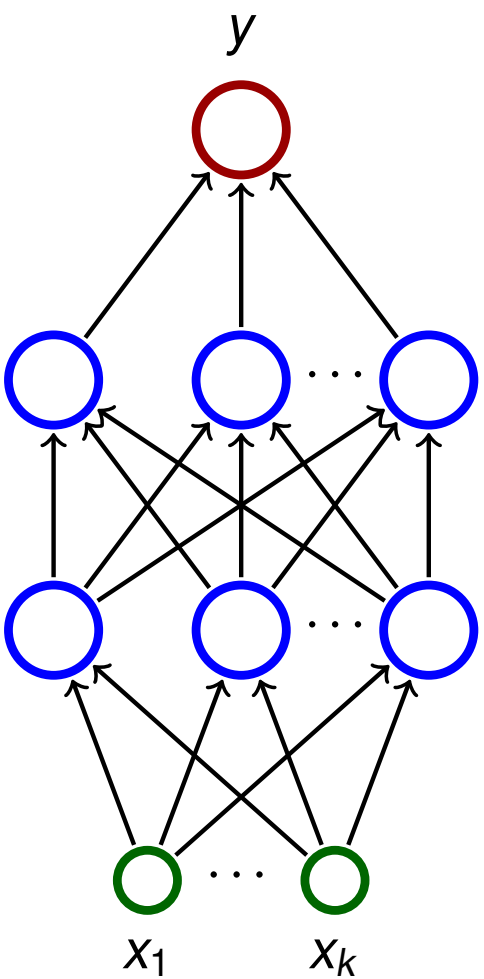

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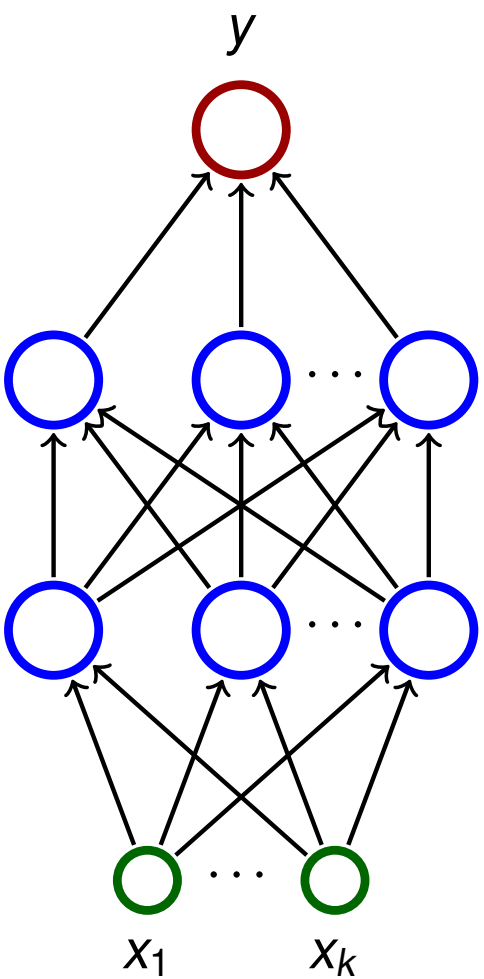

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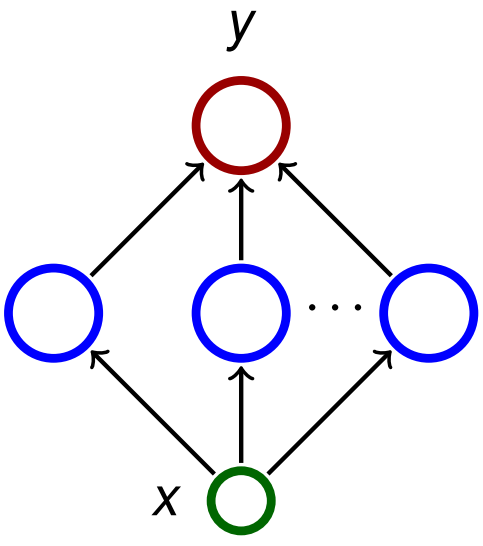
Power of ReLU



Consider a two layer network

- with a single input and single output;
- hidden neurons with the ReLU activation: $\sigma(\xi) = \max(\xi, 0)$;
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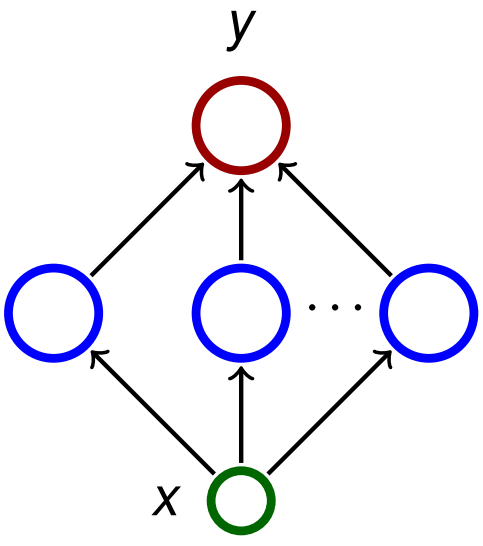

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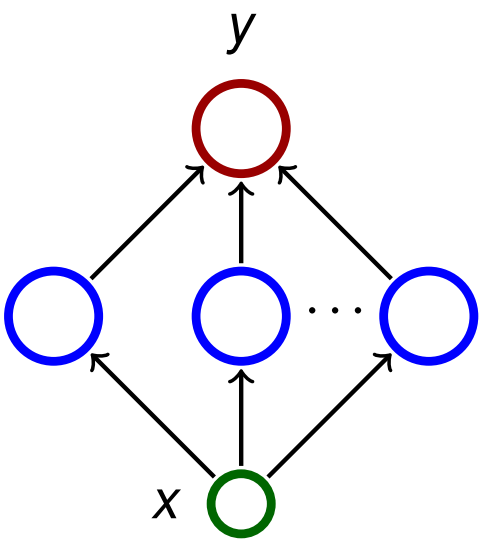

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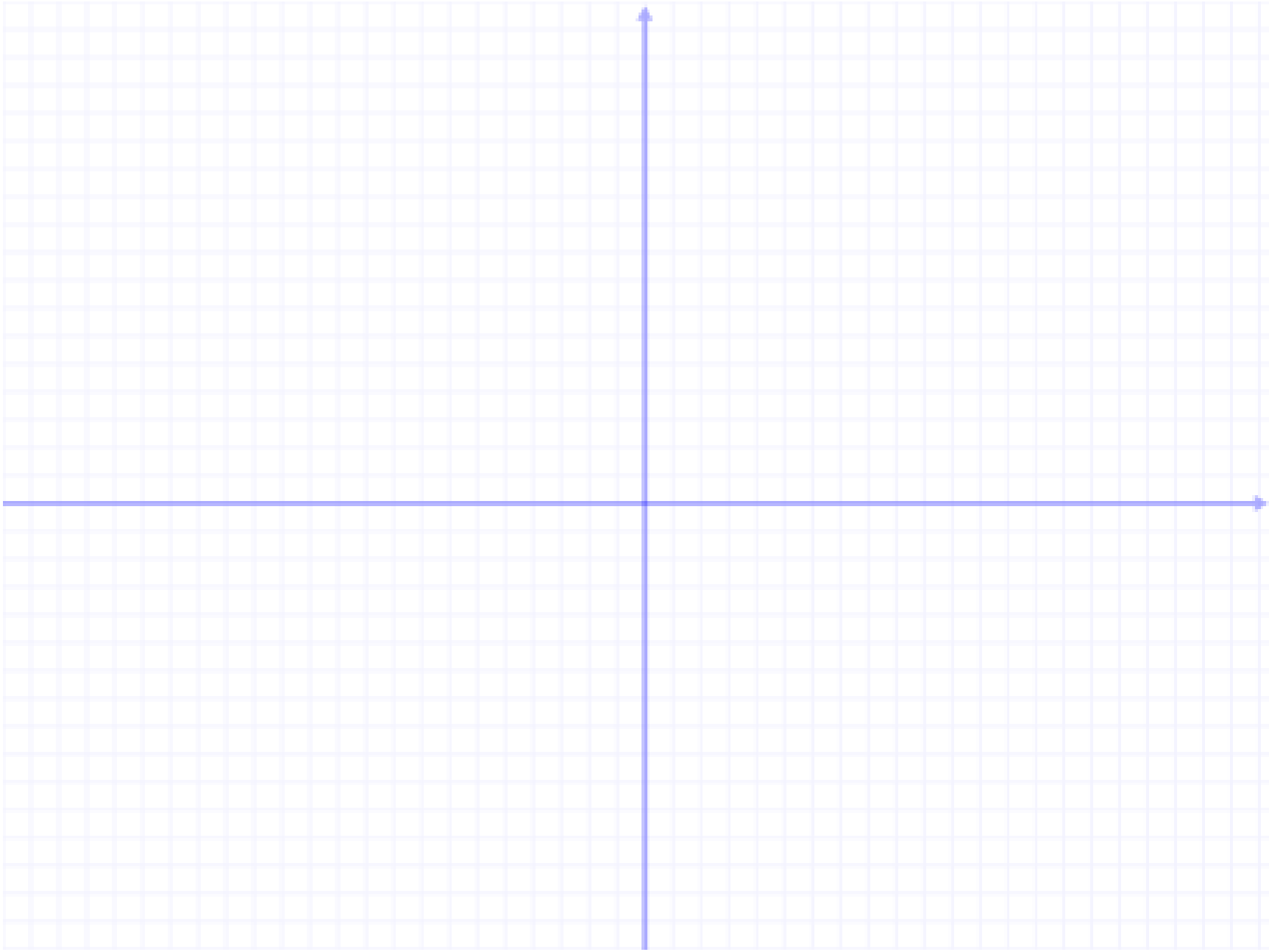
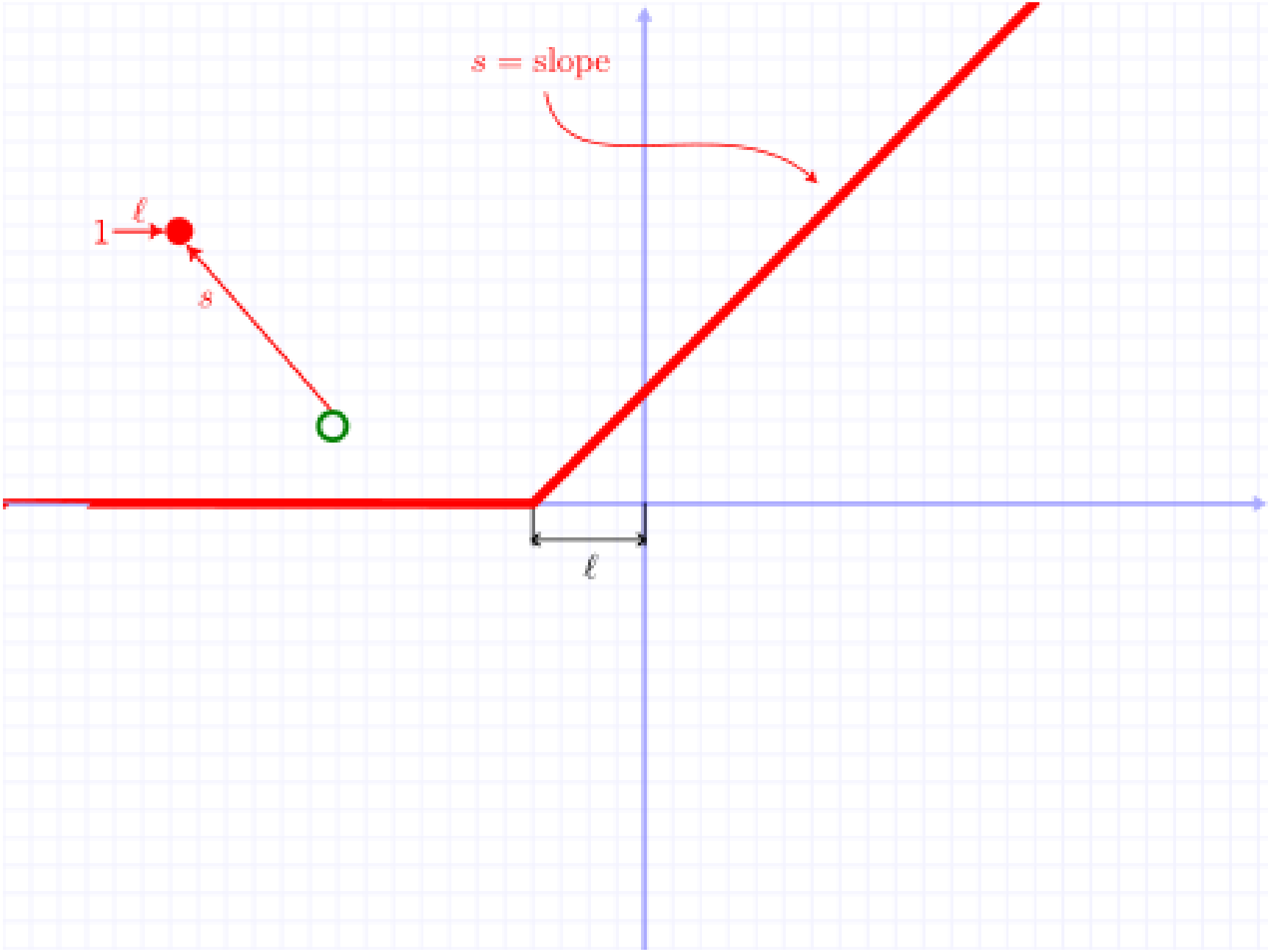
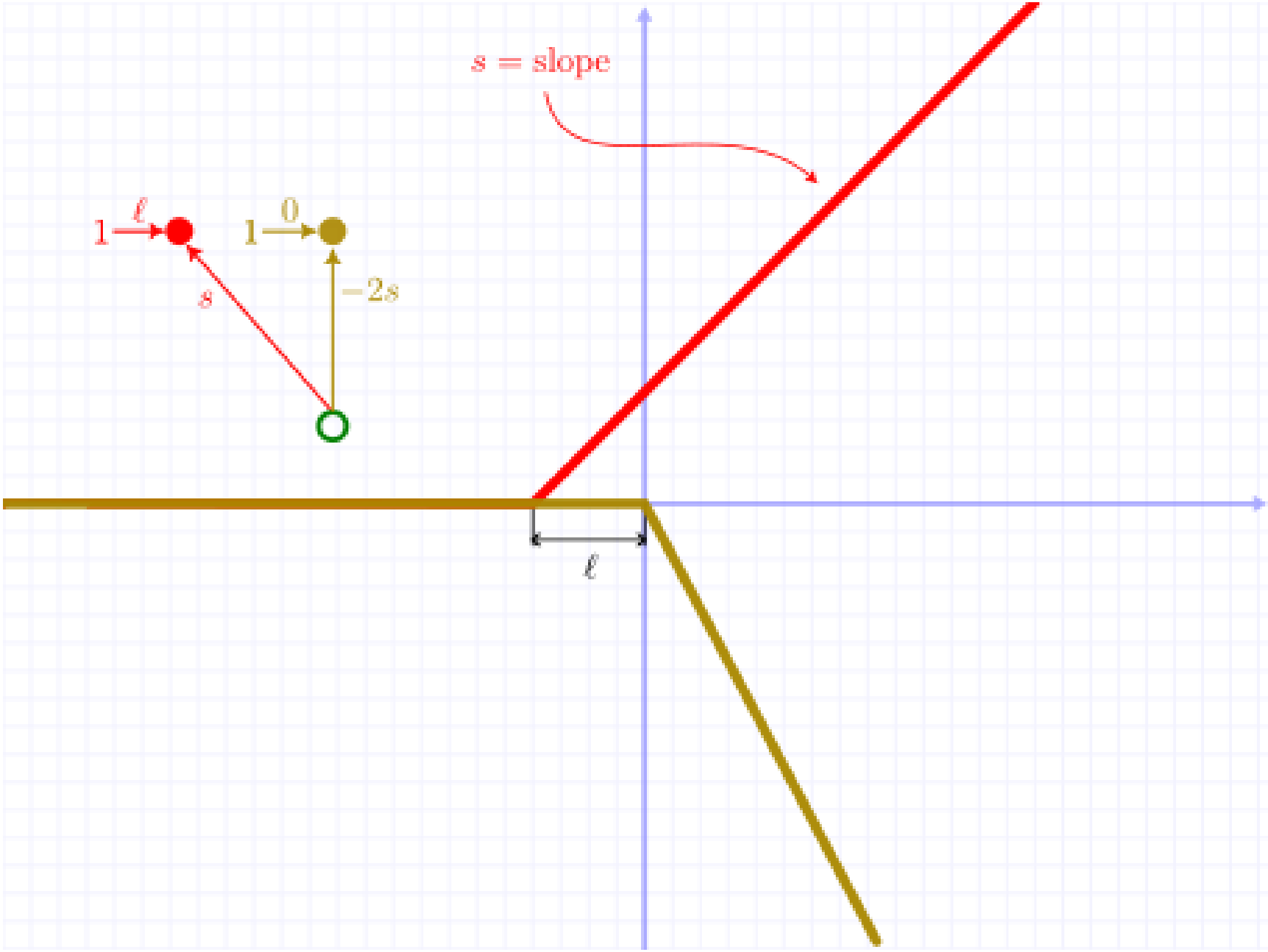
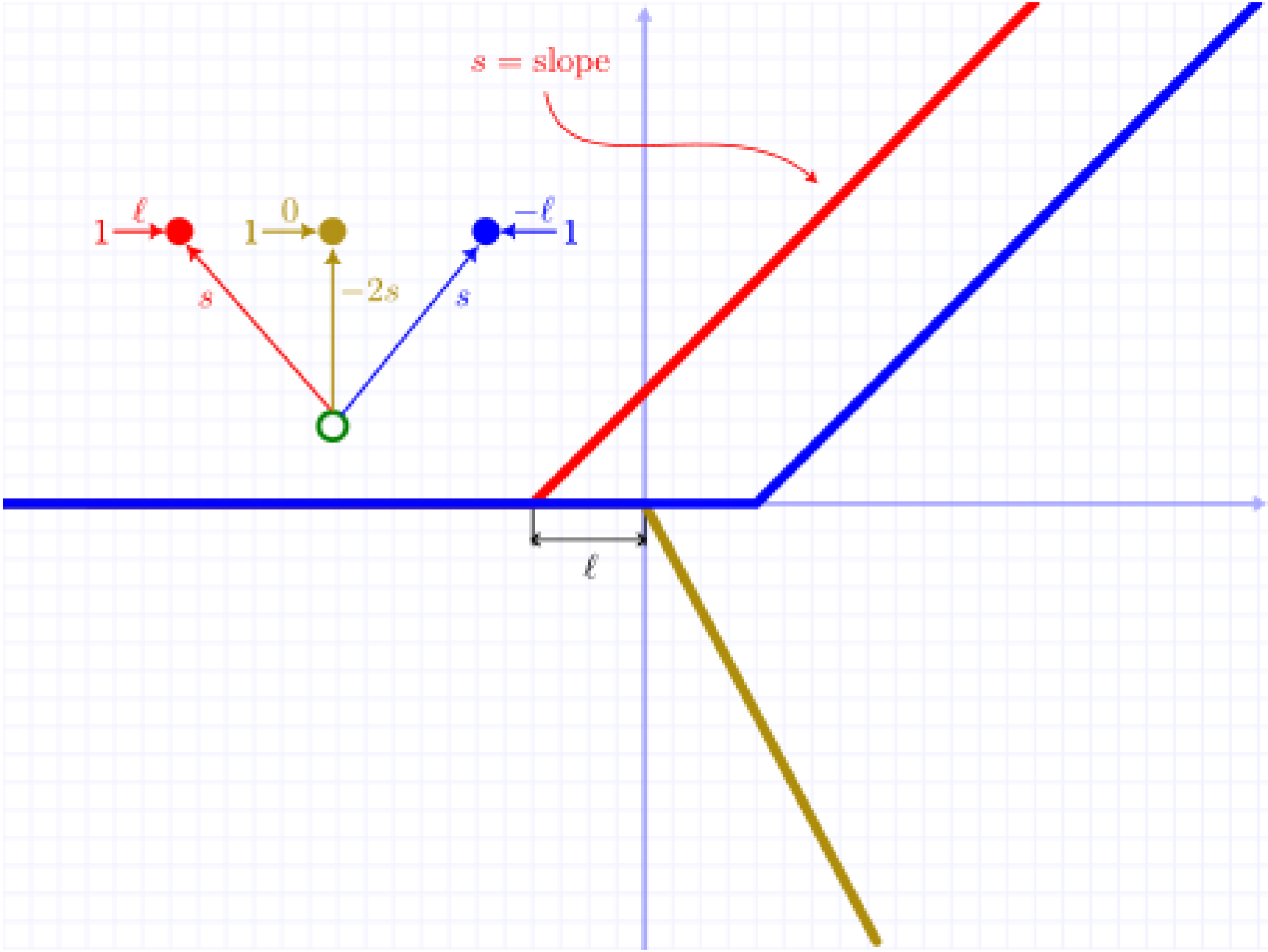
For every open subset $A \subseteq [0,1]$ there is a network of the above type such that for "most" $x \in [0,1]$ we have that $x \in A$ iff the network's output is > 0 for the input x.

Just consider a continuous function f where $f(x)$ is the minimum difference between x and a point on the boundary of A. Then uniformly approximate f using the networks.




