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Learning by Michael Nielsen http://neuralnetworksanddeeplearning.com/ (Extremely well written online textbook (a little outdated))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("Classical" overview of the theory of neural networks (a little outdated))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

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.

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

Machine learning algorithms typically construct mathematical models of given data. The models may be subsequently applied to fresh data.

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There are many types of models:

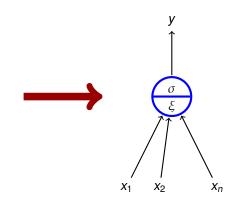
- decision trees
- support vector machines
- hidden Markov models
- Bayes networks and other graphical models
- neural networks
- • •

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/

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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Neural networks in machine learning.

 Typically primitive models, far from their biological counterparts (but often inspired by biology).

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Neural networks in machine learning.

- Typically primitive models, far from their biological counterparts (but often inspired by biology).
- Strongly oriented towards concrete application domains:
 - decision making and control autonomous vehicles, manufacturing processes, control of natural resources
 - games backgammon, poker, GO, Starcraft, ...
 - finance stock prices, risk analysis
 - medicine diagnosis, signal processing (EKG, EEG, ...), image processing (MRI, 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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 - 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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 - Simple applications of these models (image processing, a little bit of text processing)

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- Basic information about current implementations (TensorFlow-Keras, Pytorch)

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- ► Each neuron is connected with approx. 10⁴ neurons.
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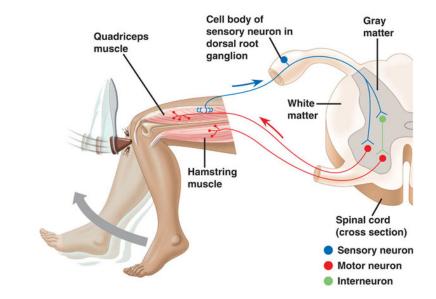
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- Afterwards, the output signal is transferred via PNS to effectors (e.g. muscle cells).

Biological neural network



Summation

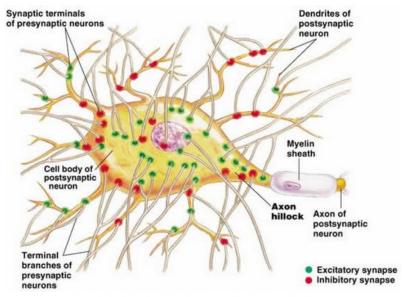
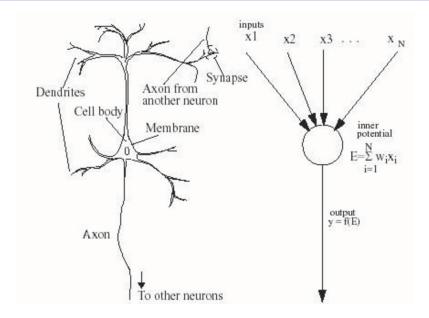
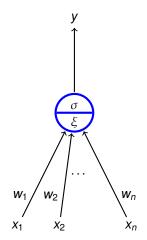
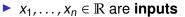


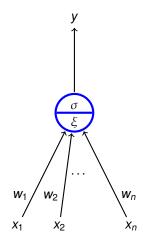
Figure 48.11(a), page 972, Campbell's Biology, 5th Edition

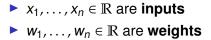
Biological and Mathematical neurons

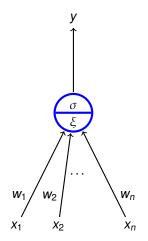




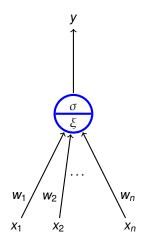








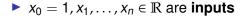
- $x_1, \ldots, x_n \in \mathbb{R}$ are inputs
- $w_1, \ldots, w_n \in \mathbb{R}$ are weights
- ξ is an inner potential; almost always ξ = Σⁿ_{i=1} w_ix_i

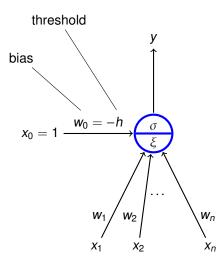


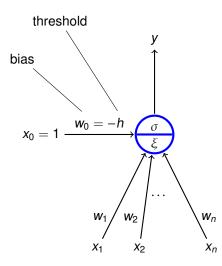
- $x_1, \ldots, x_n \in \mathbb{R}$ are inputs
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- ► ξ is an inner potential; almost always $\xi = \sum_{i=1}^{n} w_i x_i$
- y is an output given by y = σ(ξ)
 where σ is an activation function;
 e.g. a unit step function