$s = \text{slope}$
1
ℓ
s
ℓ


s = slope
ℓ
1
1
0
s
$-2s$
ℓ


$s = \text{slope}$
1
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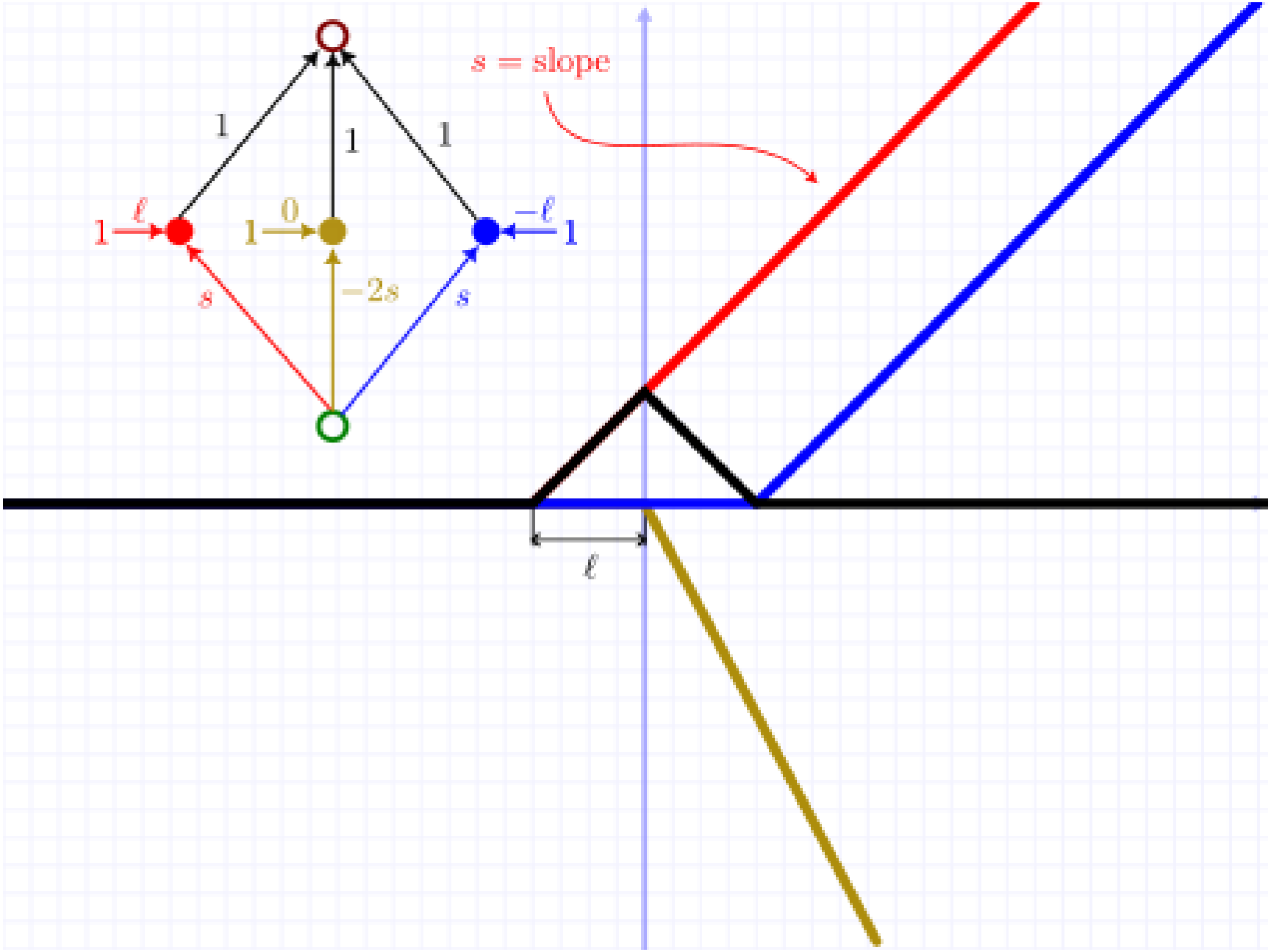
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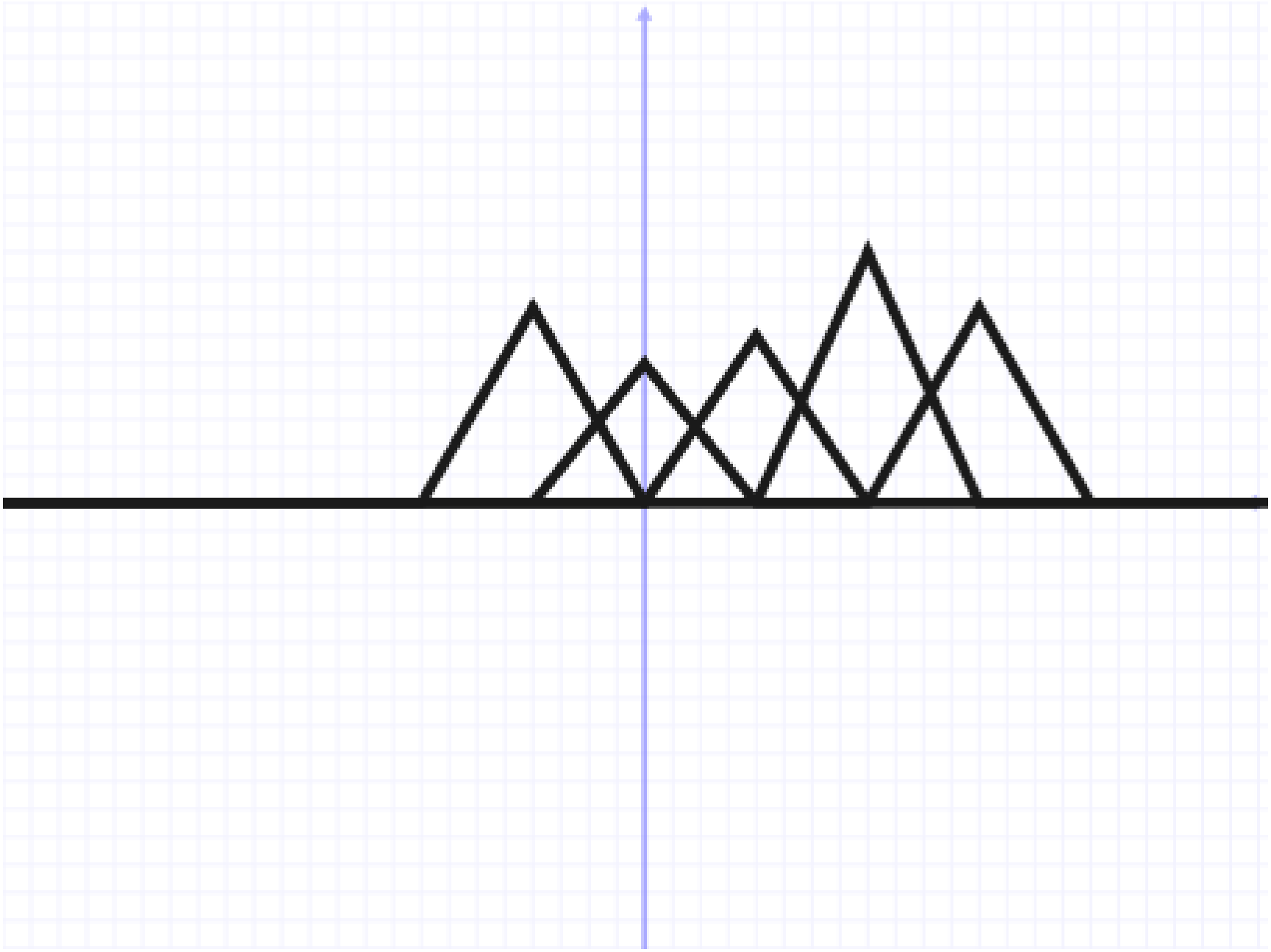
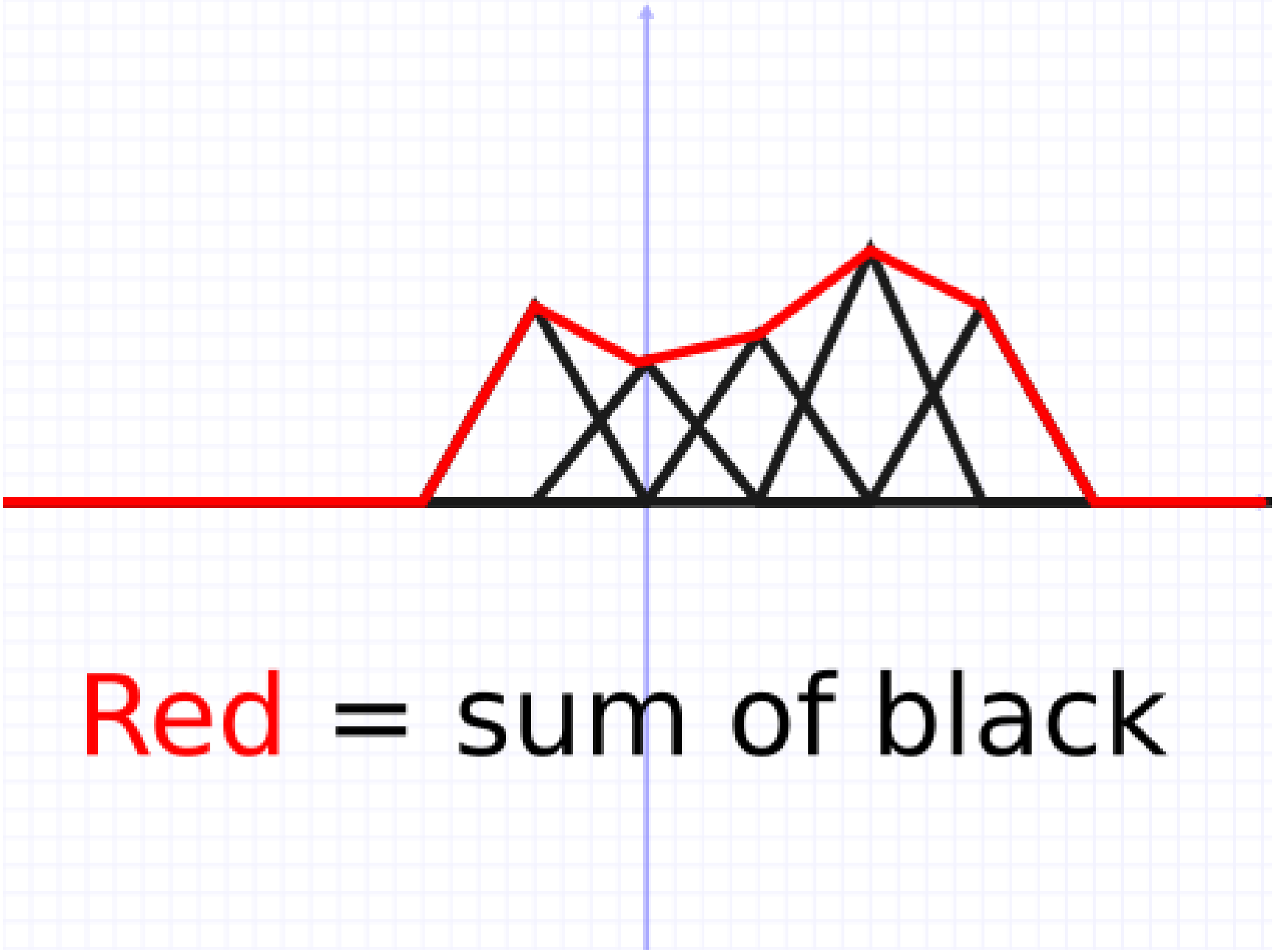




Red = sum of black

Non-linear separation - sigmoid

Theorem (Cybenko 1989 - informal version)

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

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

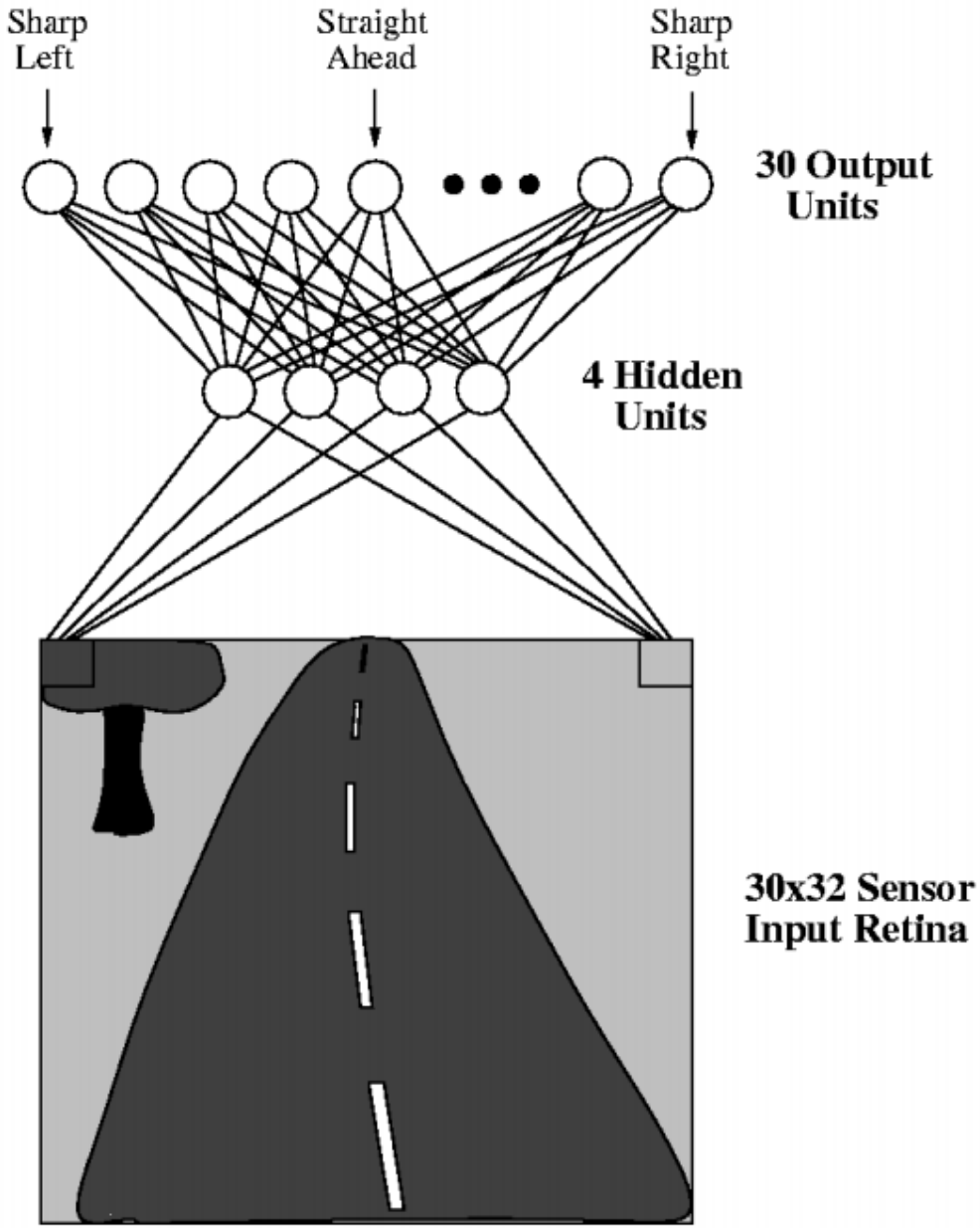
For every "reasonable" set $A \subseteq [0,1]^n$, there is a **two layer network** *where each hidden neuron has the activation function σ (output neurons are linear), that satisfies the following:*

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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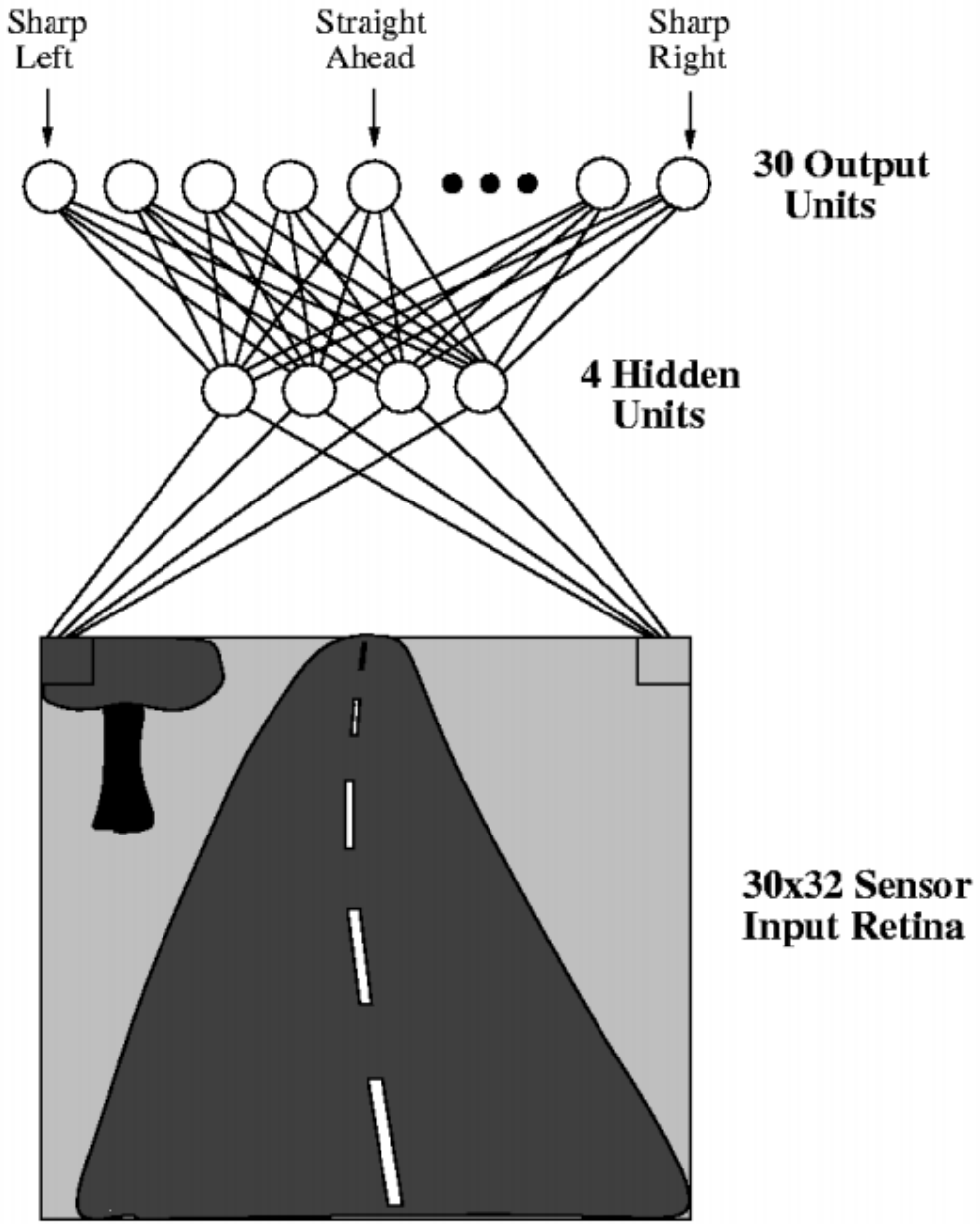

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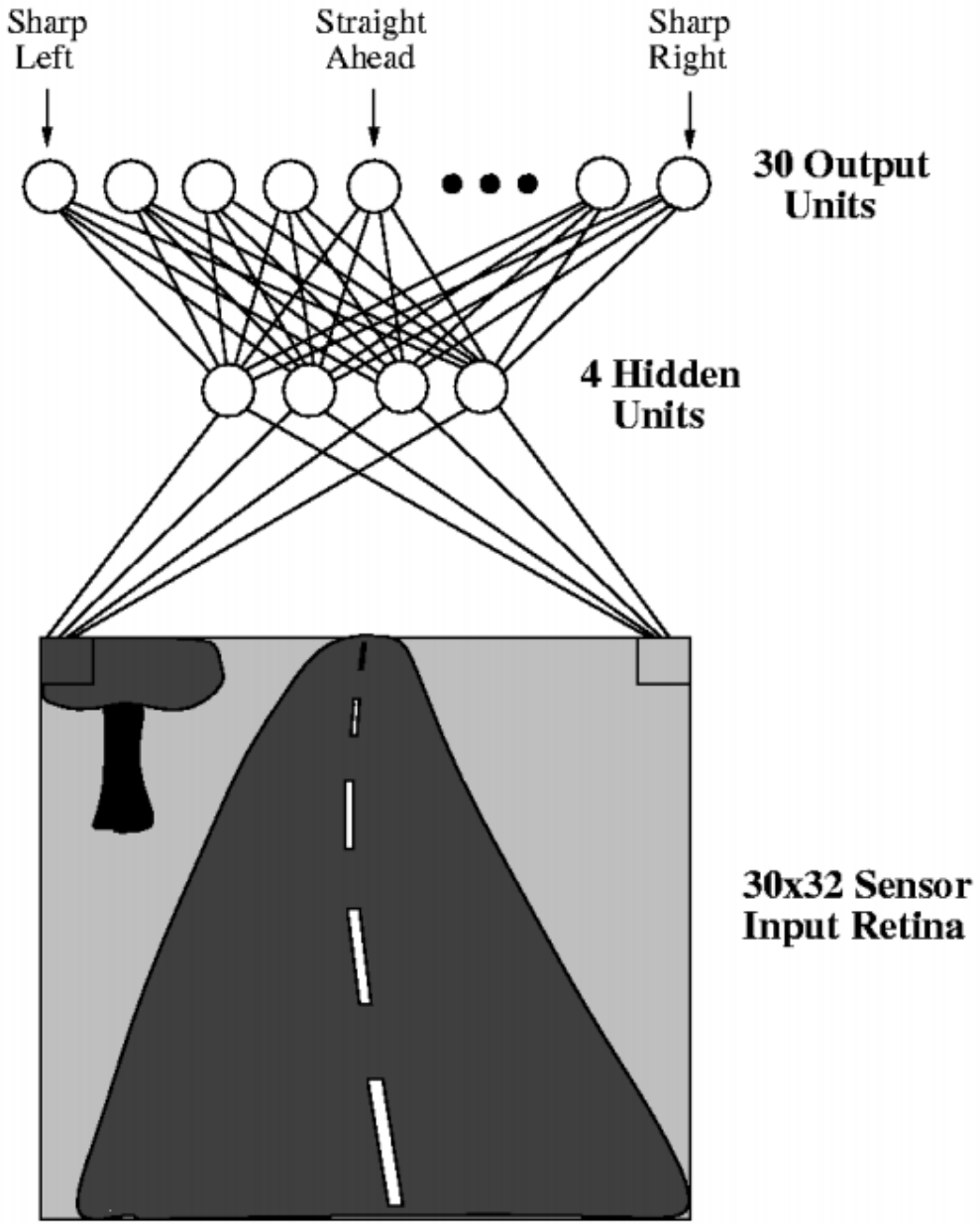

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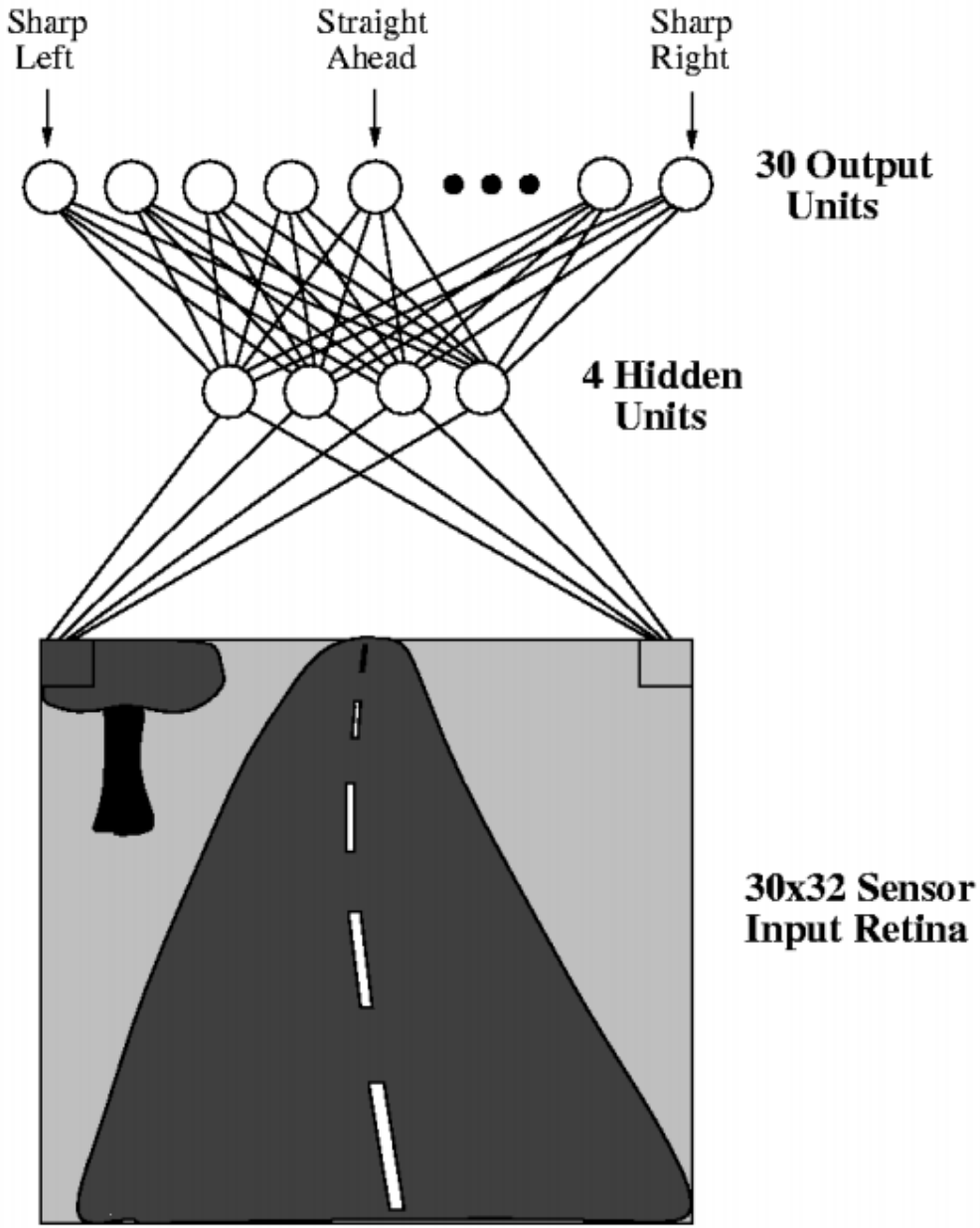

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- Output neurons "classify" images of the road based on their "curvature".

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

Function approximation - two-layer networks

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

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

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

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

Neural networks and computability

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

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

Summary of theoretical results

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

Summary of theoretical results

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

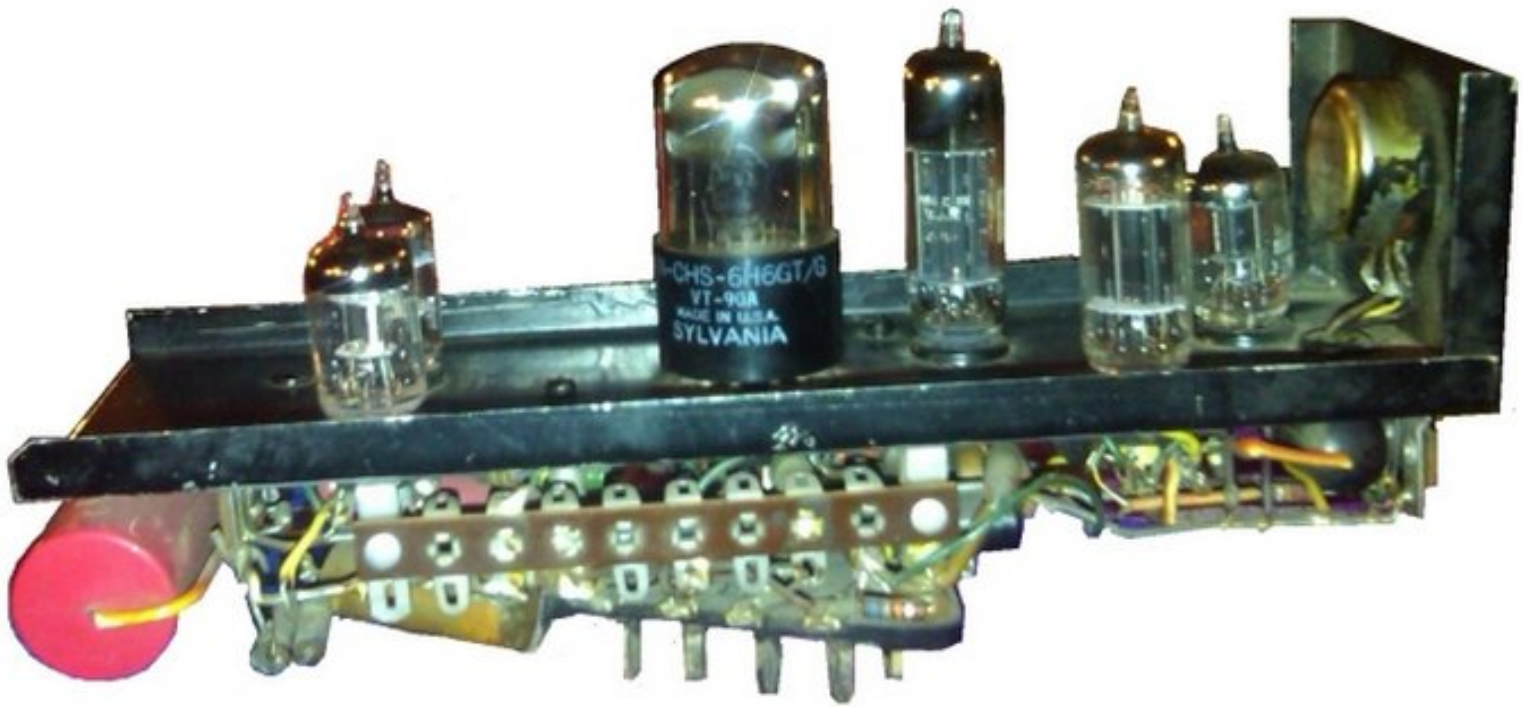
Neural networks vs classical computers

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

History & implementations

History of neurocomputers

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



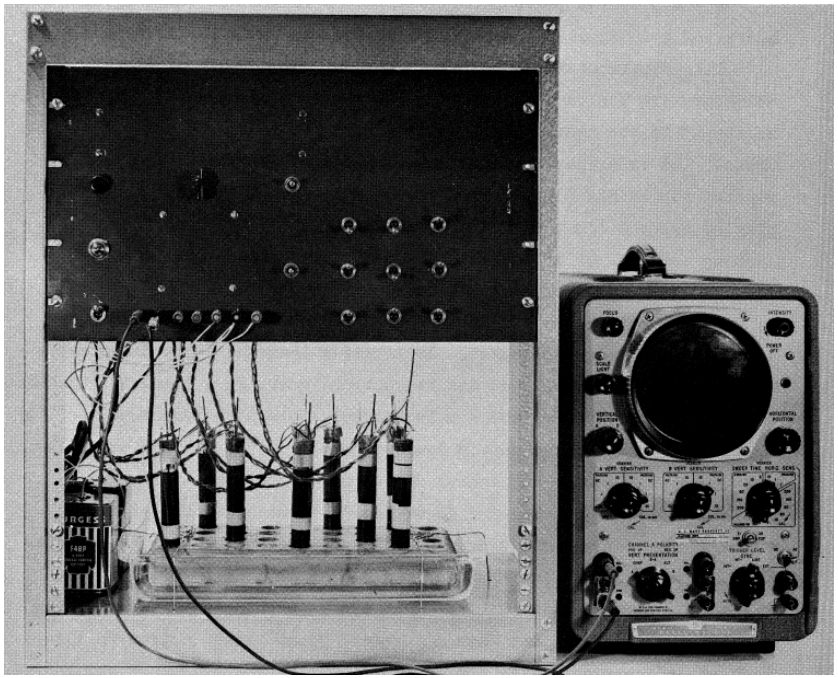
History of neurocomputers

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

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

History of neurocomputers

- 1960: ADALINE (Widrow & Hof)



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

History of neurocomputers

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

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

Some highlights

- Breakthrough in image recognition.
  Accuracy of image recognition improved by an order of magnitude in 5 years.
- Breakthrough in game playing.
  Superhuman results in Go and Chess almost without any human intervention. Master level in Starcraft, poker, etc.
- Breakthrough in machine translation.
  Switching to deep learning produced a 60% increase in translation accuracy compared to the phrase-based approach previously used in Google Translate (in human evaluation)
- Breakthrough in speech processing.
- Breakthrough in text generation.
  GPT-4 generates pretty realistic articles, short plays (for a theatre) have been successfully generated, etc.

History in waves ...

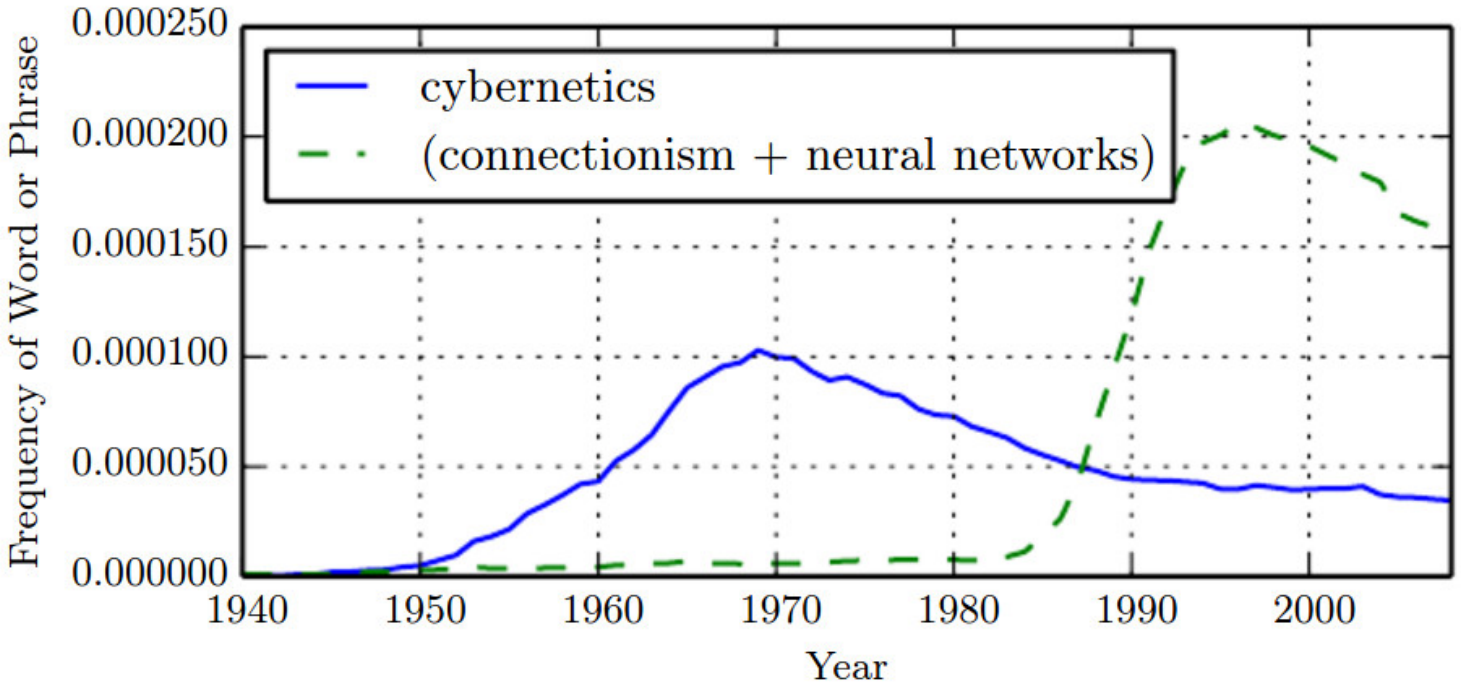
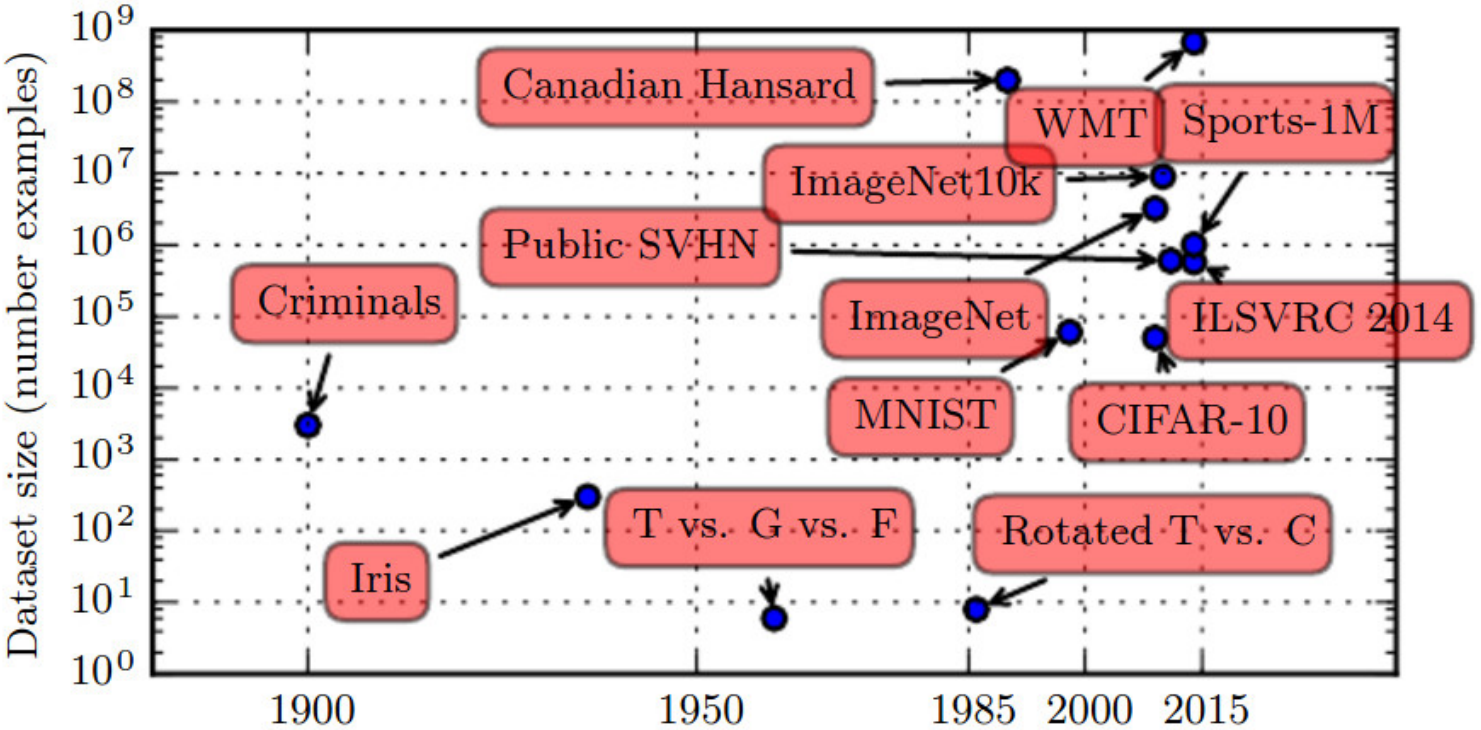


Figure: The figure shows two of the three historical waves of artificial neural nets research, as measured by the frequency of the phrases "cybernetics" and "connectionism" or "neural networks" according to Google Books (the third wave is too recent to appear).

Current hardware – What do we face?

Increasing dataset size ...



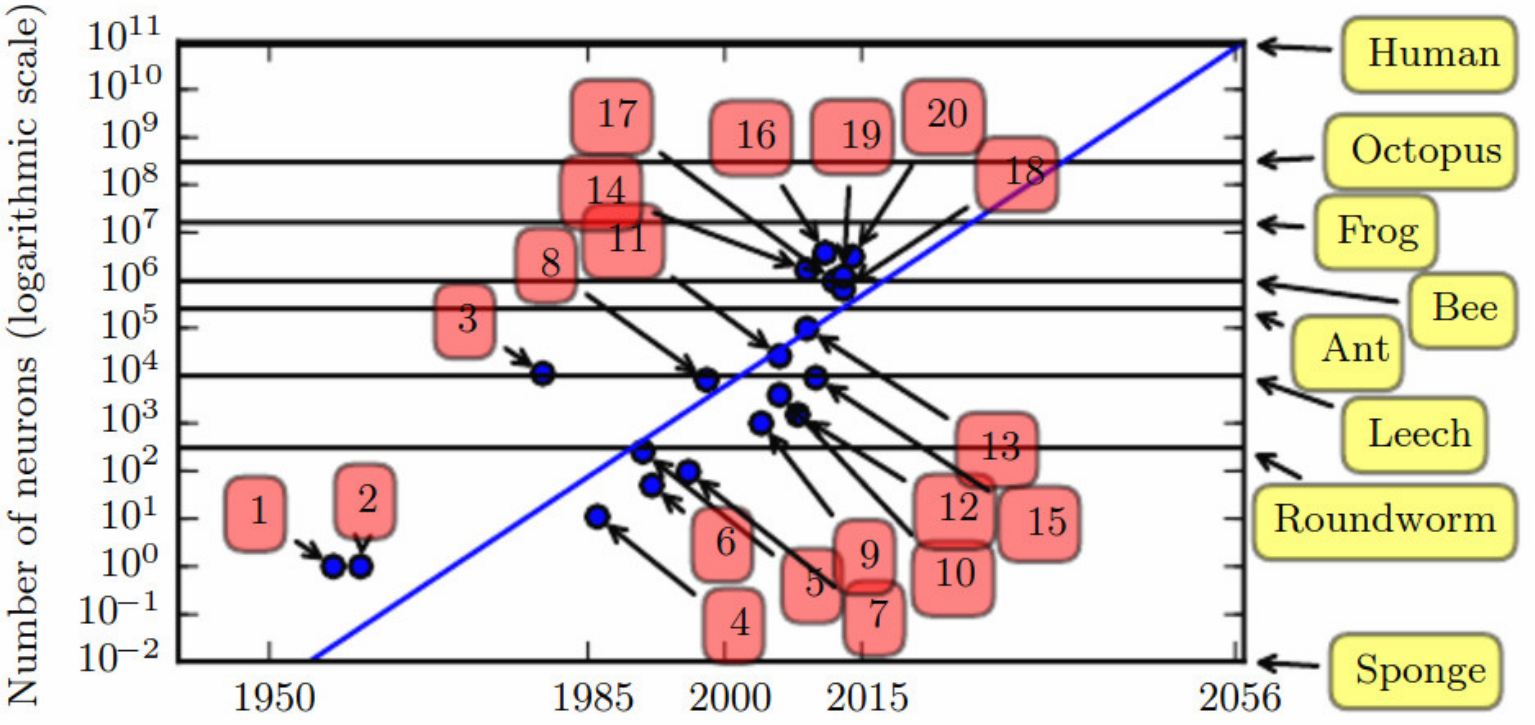
... weakly-supervised pre-training using hashtags from the Instagram uses $3.6 * 10^9$ images.

Revisiting Weakly Supervised Pre-Training of Visual Perception Models. Singh et al.

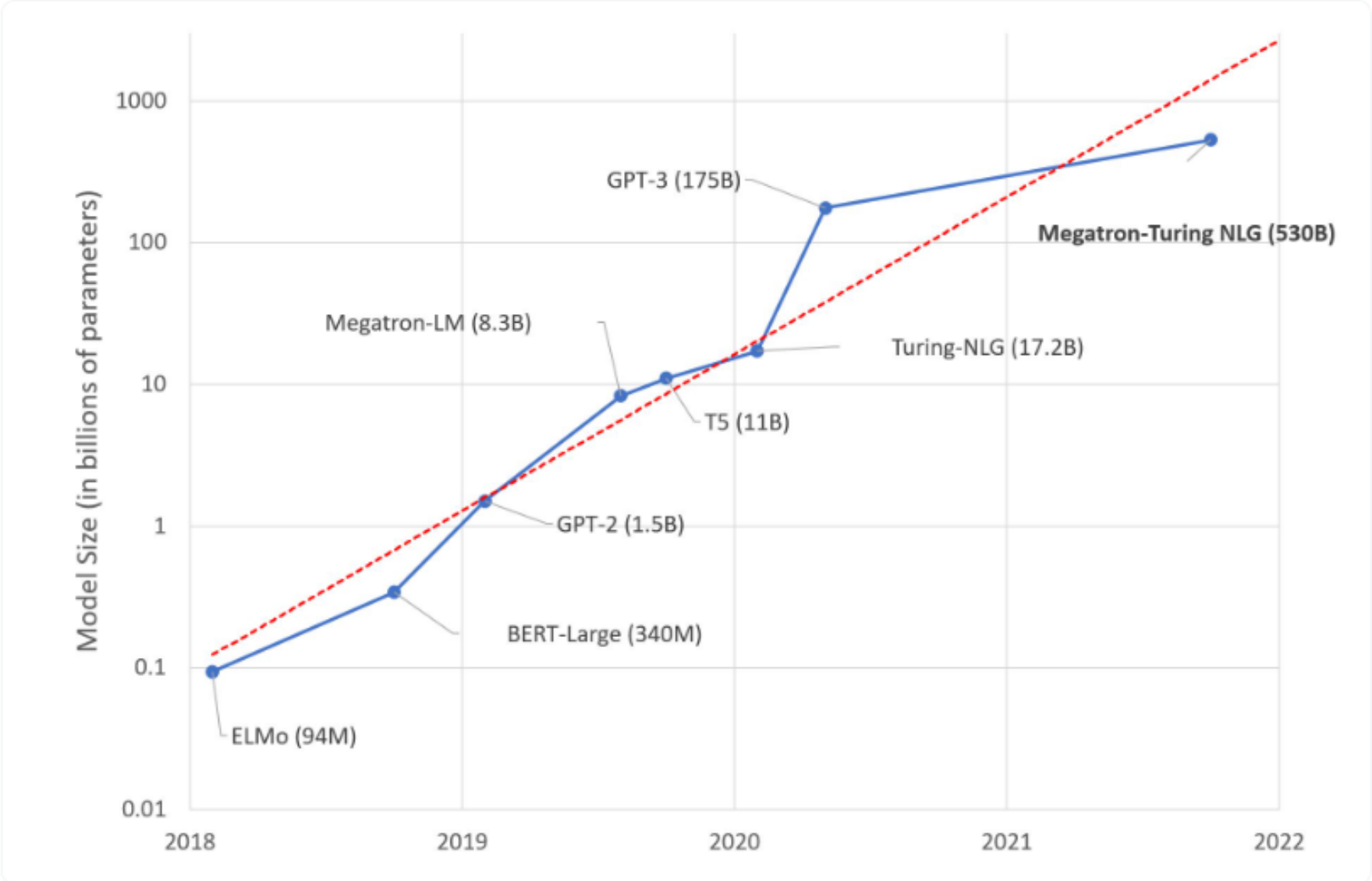
https://arxiv.org/pdf/2201.08371.pdf, 2022

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)



GPT-4's Scale: GPT-4 has 1.8 trillion parameters across 120 layers, which is over 10 times larger than GPT-3.

Current hardware – What do we face?

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

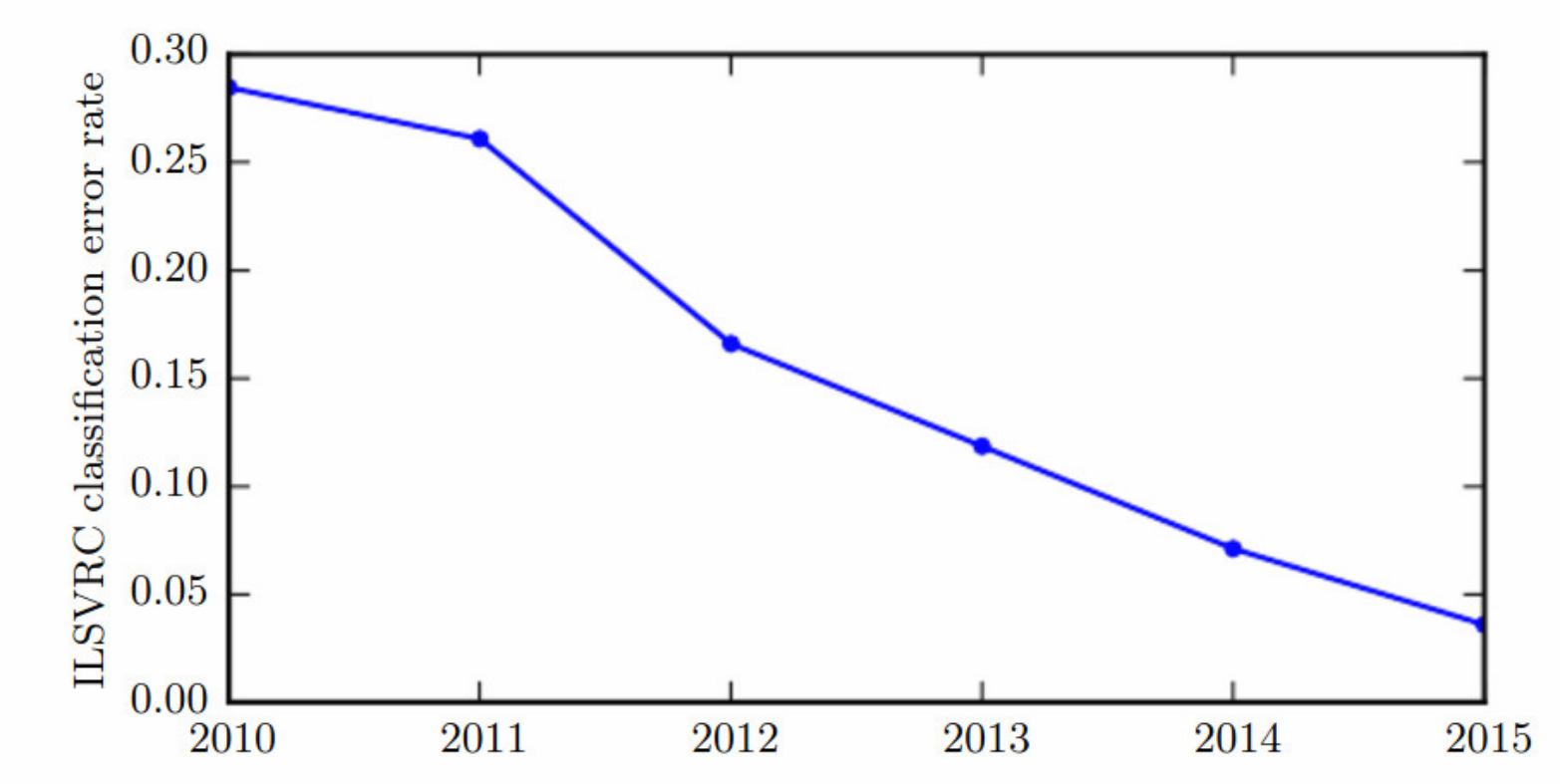


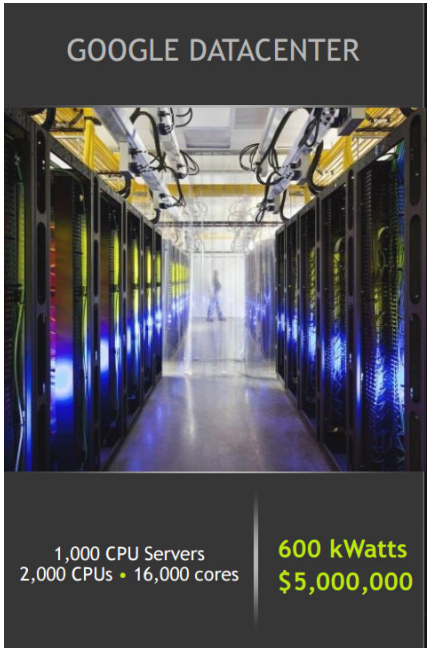
Figure: Since deep networks reached the scale necessary to compete in the ImageNetLarge Scale Visual Recognition Challenge, they have consistently won the competition every year, and yielded lower and lower error rates each time. Data from Russakovsky et al. (2014b) and He et al. (2015).

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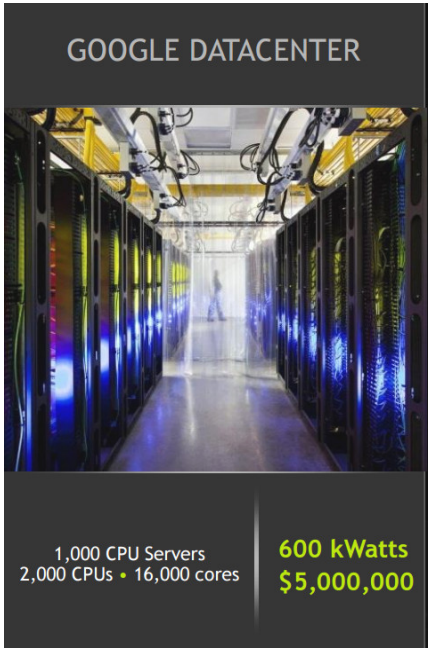
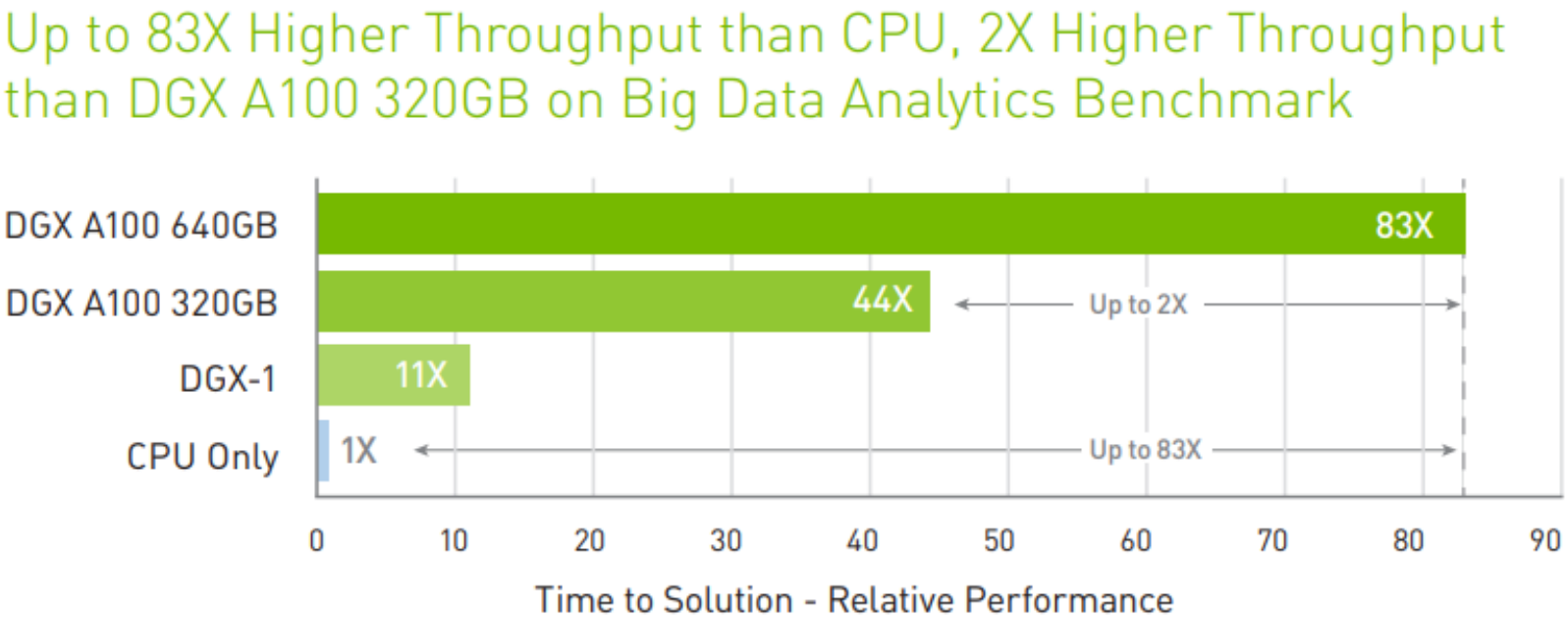
In 2014, similar task performed on Commodity Off-The-Shelf High Performance Computing (COTS HPC) technology: a cluster of GPU servers with Infiniband interconnects and MPI.

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

- 8x GPU (Nvidia A100 80GB Tensor Core)
- 5 petaFLOPS
- System memory: 2 TB
- Network: 200 Gb/s InfiniBand



Deep learning in clouds

Big companies offer cloud services for deep learning:

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

Advantages:

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

Disadvatages:

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

Current software

- **TensorFlow** (Google)
  - open source software library for numerical computation using data flow graphs
  - allows implementation of most current neural networks
  - allows computation on multiple devices (CPUs, GPUs, ...)
  - Python API
  - **Keras**: a part of TensorFlow that allows easy description of most modern neural networks
- **PyTorch** (Facebook)
  - similar to TensorFlow
  - object oriented
  - ... majority of new models in research papers implemented in PyTorch

    https://www.cioinsight.com/big-data/pytorch-vs-tensorflow/
- **Theano (dead)**:
  - The "academic" grand-daddy of deep-learning frameworks, written in Python. Strongly inspired TensorFlow (some people developing Theano moved on to develop TensorFlow).
- There are others: Caffe, Deeplearning4j, ...

Current software – Keras

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

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

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

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

Current software – Keras functional API

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

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

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

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

Current software – TensorFlow

```
41  # tf Graph input
42  X = tf.placeholder("float", [None, n_input])
43  Y = tf.placeholder("float", [None, n_classes])
44
45  # Store layers weight & bias
46  weights = {
47      'h1': tf.Variable(tf.random_normal([n_input, n_hidden_1])),
48      'h2': tf.Variable(tf.random_normal([n_hidden_1, n_hidden_2])),
49      'out': tf.Variable(tf.random_normal([n_hidden_2, n_classes]))
50  }
51  biases = {
52      'b1': tf.Variable(tf.random_normal([n_hidden_1])),
53      'b2': tf.Variable(tf.random_normal([n_hidden_2])),
54      'out': tf.Variable(tf.random_normal([n_classes]))
55  }
```

Current software – TensorFlow

```
58  # Create model
59  def multilayer_perceptron(x):
60      # Hidden fully connected layer with 256 neurons
61      layer_1 = tf.add(tf.matmul(x, weights['h1']), biases['b1'])
62      # Hidden fully connected layer with 256 neurons
63      layer_2 = tf.add(tf.matmul(layer_1, weights['h2']), biases['b2'])
64      # Output fully connected layer with a neuron for each class
65      out_layer = tf.matmul(layer_2, weights['out']) + biases['out']
66      return out_layer
67
68  # Construct model
69  logits = multilayer_perceptron(X)
```

Current software – PyTorch

```
36  class Net(nn.Module):
37      def __init__(self, input_size, hidden_size, num_classes):
38          super(Net, self).__init__()
39          self.fc1 = nn.Linear(input_size, hidden_size)
40          self.relu = nn.ReLU()
41          self.fc2 = nn.Linear(hidden_size, num_classes)
42
43      def forward(self, x):
44          out = self.fc1(x)
45          out = self.relu(out)
46          out = self.fc2(out)
47          return out
48
49  net = Net(input_size, hidden_size, num_classes)
```

Other software implementations

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

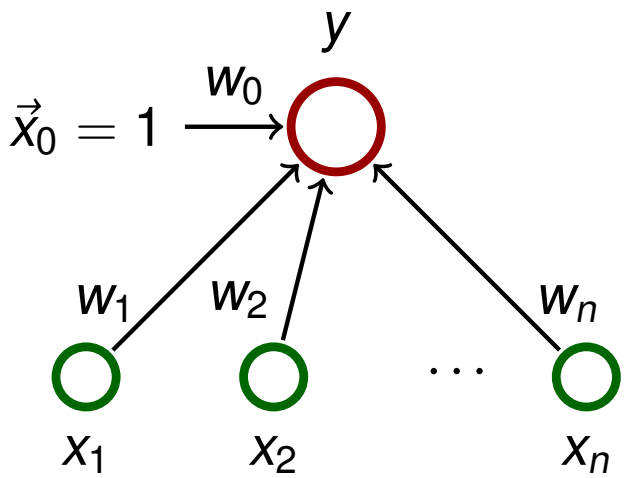
- MATLAB
- R
- STATISTICA
- Weka
- ...

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

Training linear models

Linear regression (ADALINE)

Architecture:



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

Activity:

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

Linear regression (ADALINE)

Learning:

- Given a **training dataset**

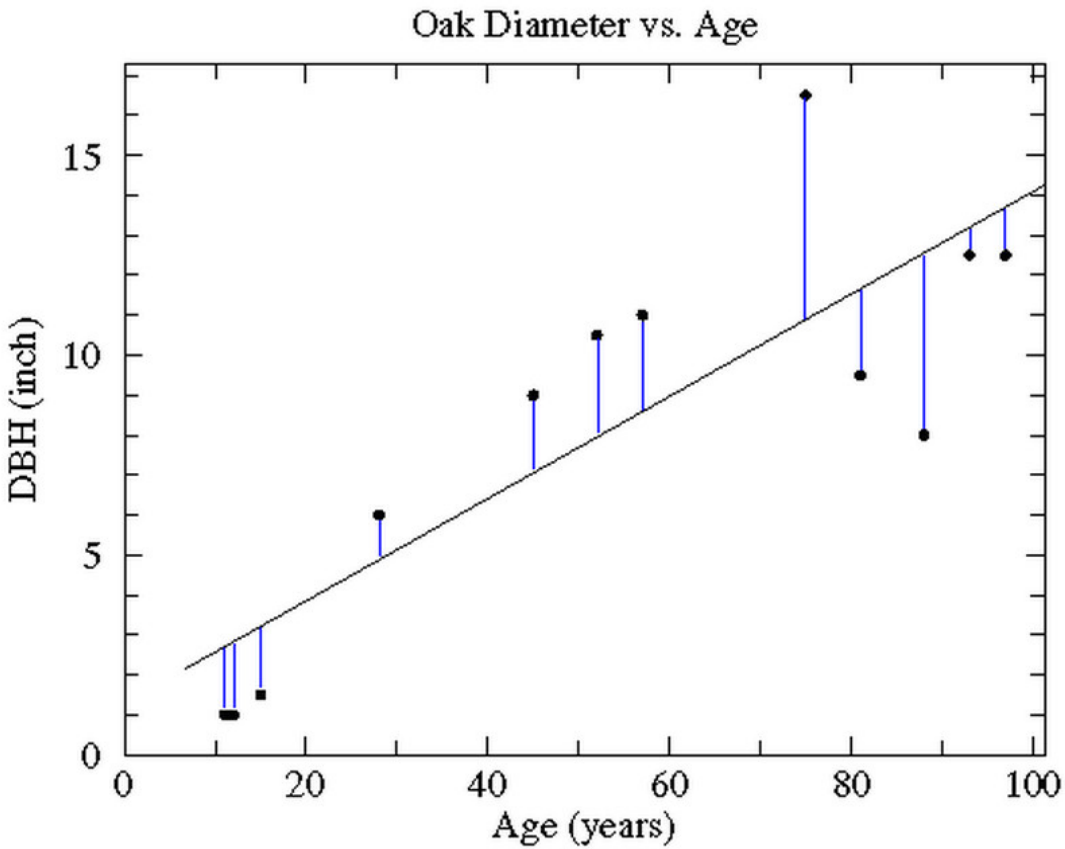
$$\mathcal{T} = \left\{\left(\vec{x}_1, d_1\right), \left(\vec{x}_2, d_2\right), \ldots, \left(\vec{x}_p, d_p\right)\right\}$$

  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

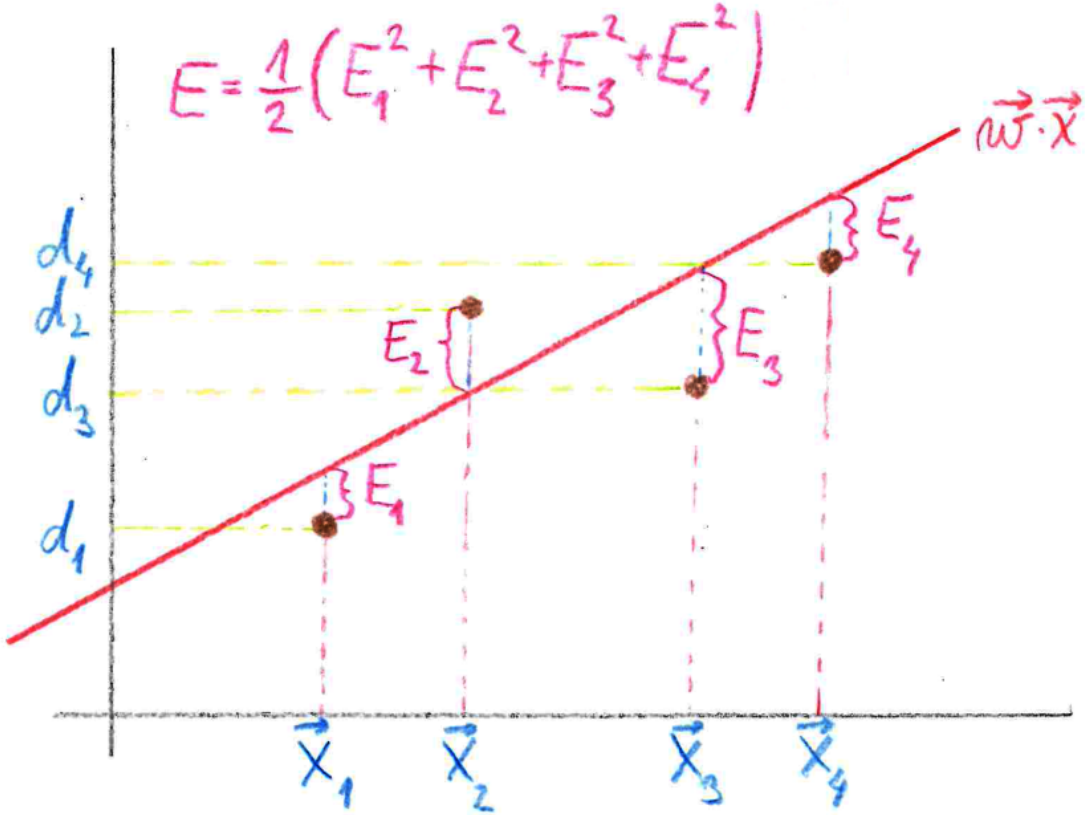
Age (years)	*DBH* (inch)
97	12.5
93	12.5
88	8.0
81	9.5
75	16.5
57	11.0
52	10.5
45	9.0
28	6.0
15	1.5
12	1.0
11	1.0



Linear regression (ADALINE)

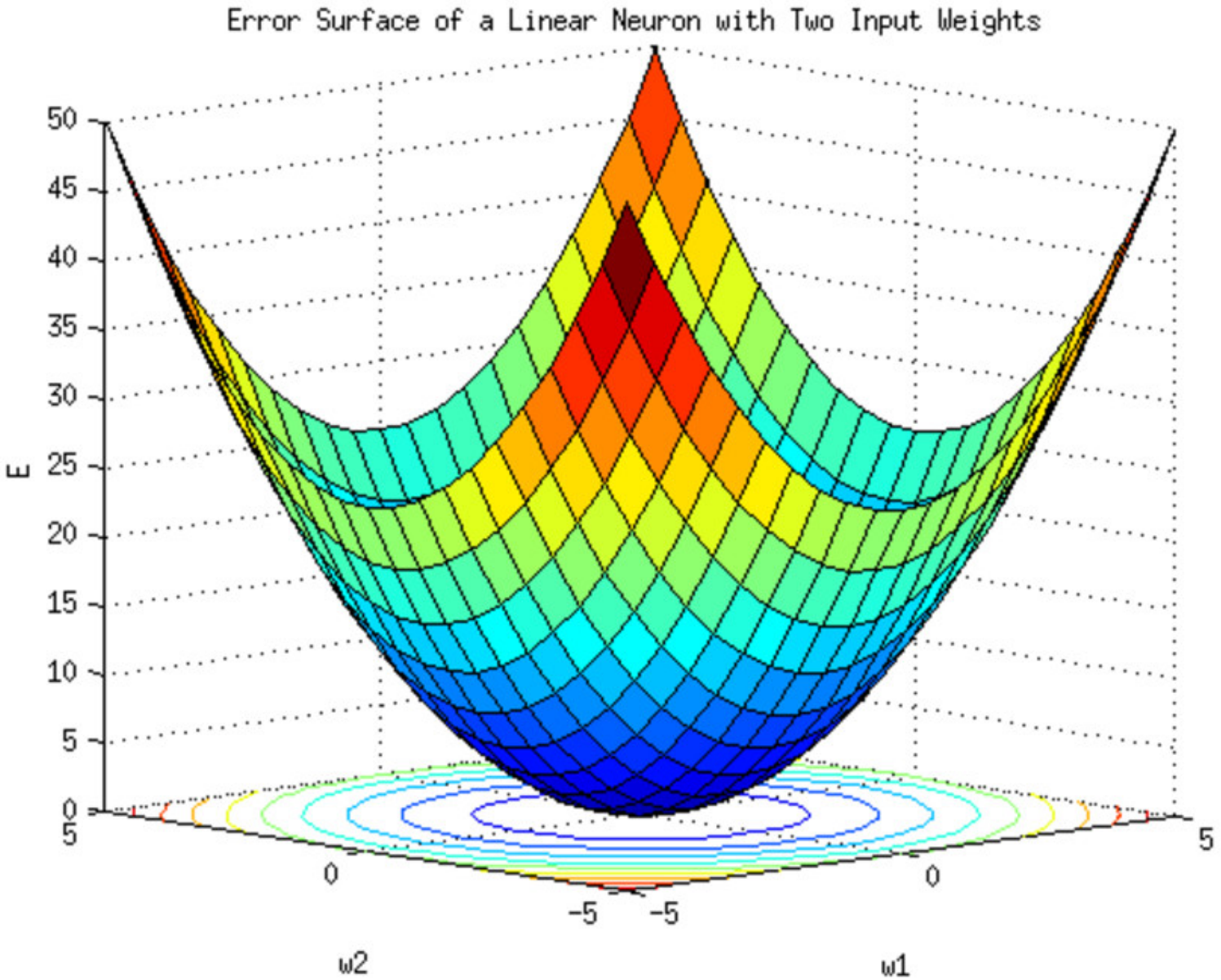
- **Error function:**

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



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

Error function



Gradient of the error function

Consider **gradient** of the error function:

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

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

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

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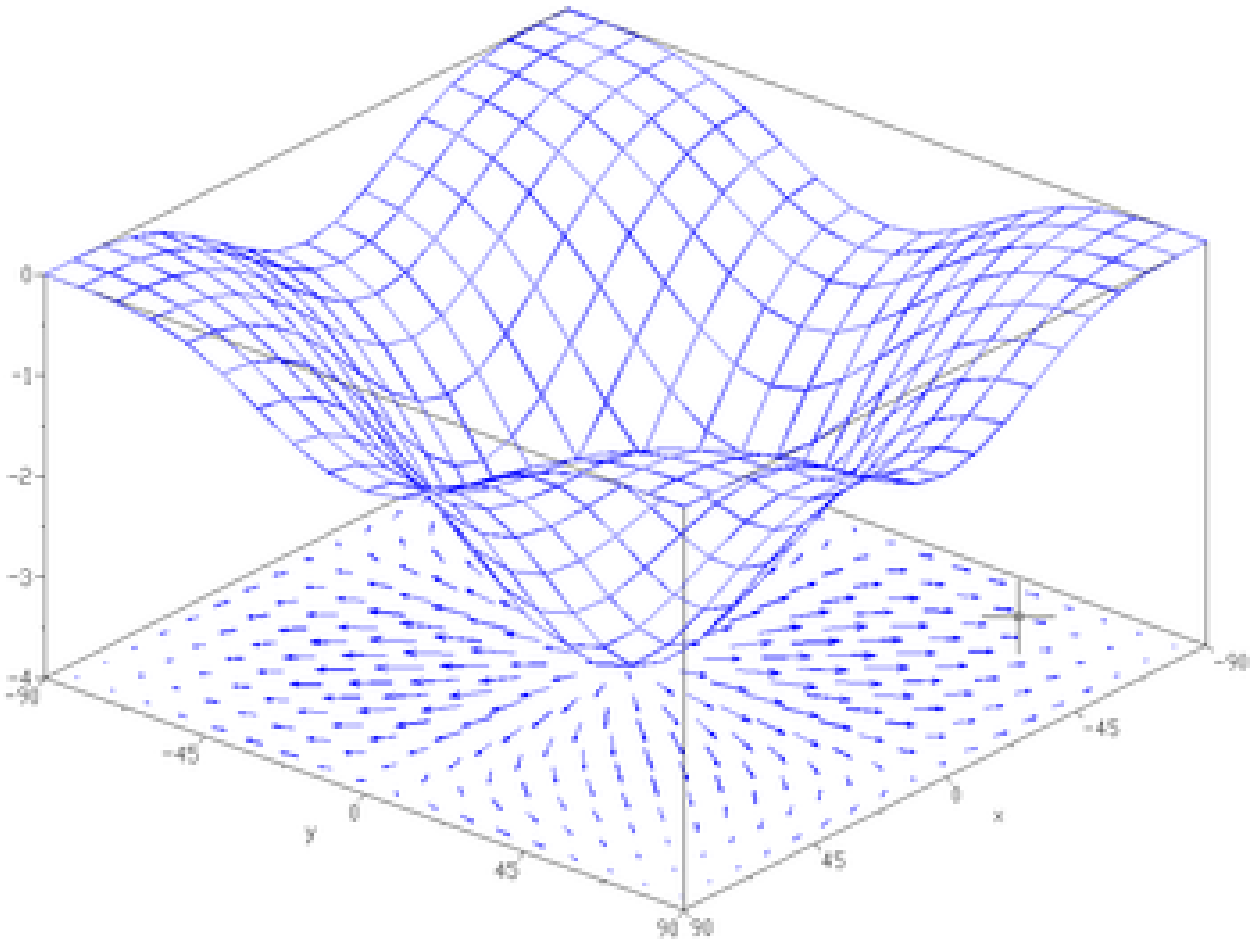
Fact

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

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

Gradient - illustration



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

Gradient of the error function

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

Gradient of the error function

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

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

Gradient of the error function

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

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

Thus

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

Linear regression - learning

Batch algorithm (gradient descent):

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

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

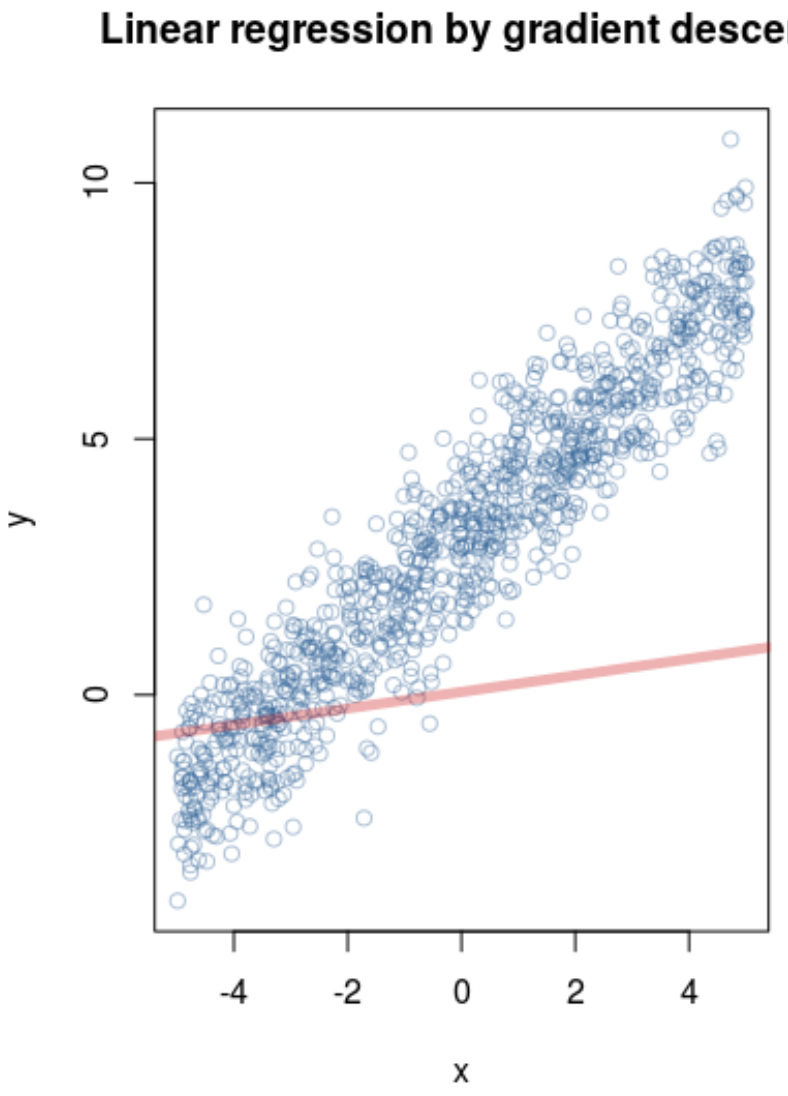
$$\begin{aligned} \vec{w}^{(t+1)} &= \vec{w}^{(t)} - \varepsilon \cdot \nabla E(\vec{w}^{(t)}) \\ &= \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(\vec{w}^{(t)} \cdot \vec{x}_k - d_k \right) \cdot \vec{x}_k \end{aligned}$$

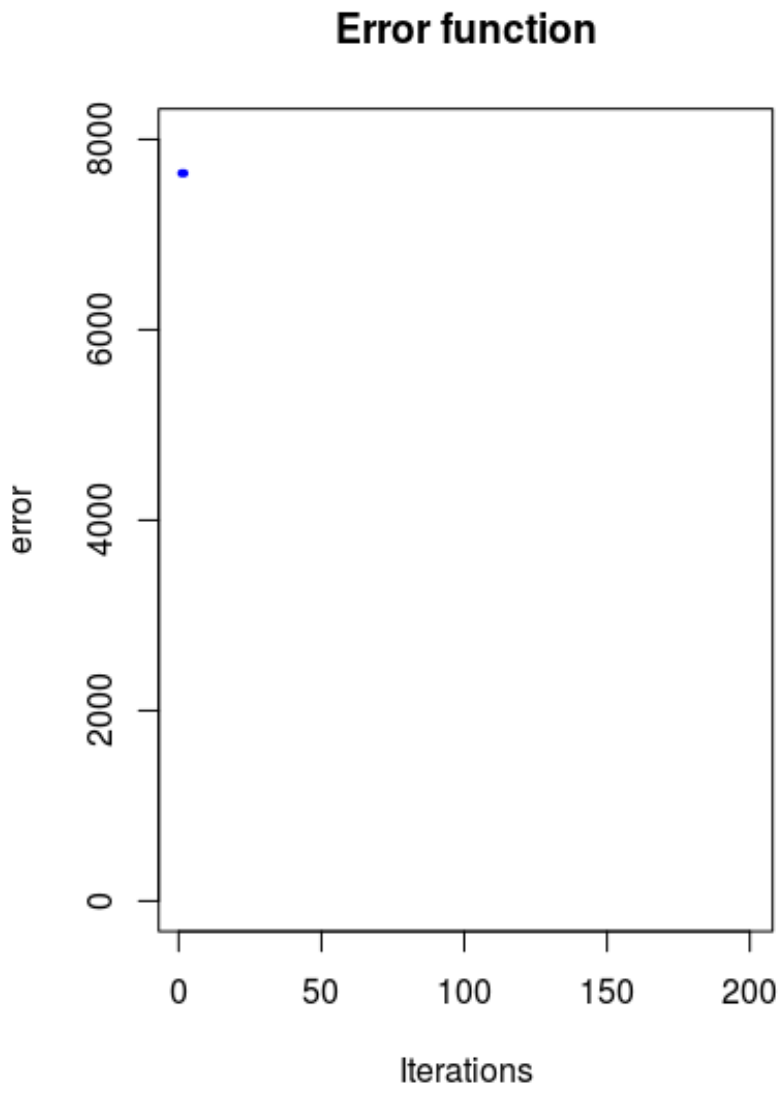
Here $k = (t \mod p) + 1$ and $0 < \varepsilon \leq 1$ is a *learning rate*.

Proposition

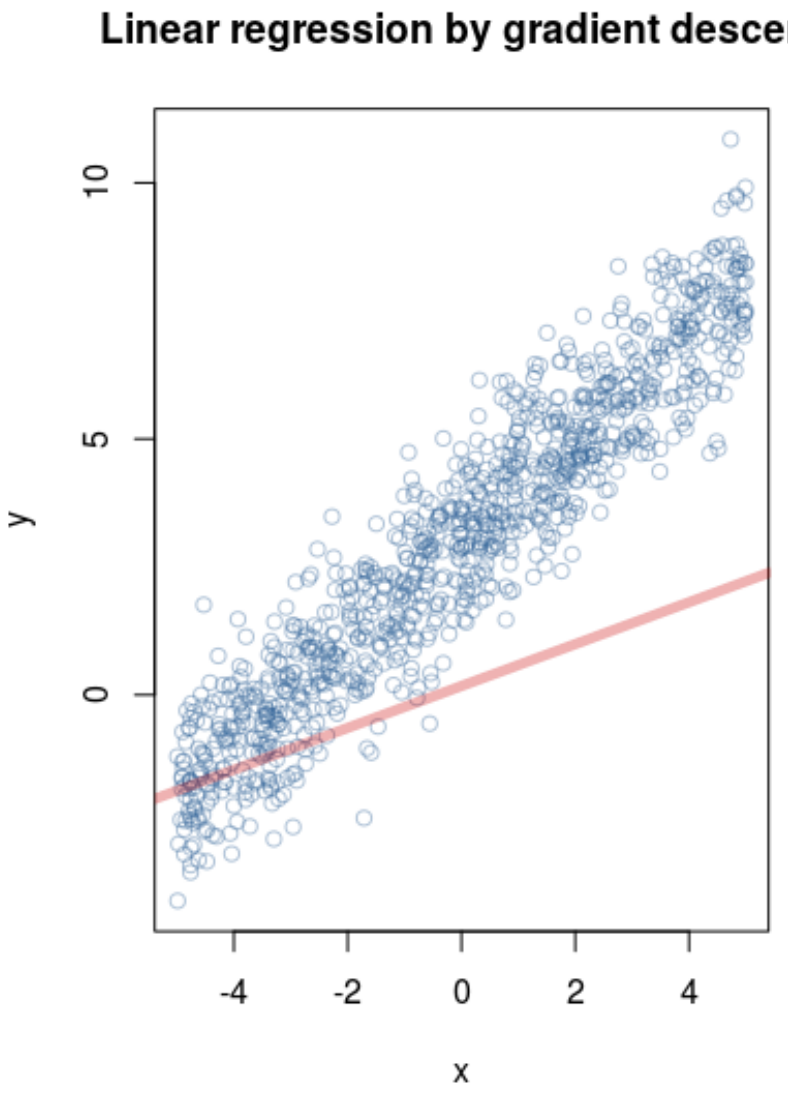
For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (componentwise) to the global minimum of E (i.e. to the vector $\vec{w}$ satisfying $\nabla E(\vec{w}) = \vec{0}$).

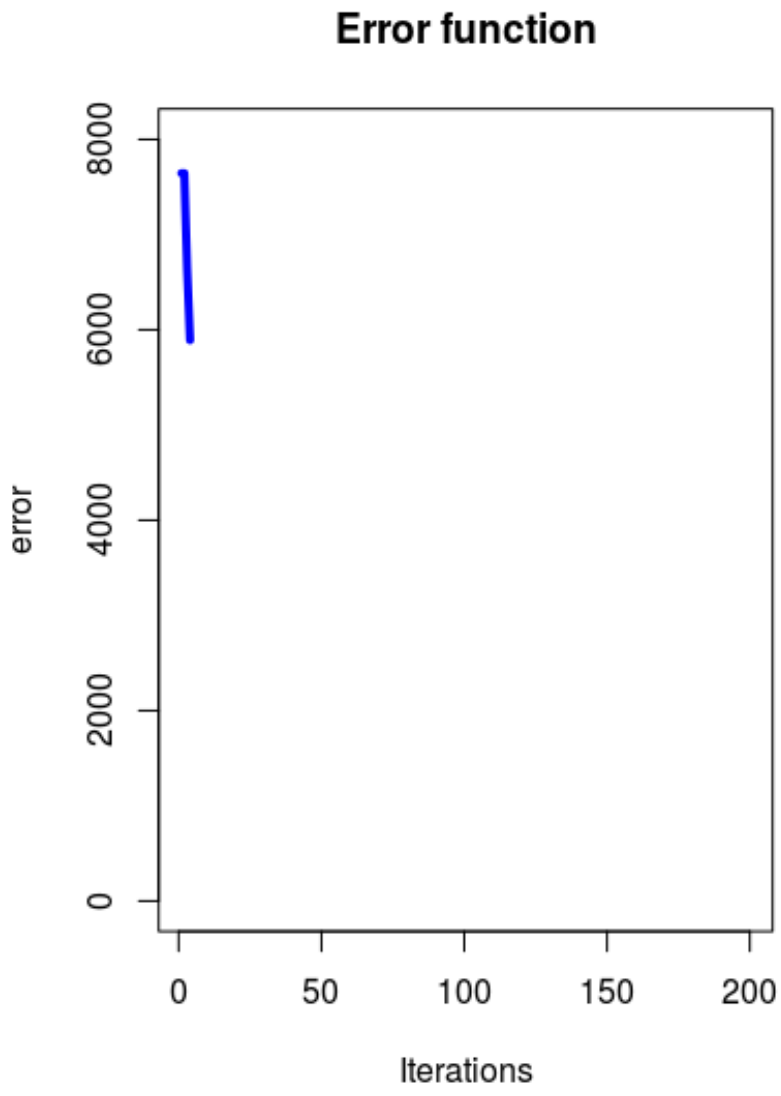
Linear regression - animation



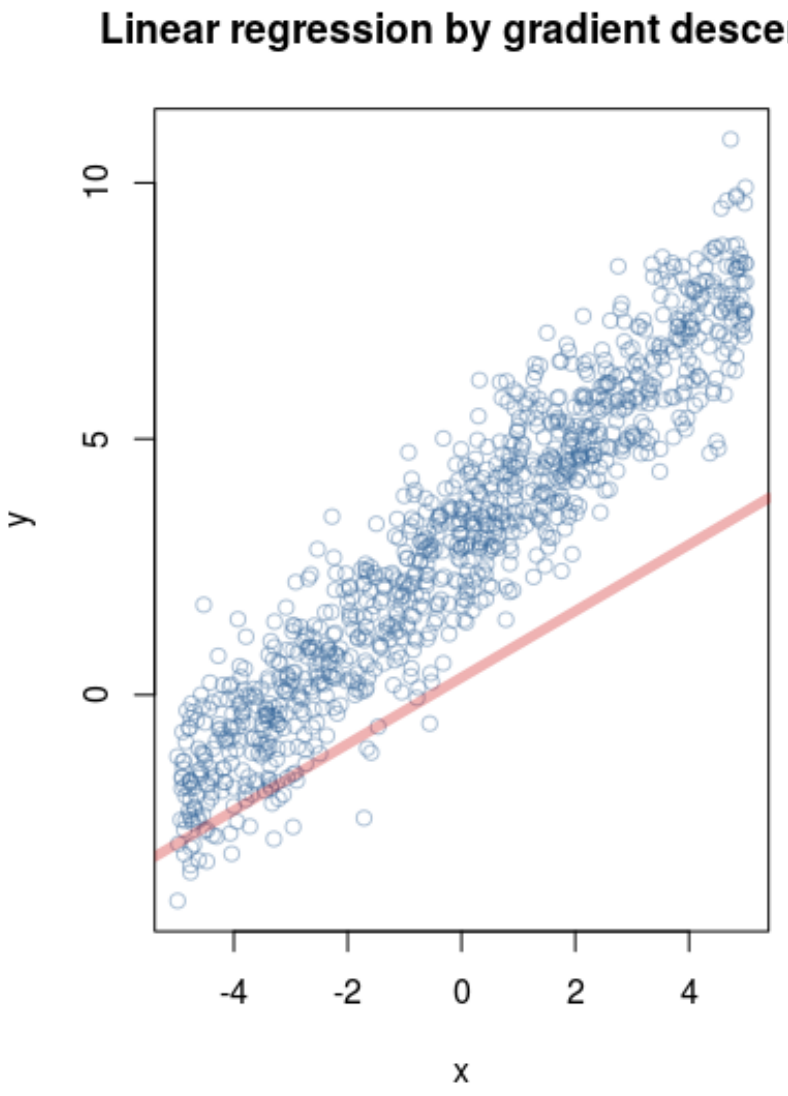


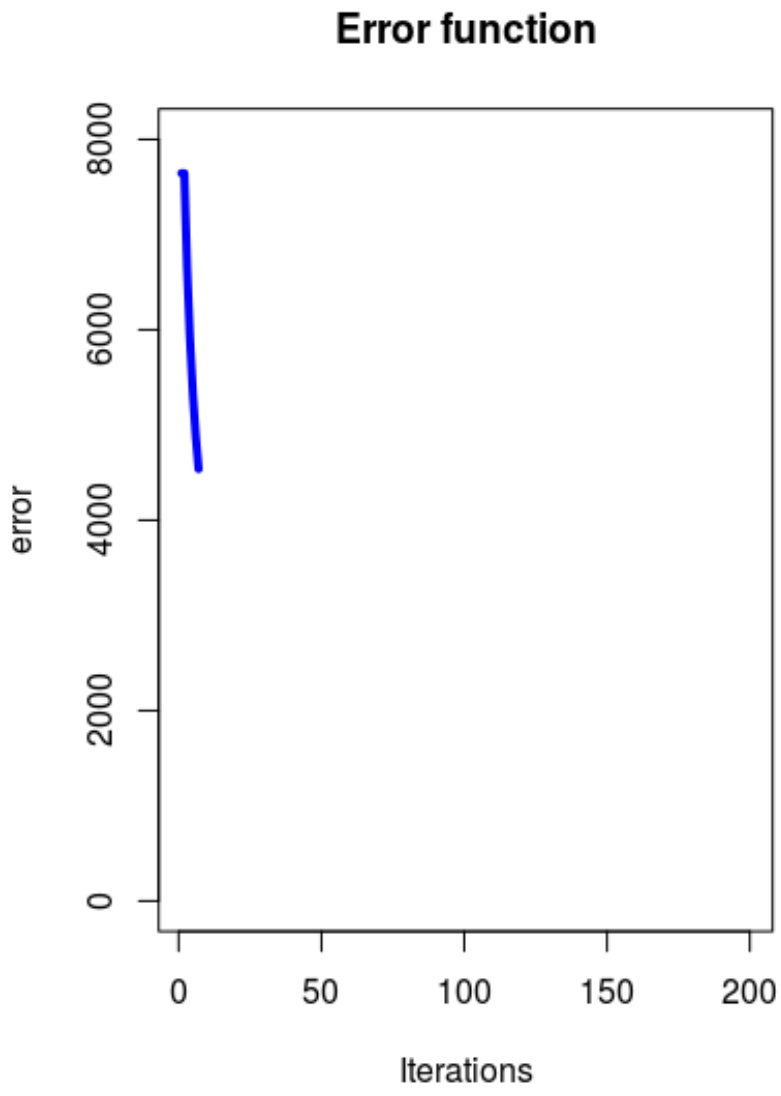
Linear regression - animation



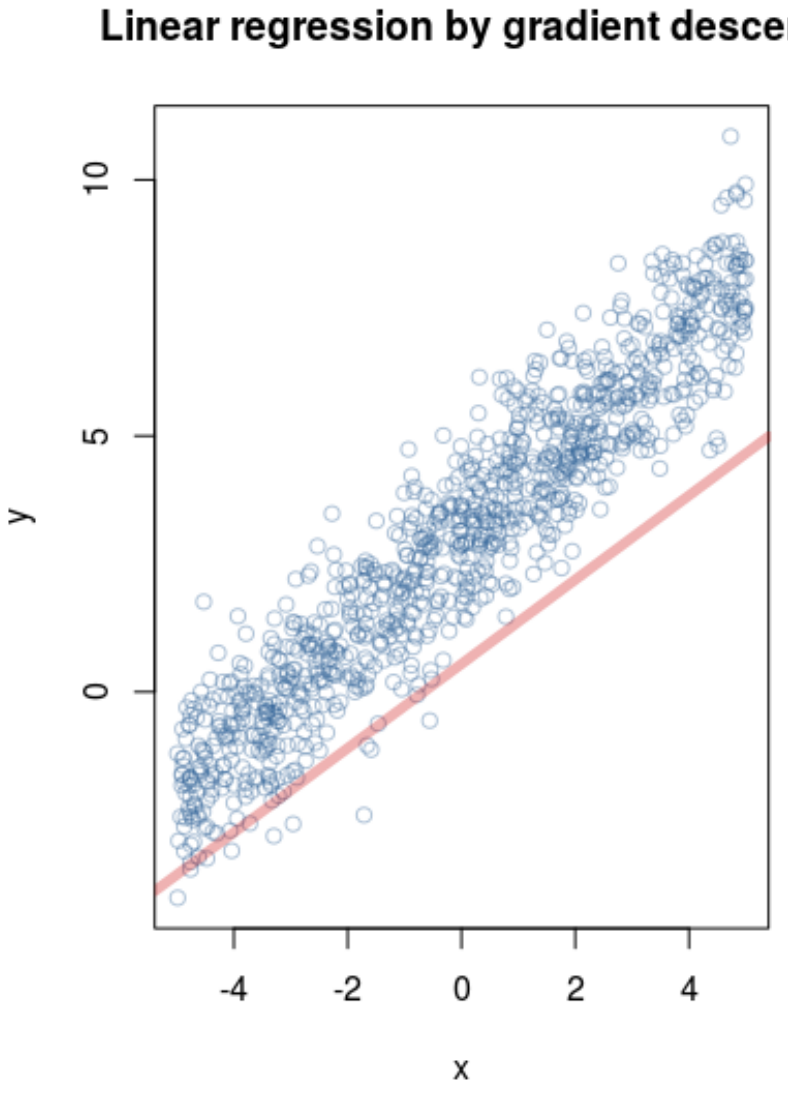


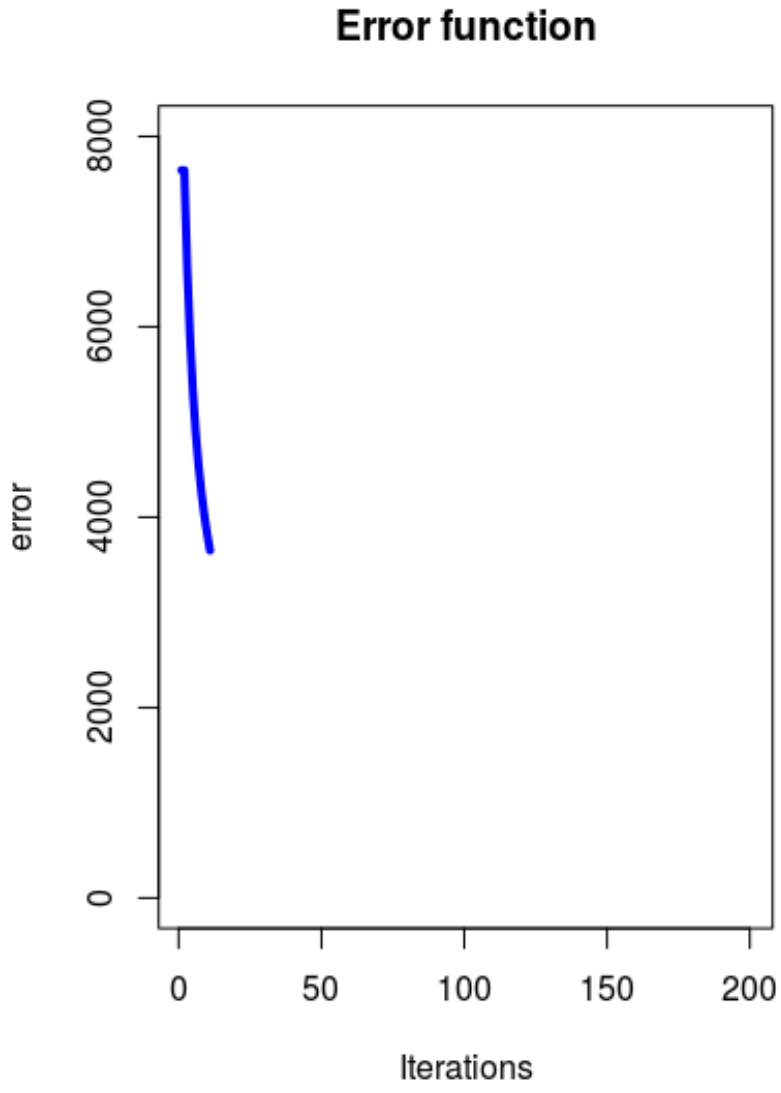
Linear regression - animation



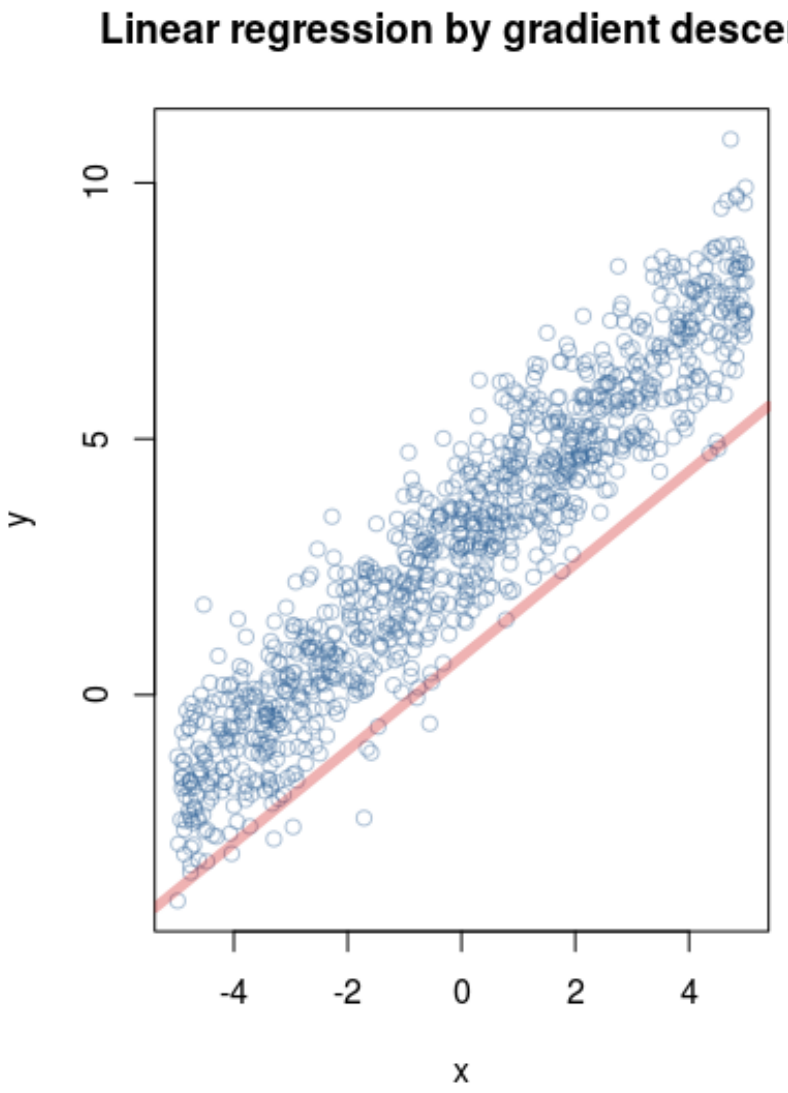


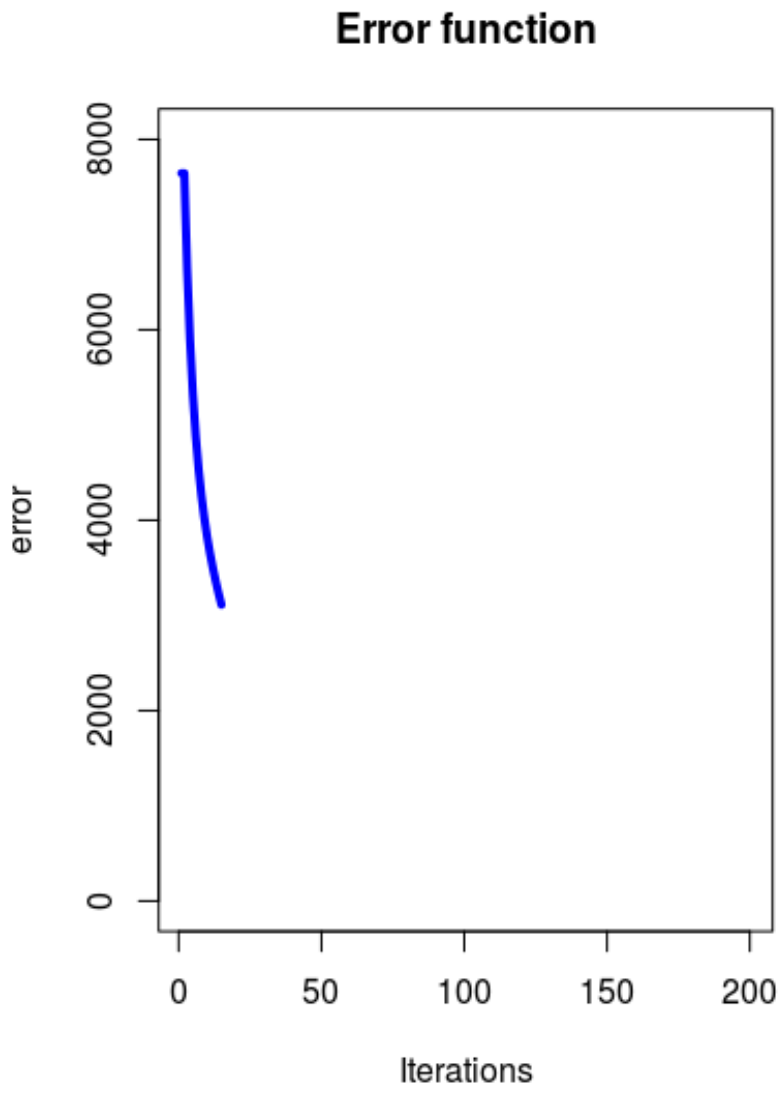
Linear regression - animation



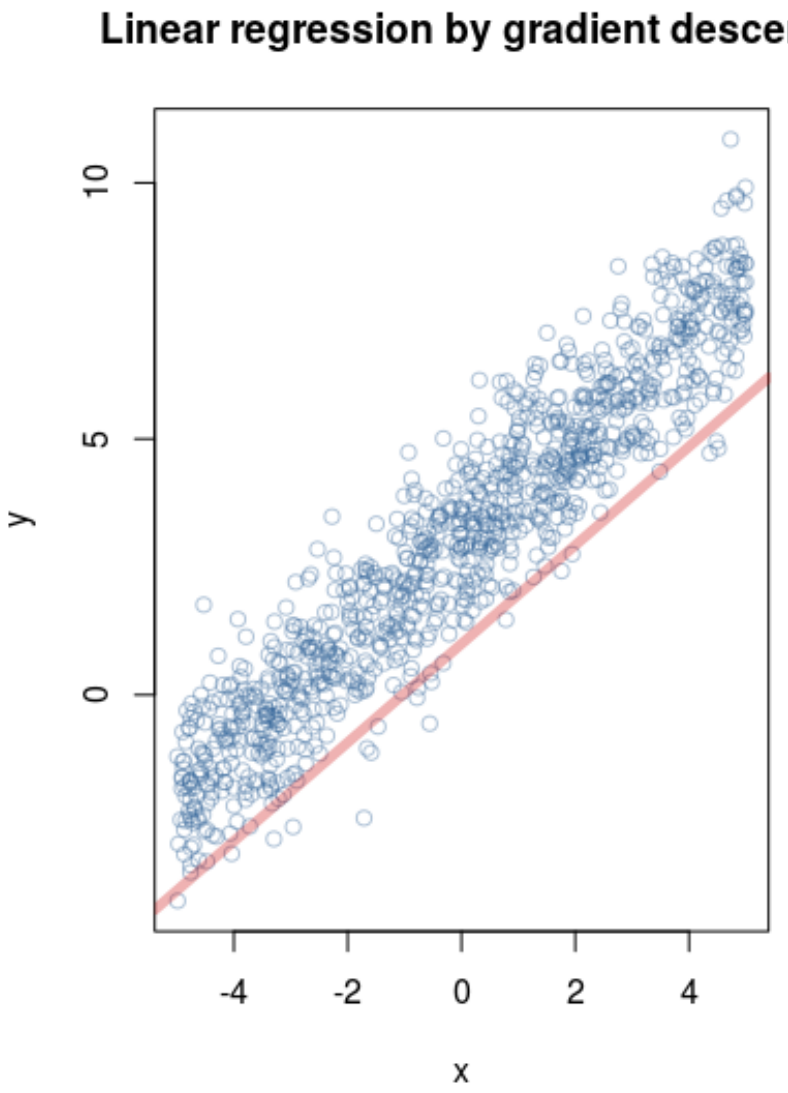


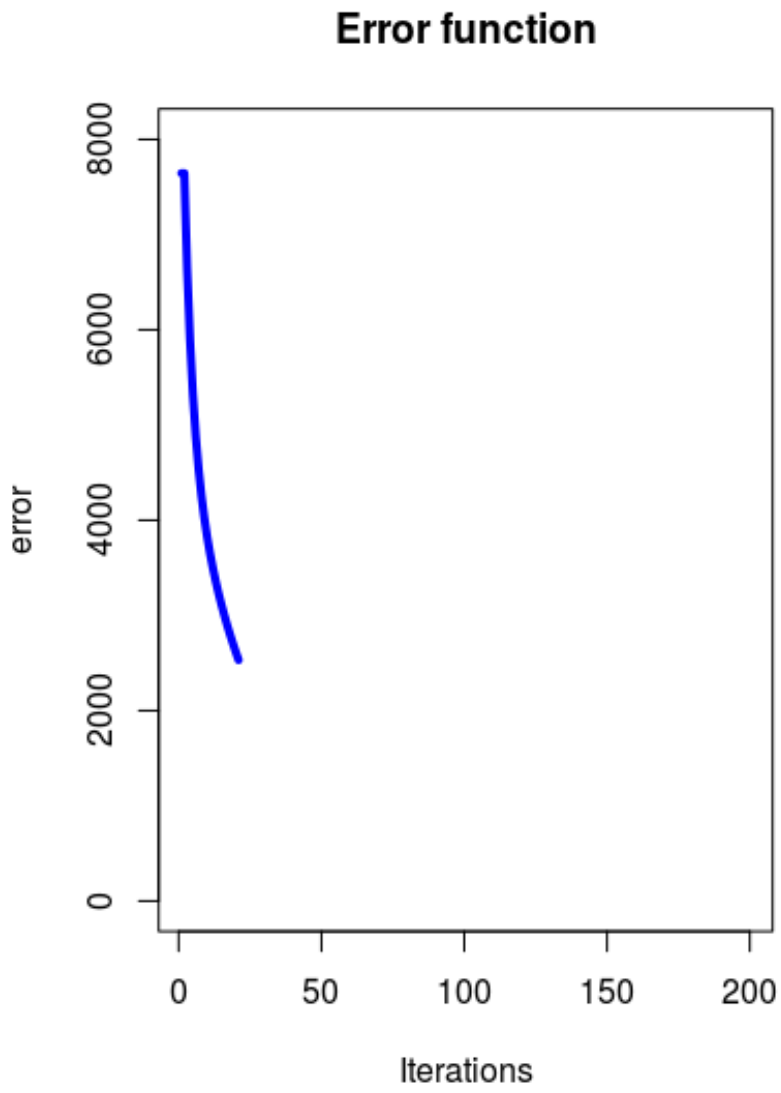
Linear regression - animation



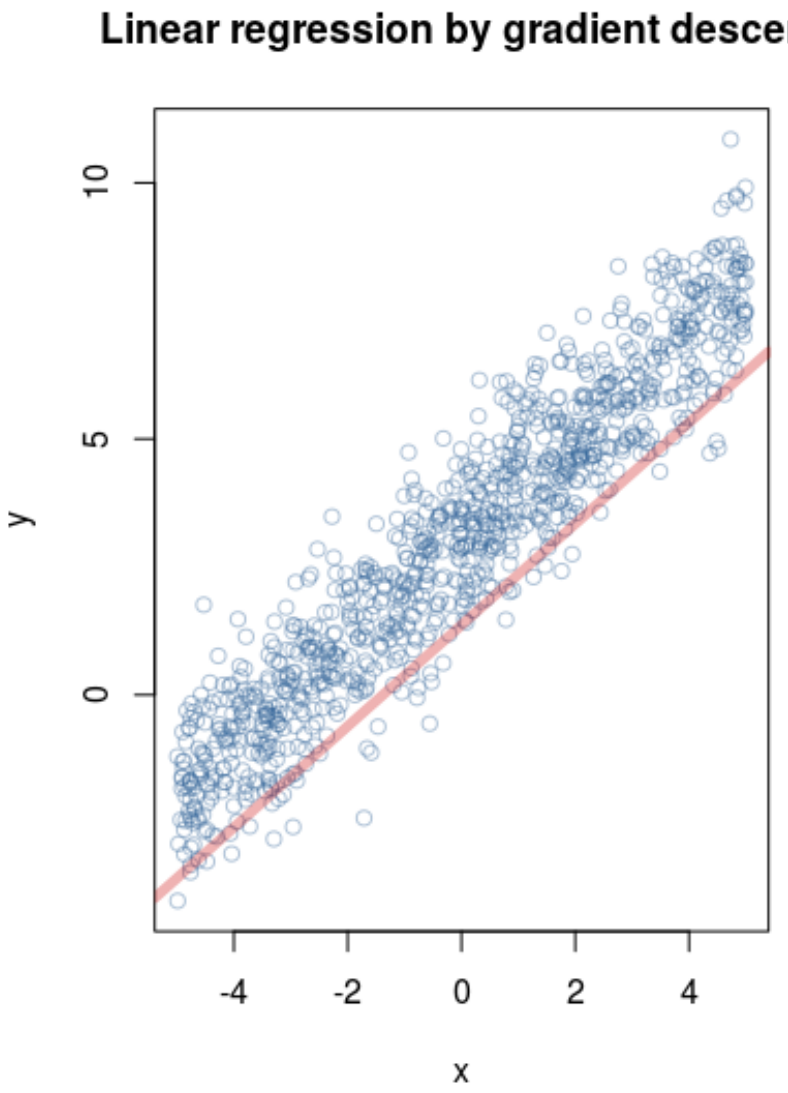


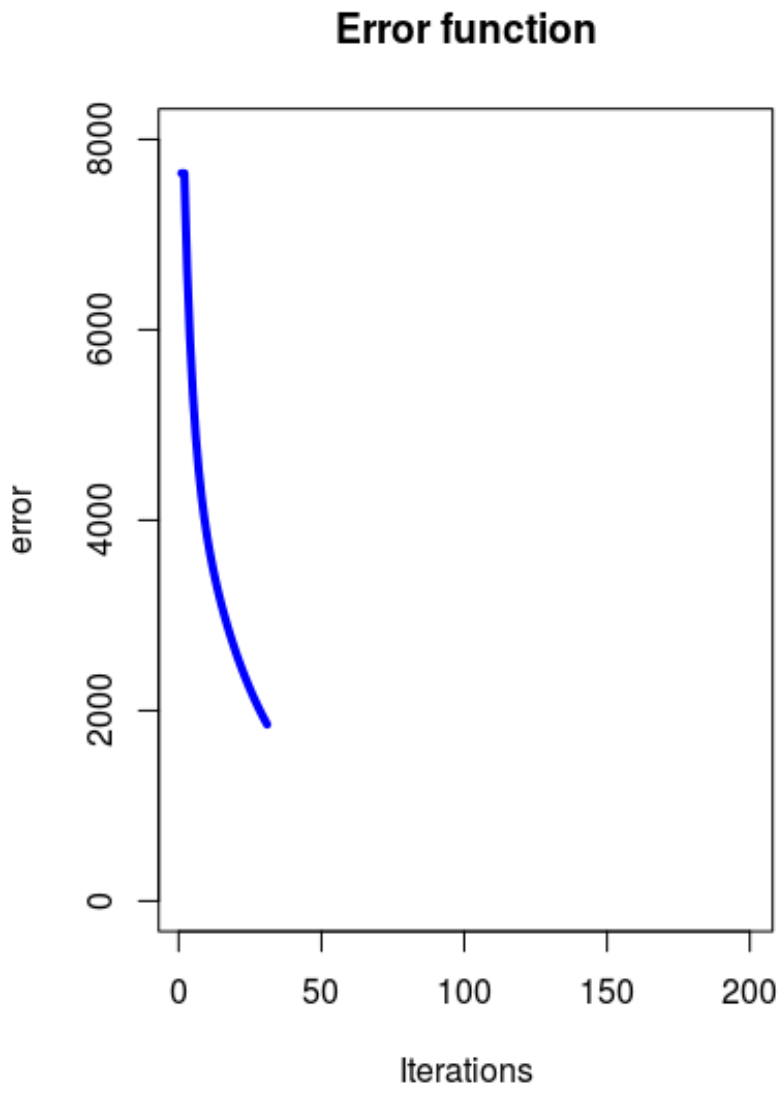
Linear regression - animation



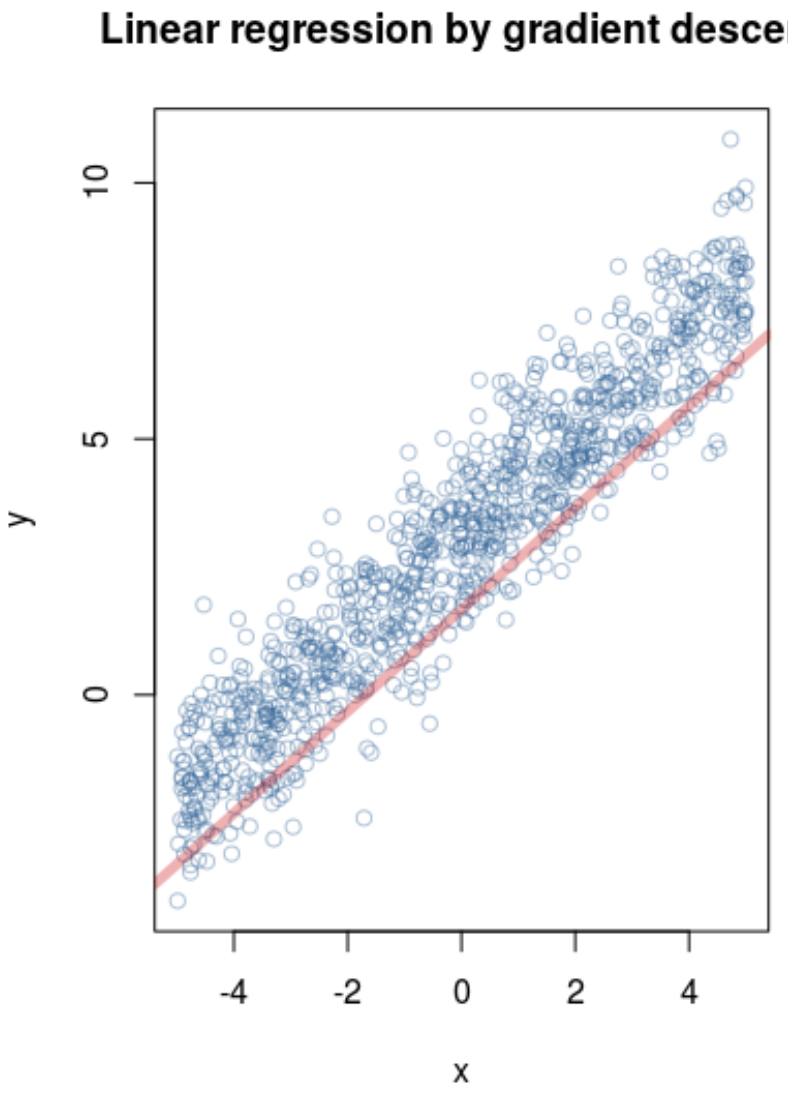


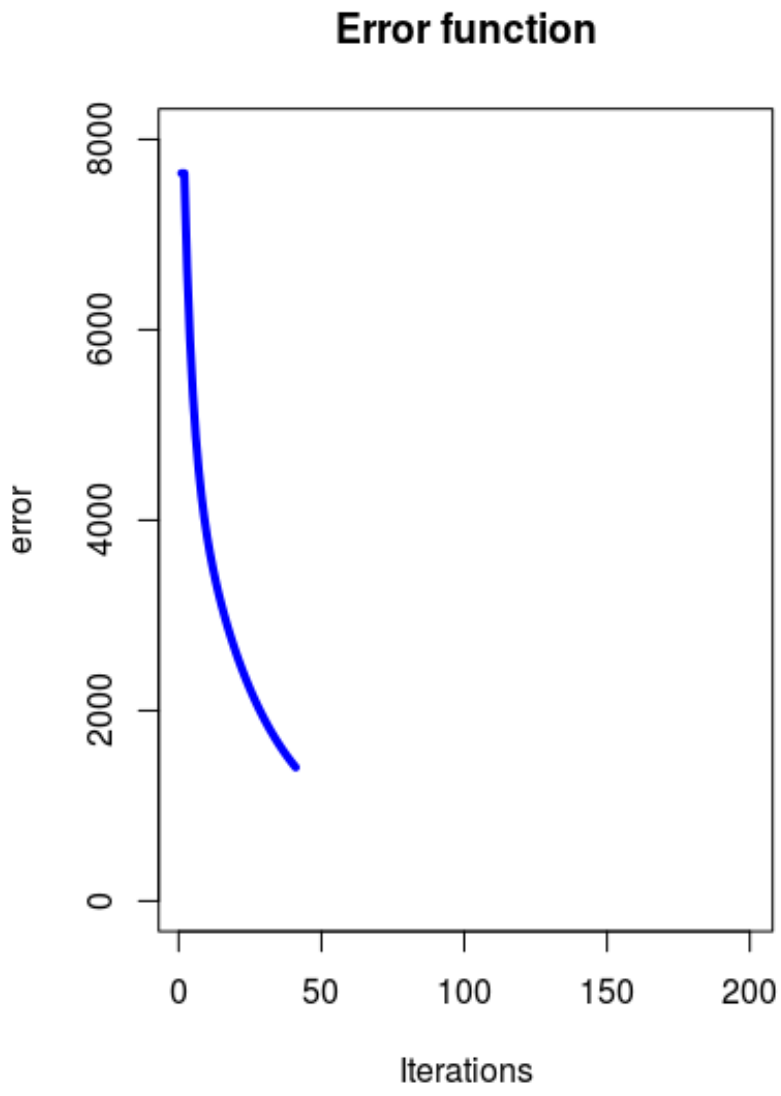
Linear regression - animation



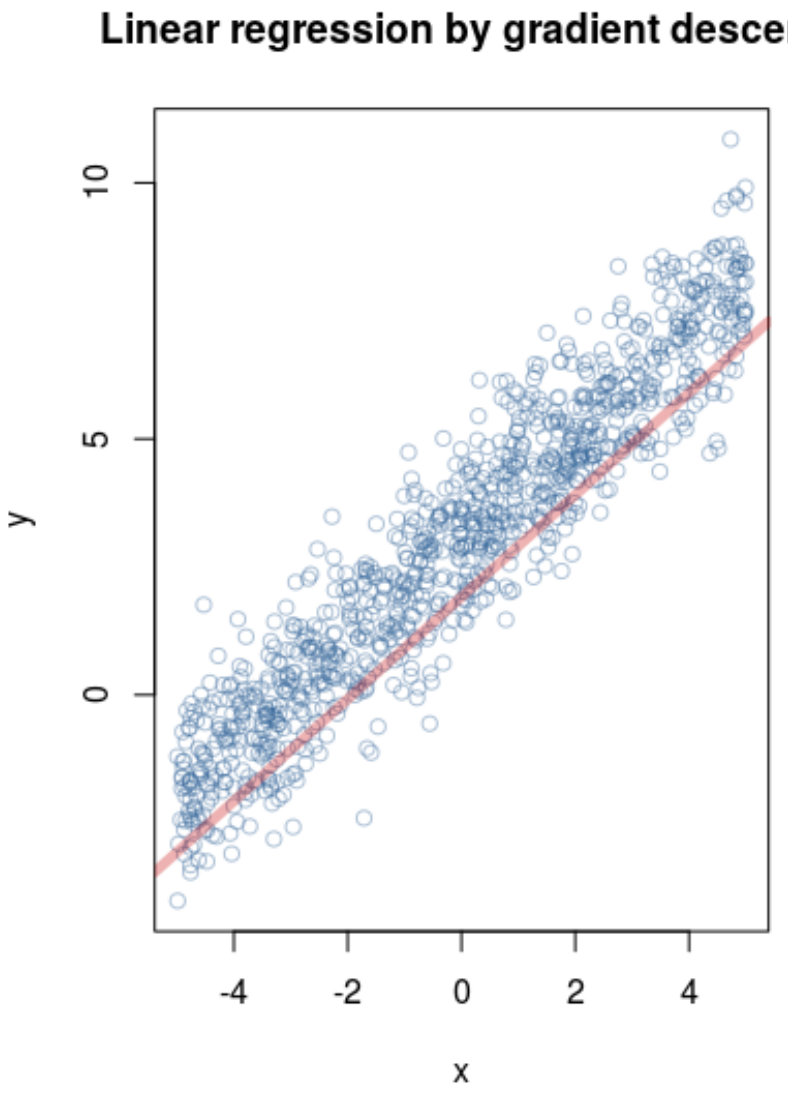


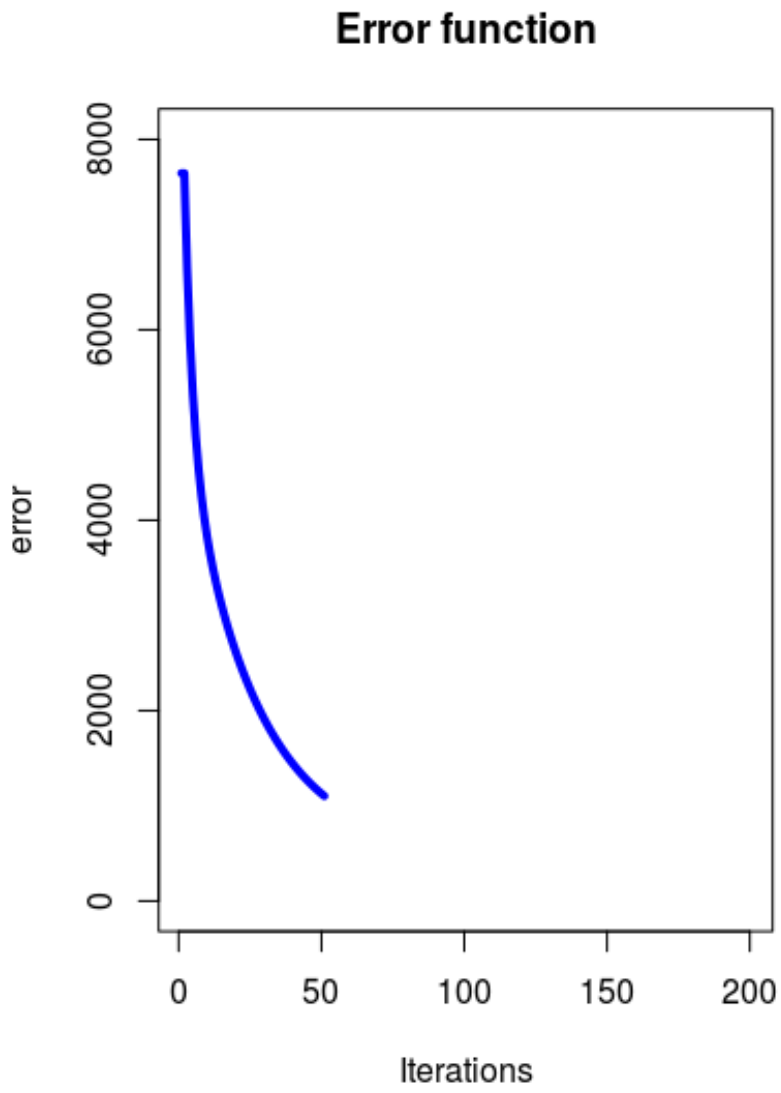
Linear regression - animation



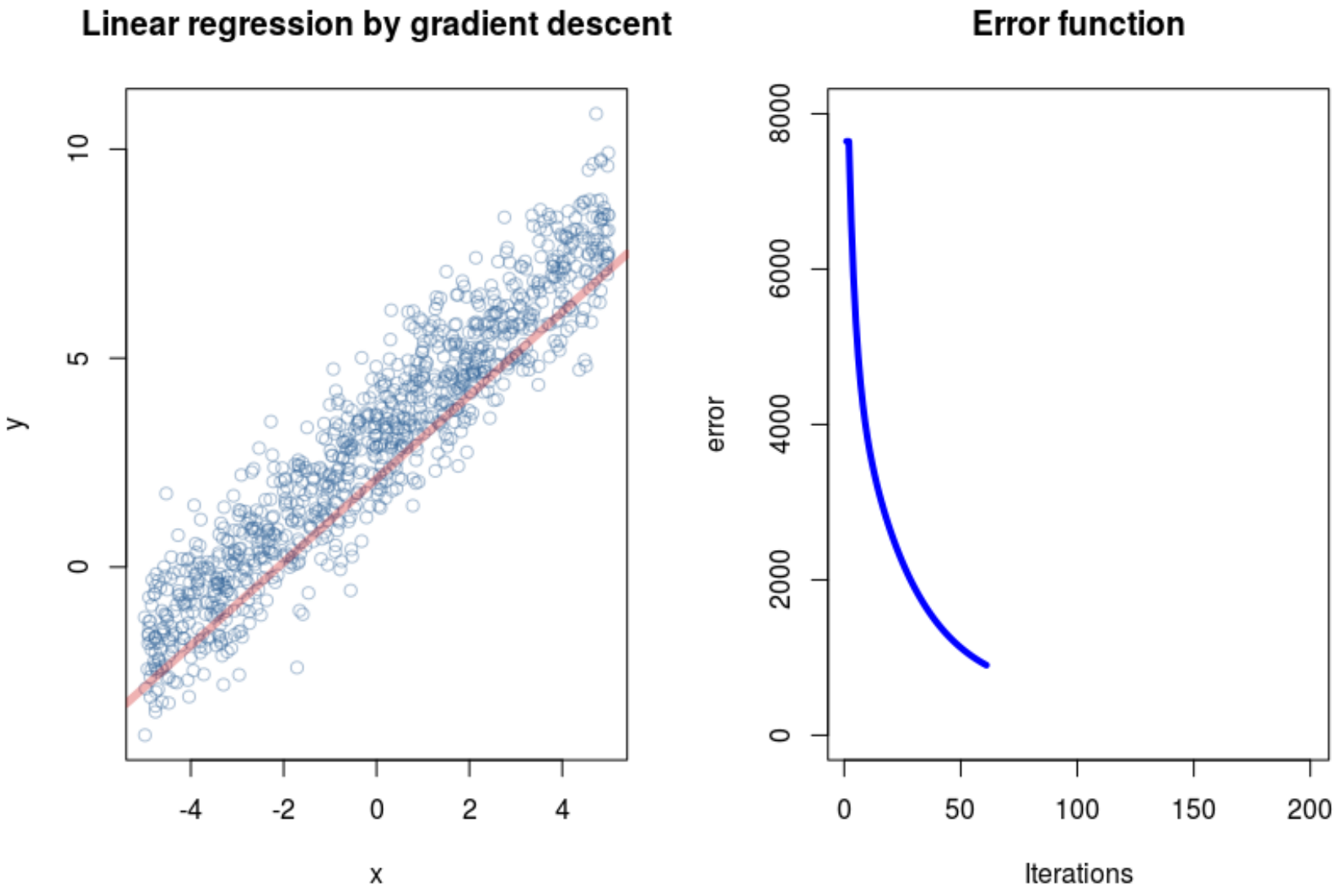


Linear regression - animation

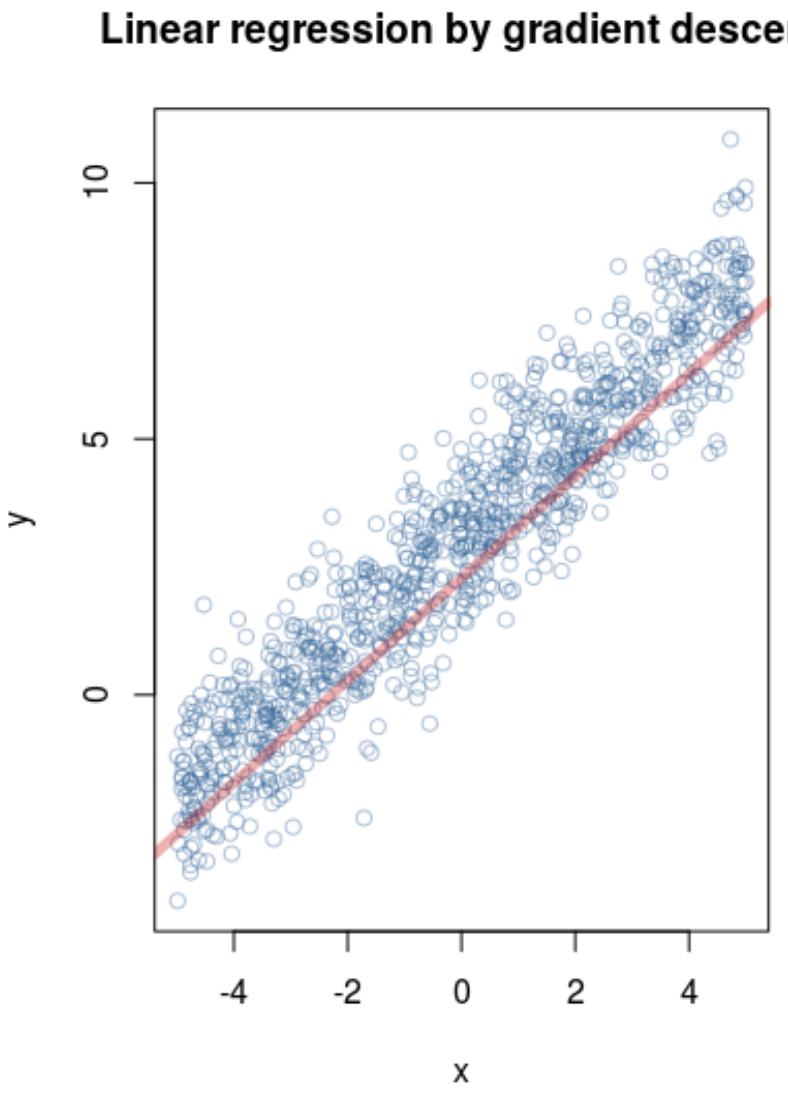


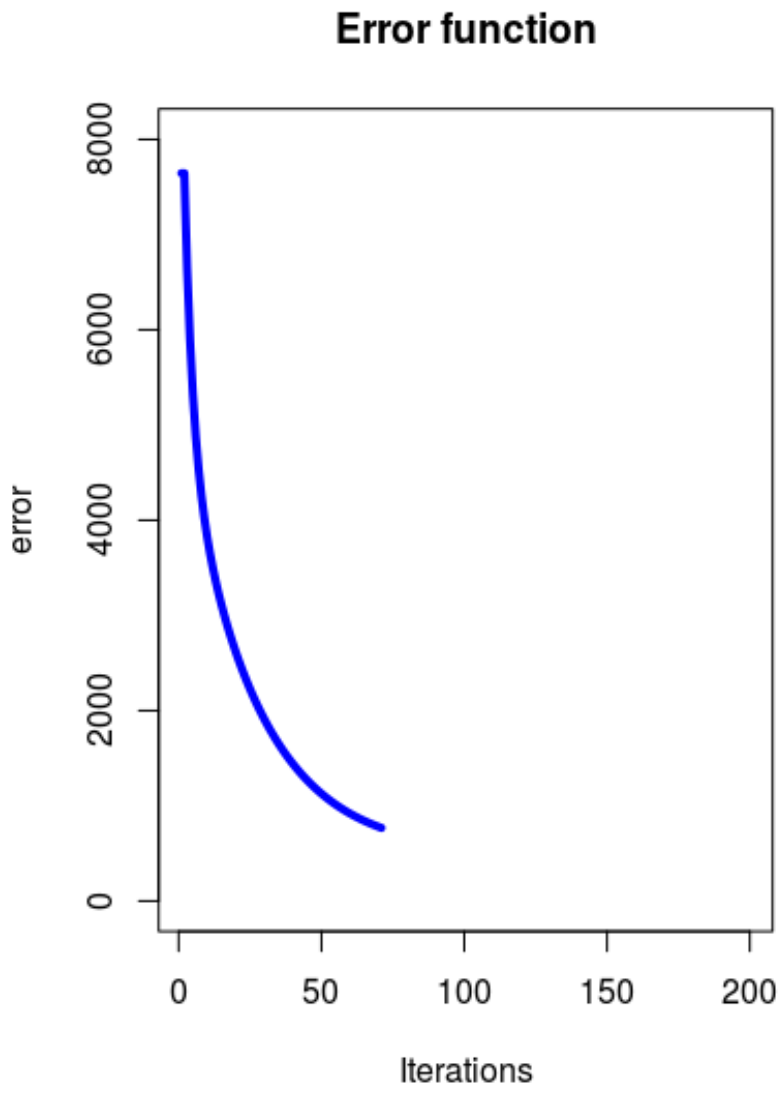


Linear regression - animation

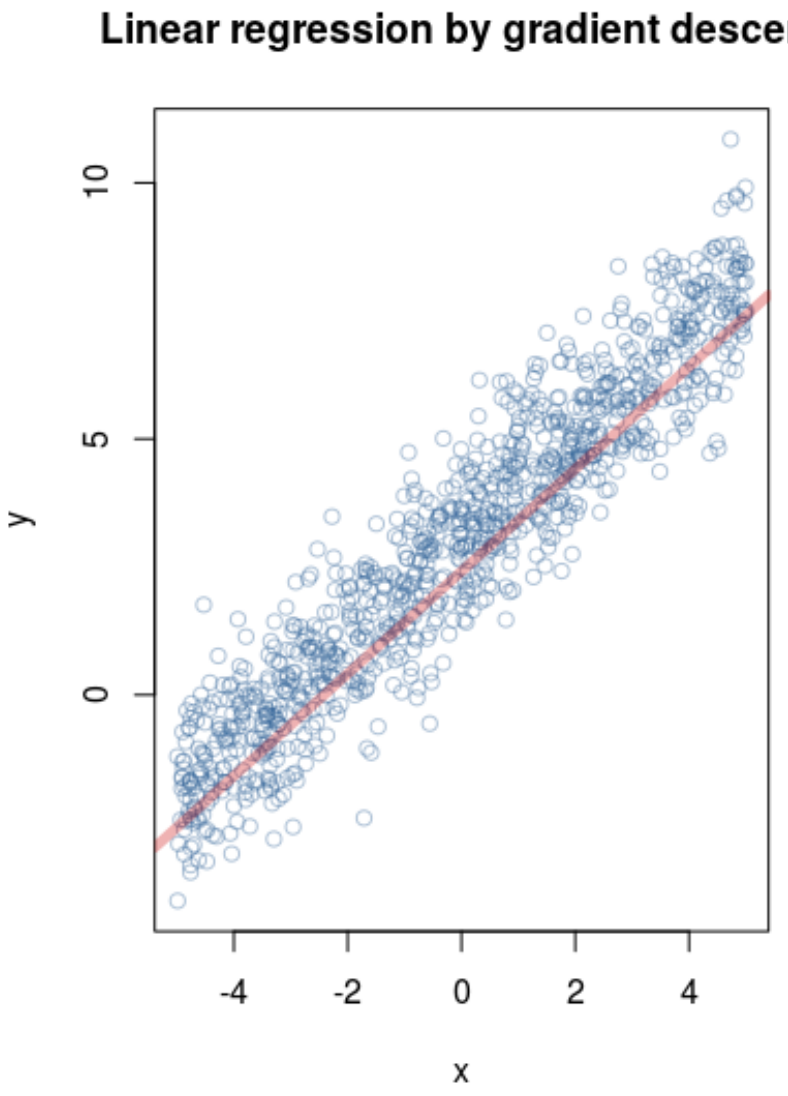


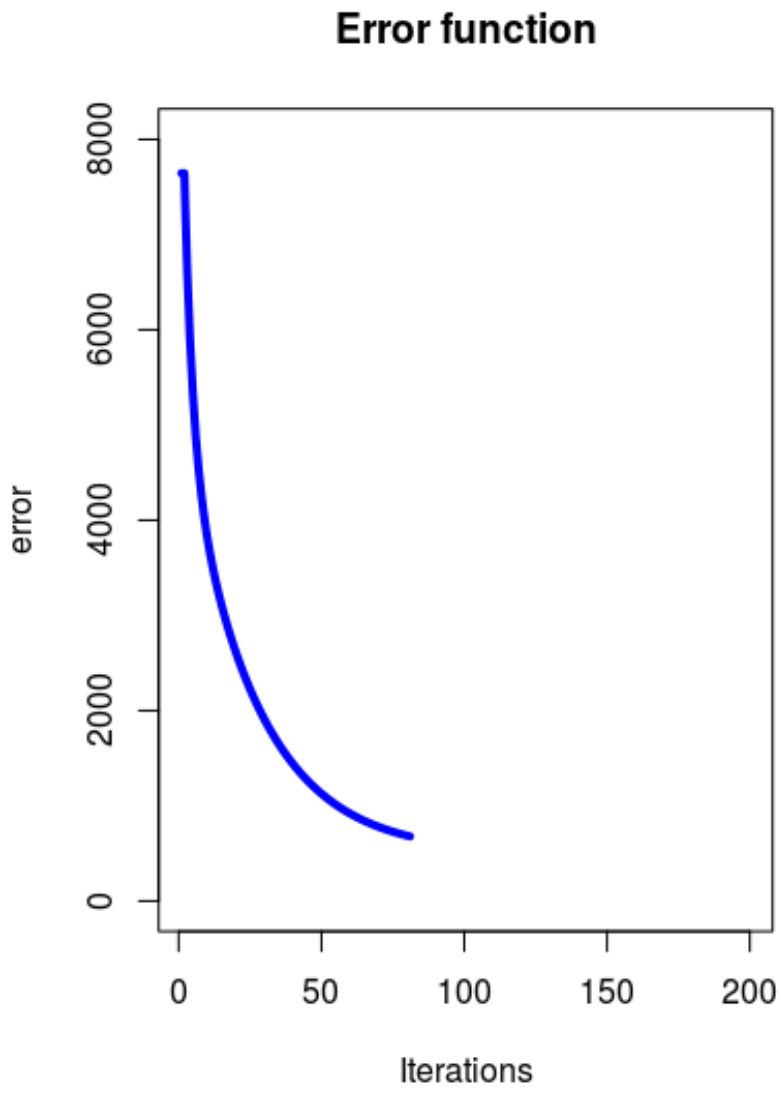
Linear regression - animation





Linear regression - animation





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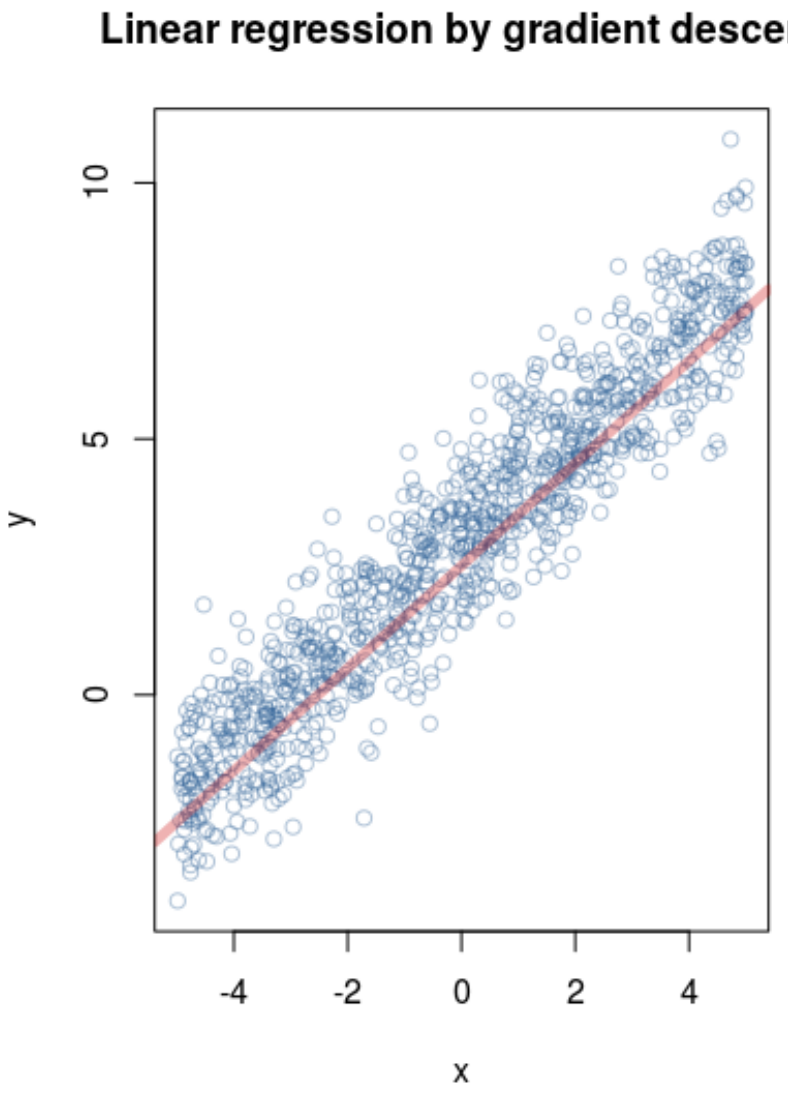
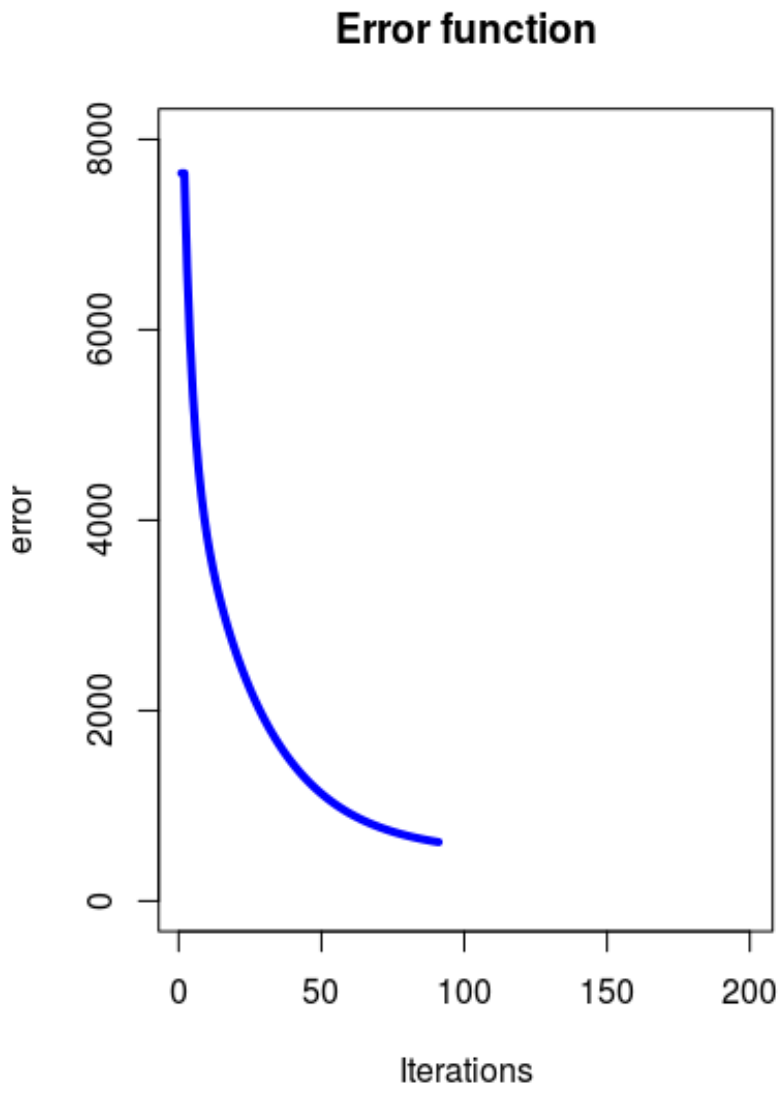
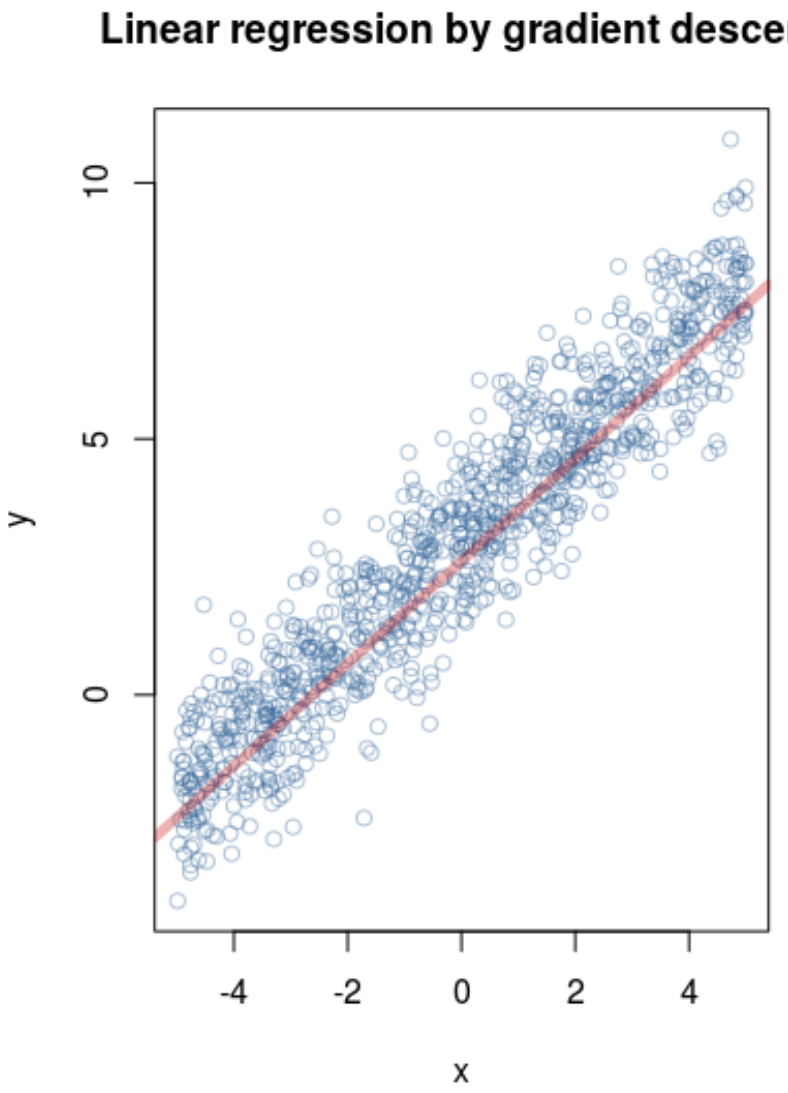
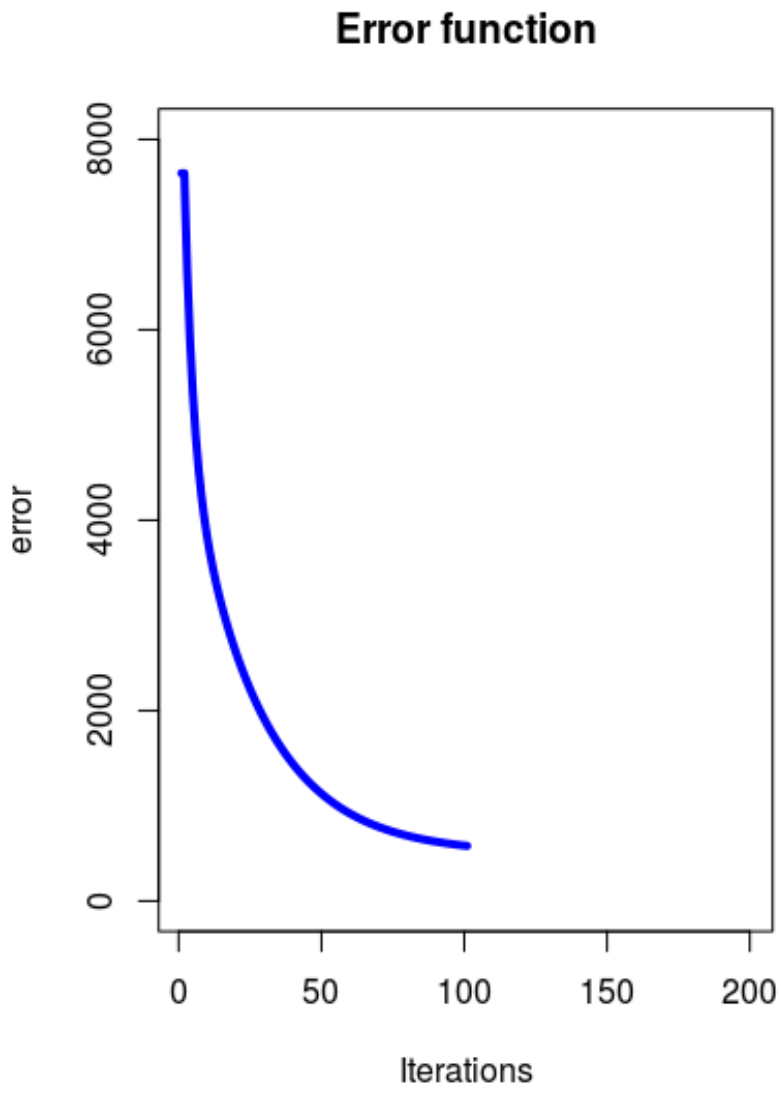


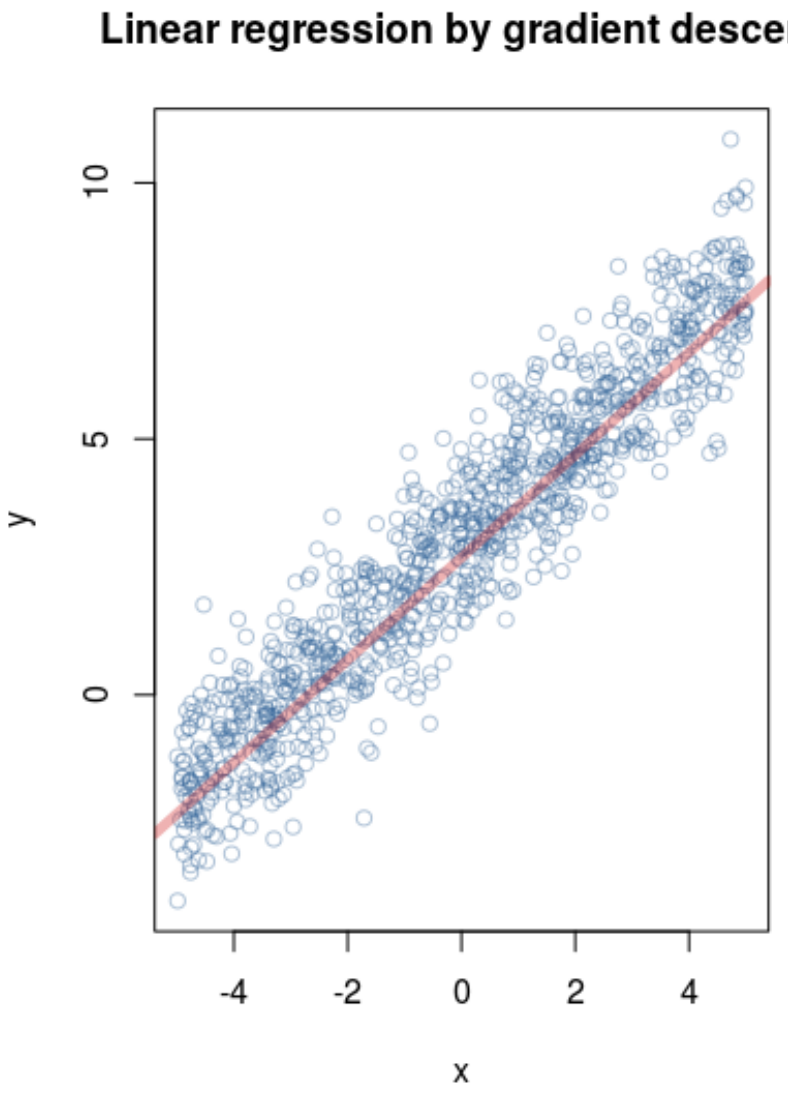


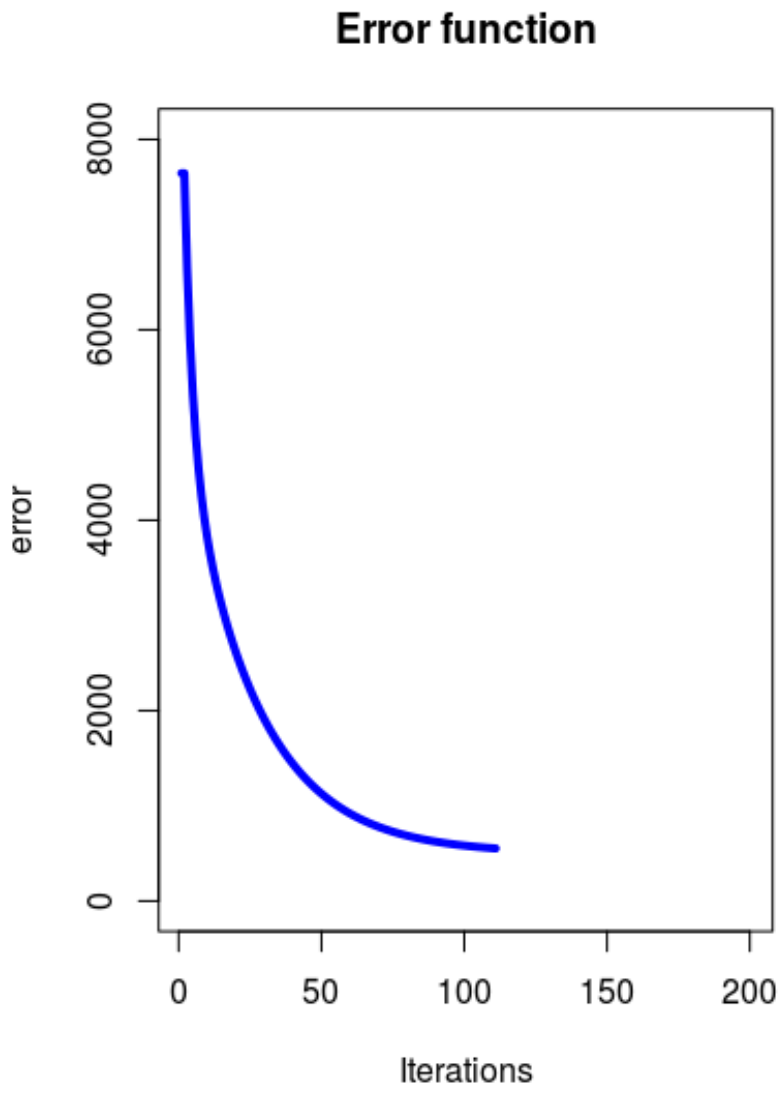
Linear regression - animation



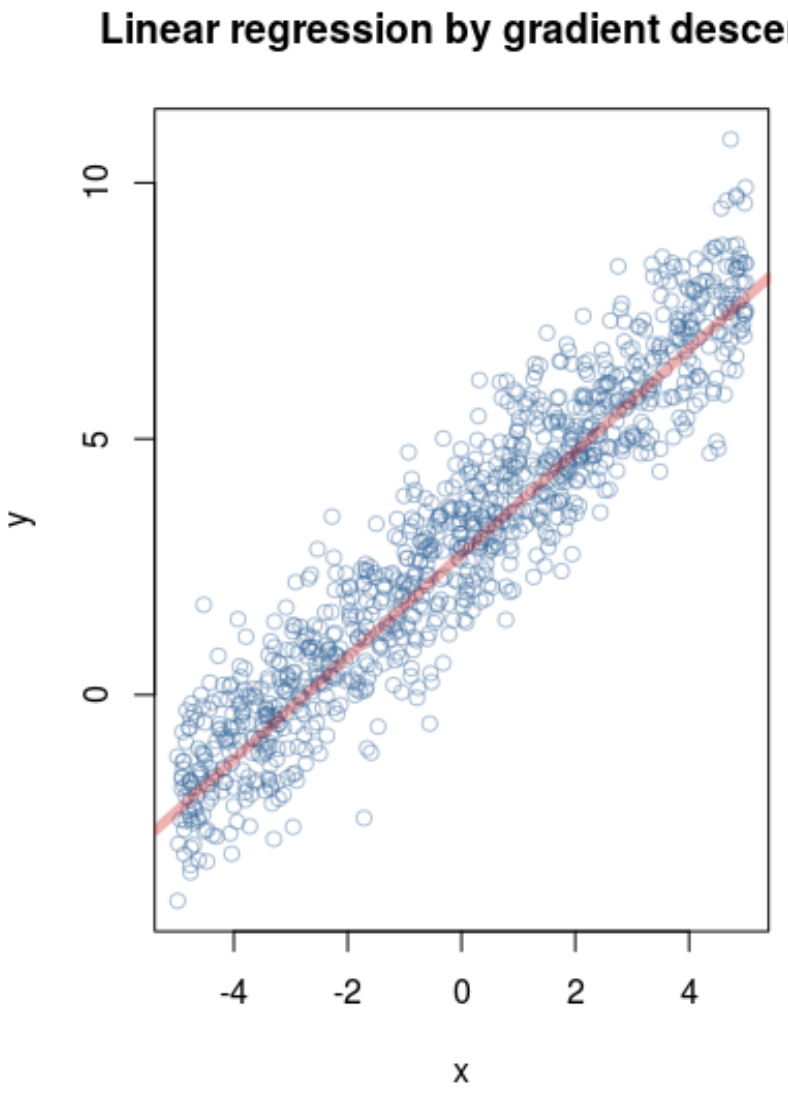


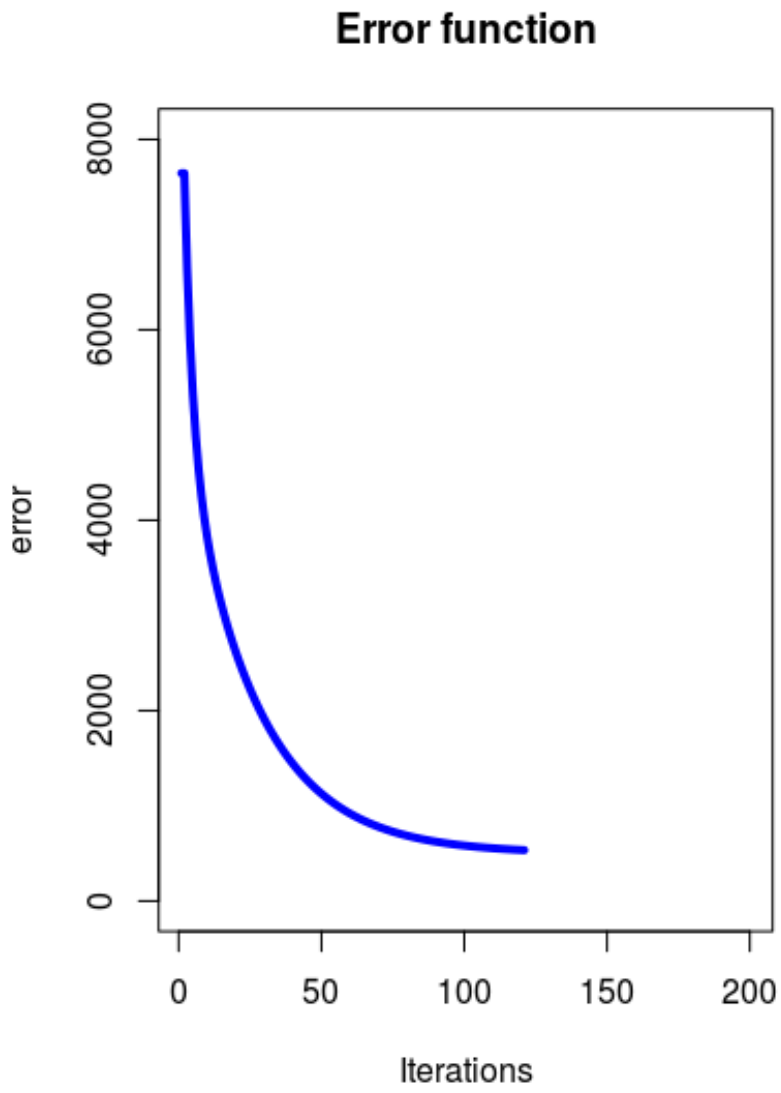
Linear regression - animation



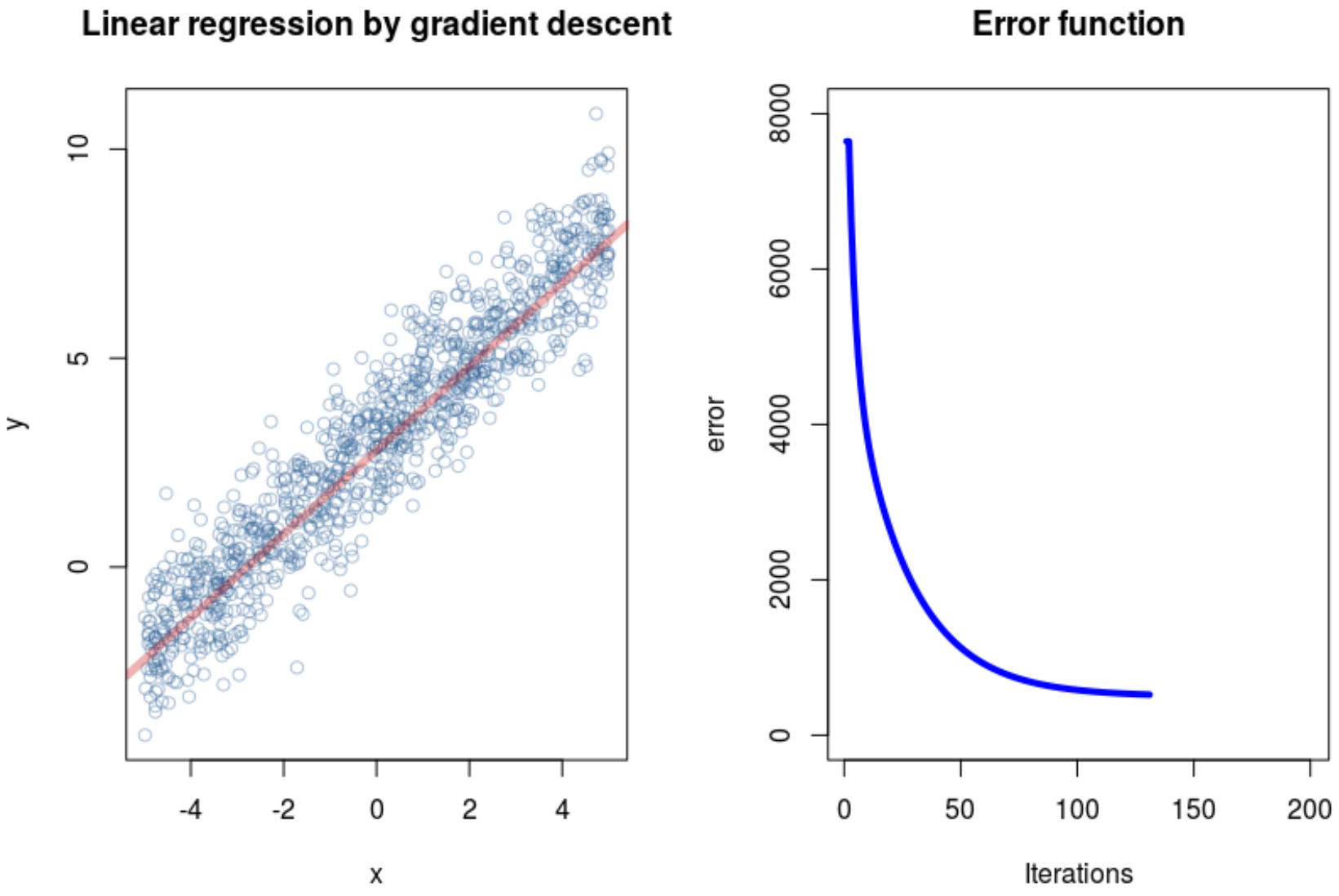


Linear regression - animation

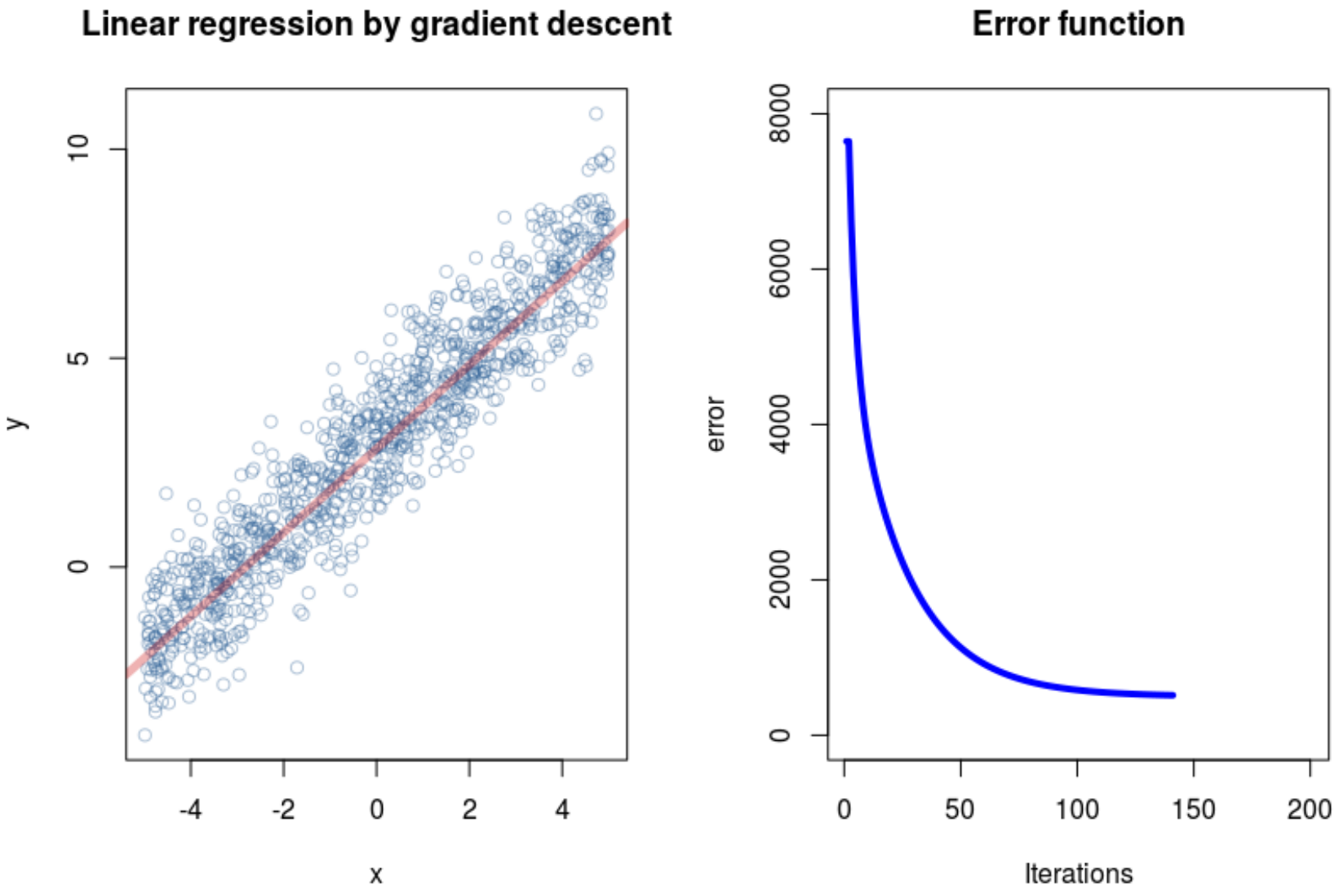




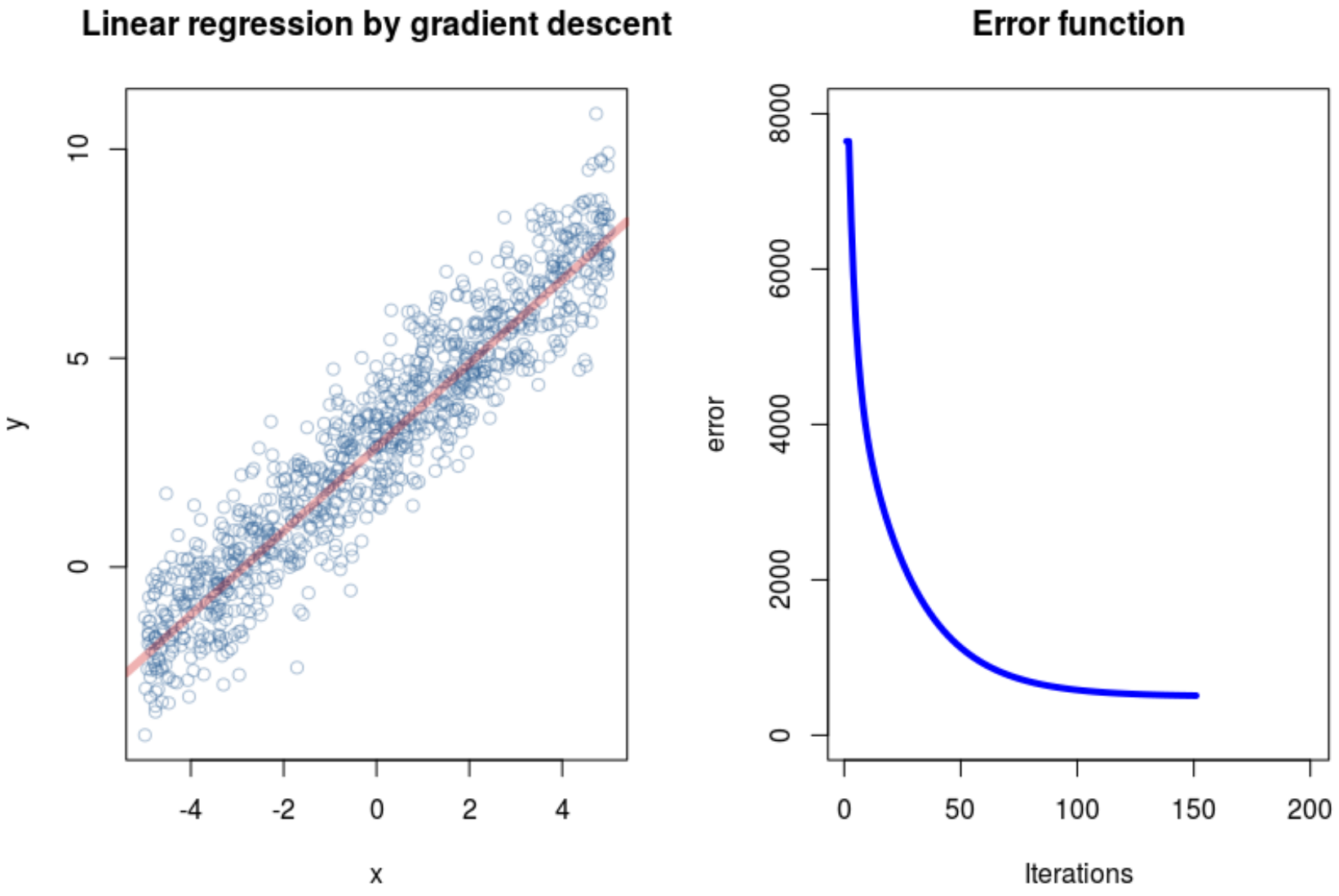
Linear regression - animation



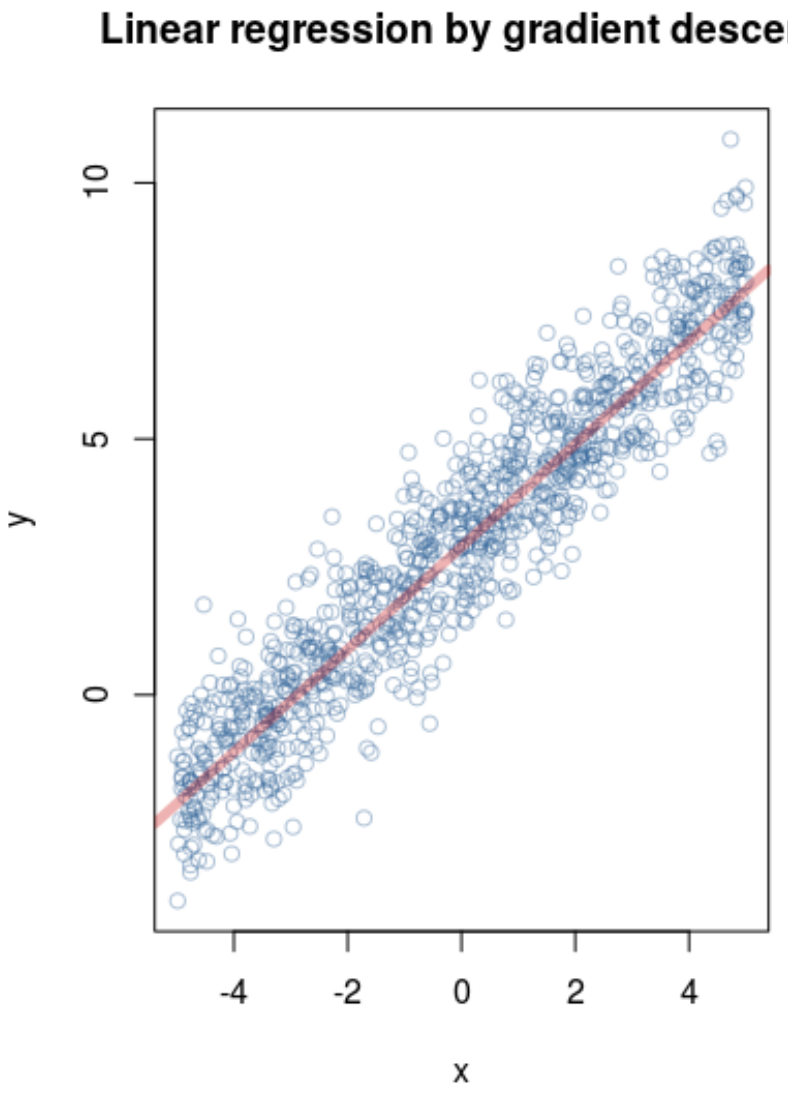
Linear regression - animation

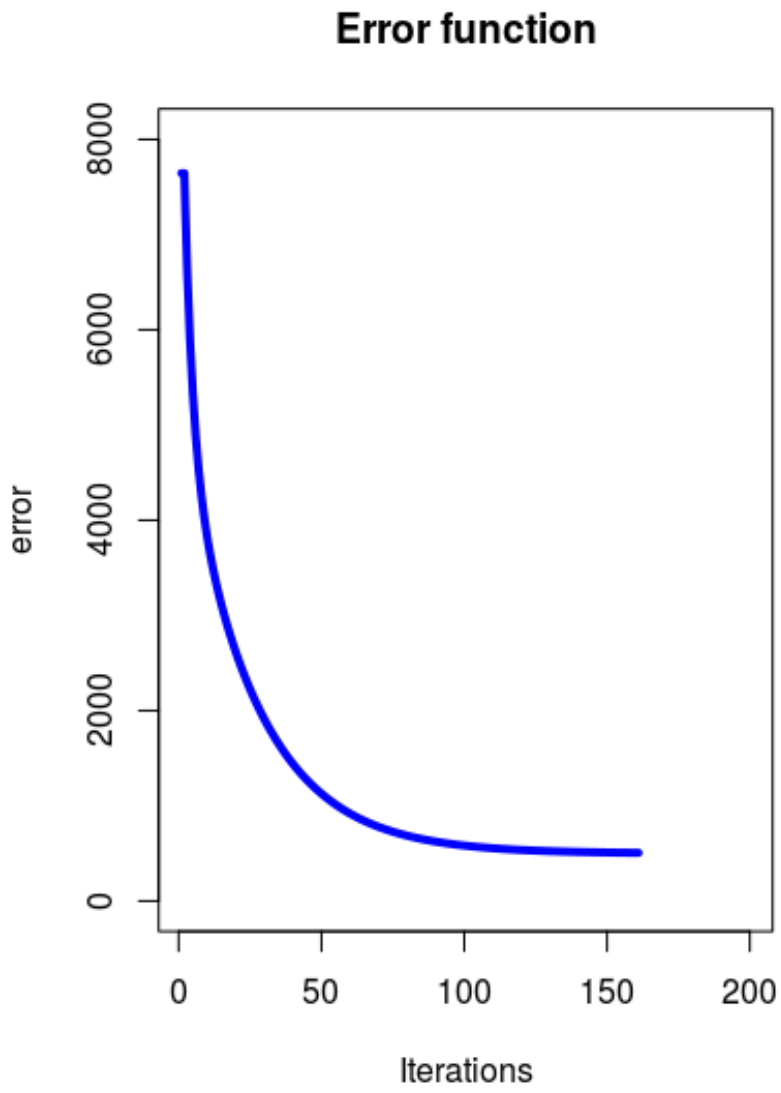


Linear regression - animation

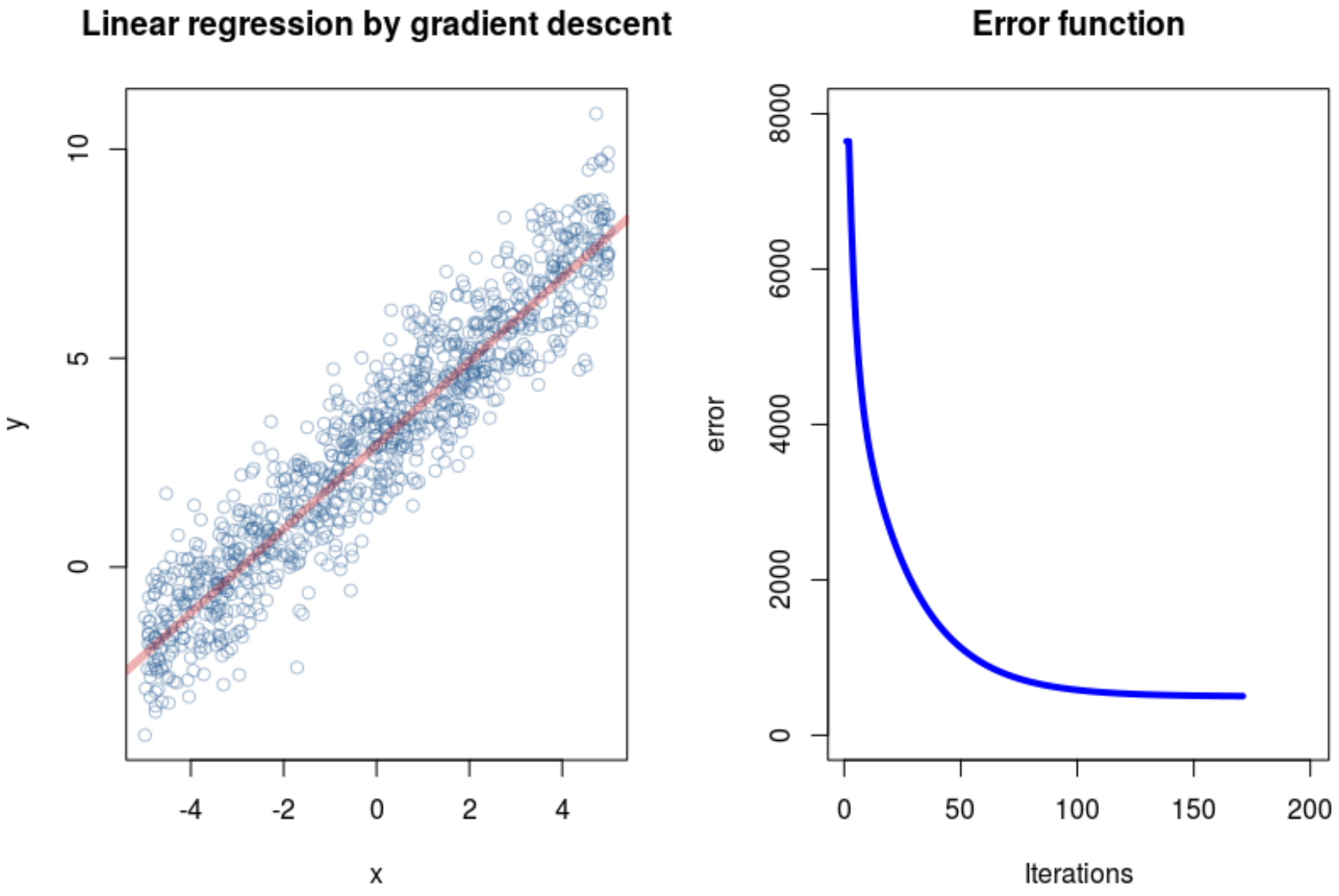


Linear regression - animation

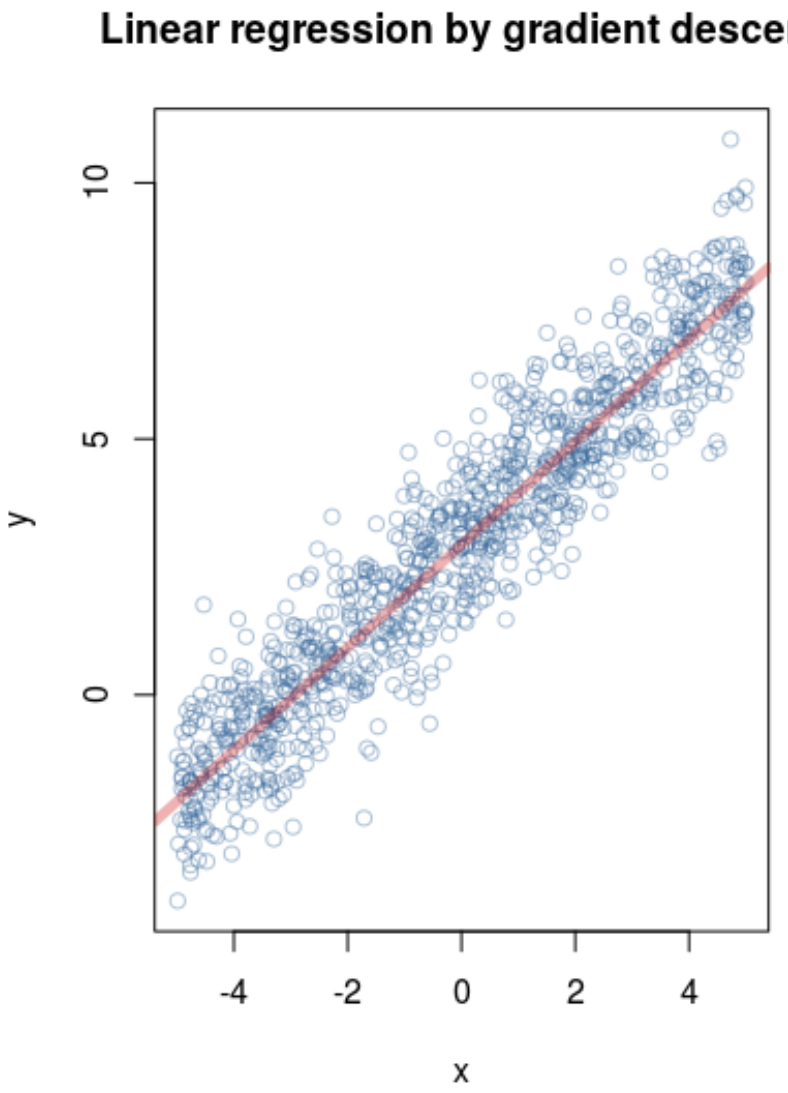


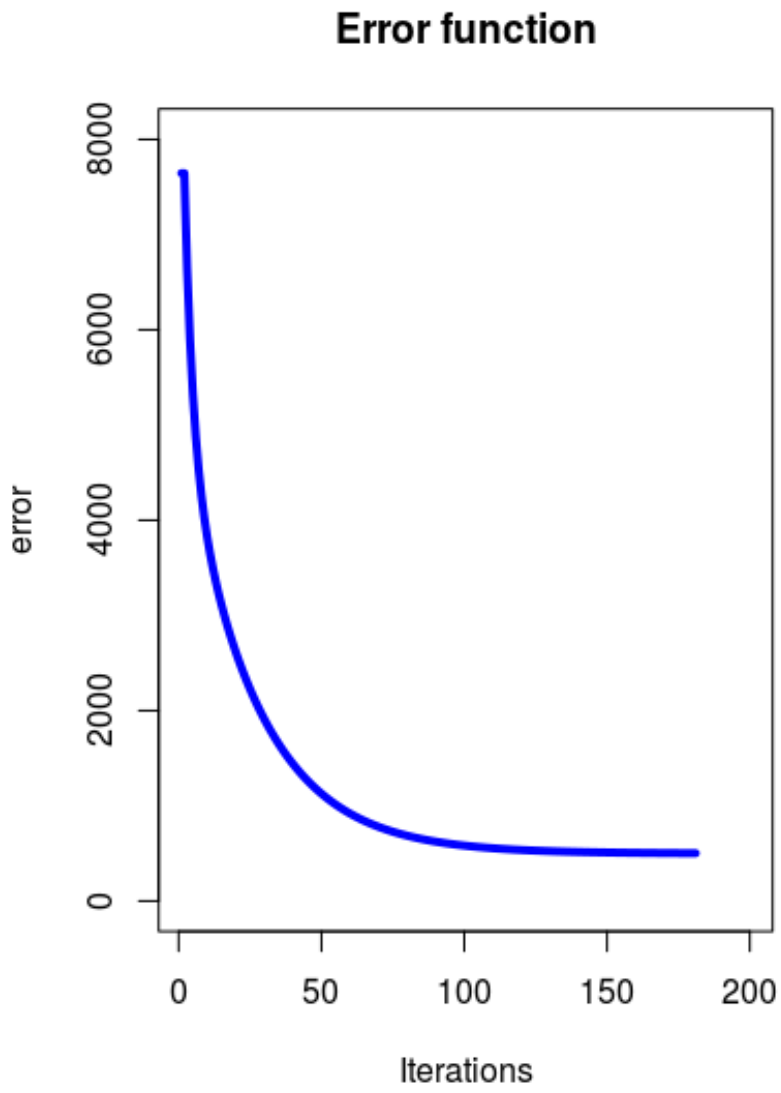


Linear regression - animation

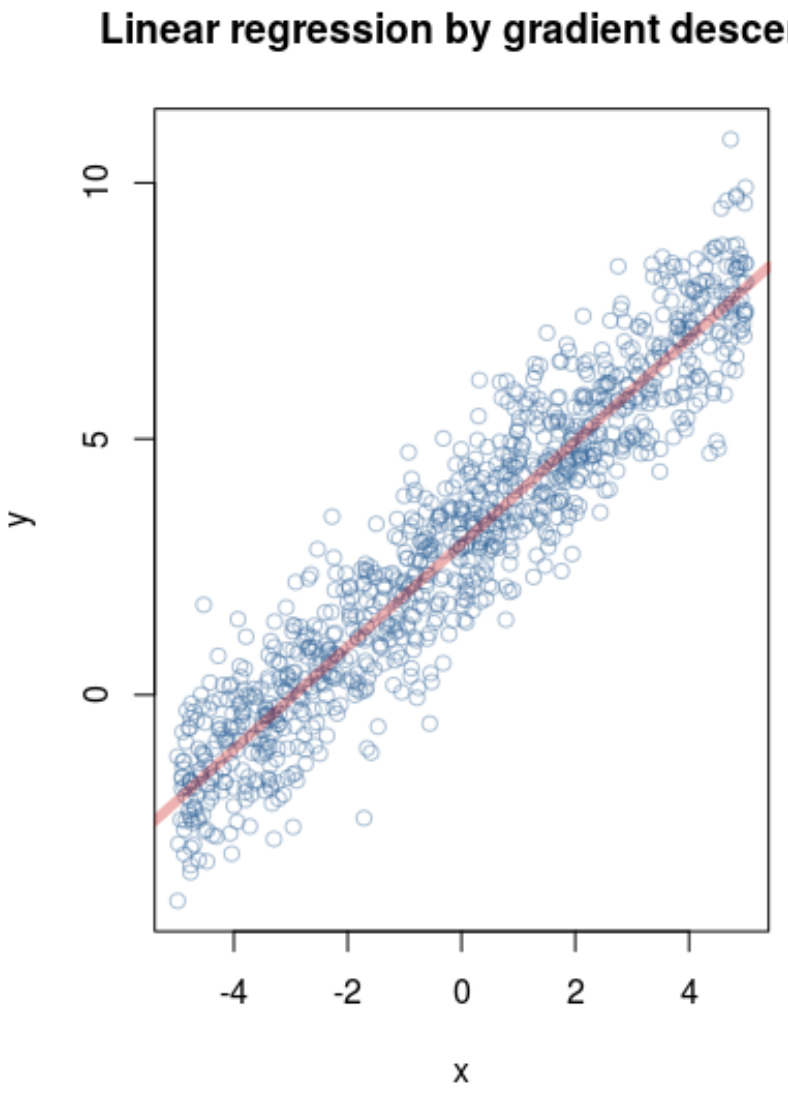


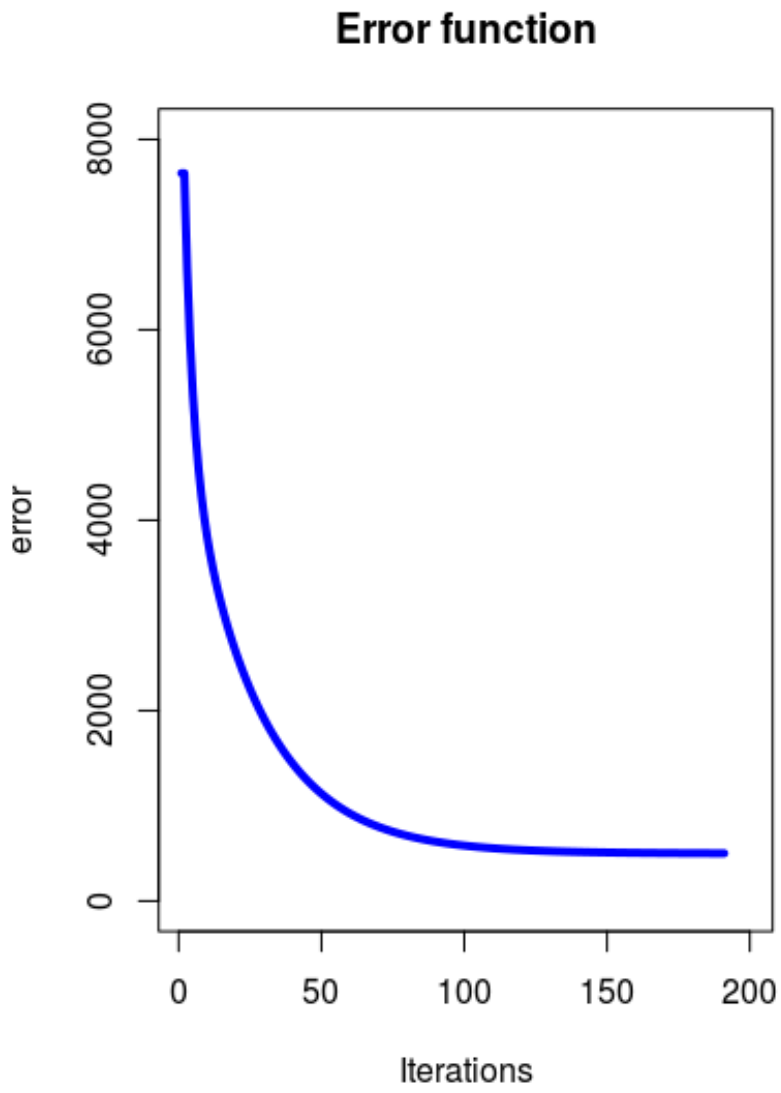
Linear regression - animation





Linear regression - animation





Linear regression - animation