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

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

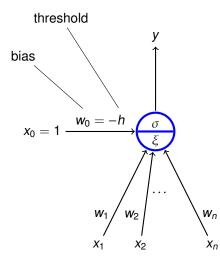




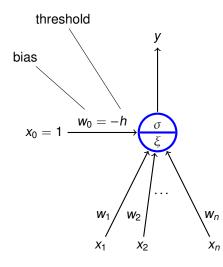


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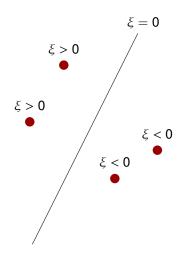


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(The threshold *h* has been substituted with the new input $x_0 = 1$ and the weight $w_0 = -h$.)



inner potential

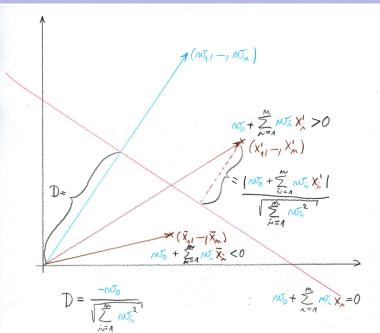
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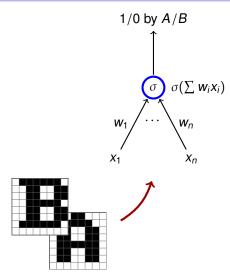
determines a separation hyperplane in the *n*-dimensional **input space**

- in 2d line
- in 3d plane

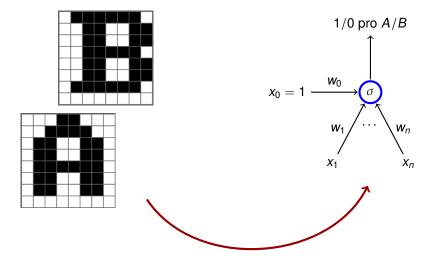
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Neuron geometry

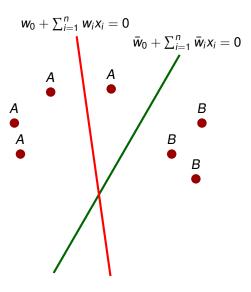




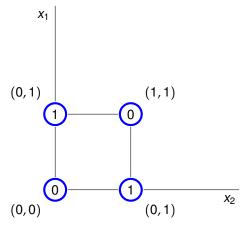
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- Red line classifies incorrectly
- Green line classifies correctly (may be a result of a correction by a learning algorithm)



No line separates ones from zeros.

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

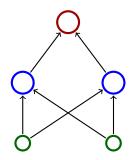
How the weights are changed during training.

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

We distinguish several categories of neurons:

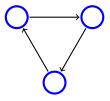
- Output neurons
- Hidden neurons
- Input neurons

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



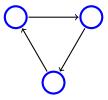
Architecture – Cycles

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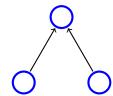


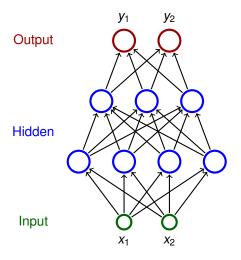
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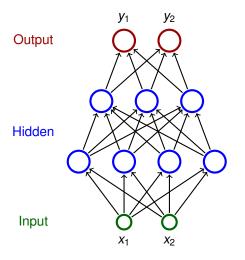


Otherwise it is acyclic (feed-forward)

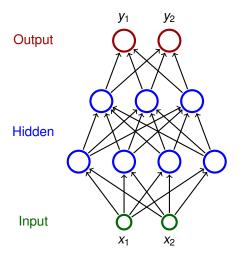




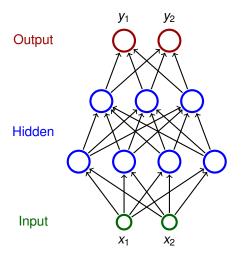
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- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

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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.

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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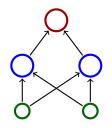
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Example 1

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



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We assume (unless otherwise specified) that

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

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

In order to specify activity of the network, we need to specify how the inner potentials ξ are computed and what are the activation functions σ .

We assume (unless otherwise specified) that

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

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

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.

There are many activation functions, typical examples:

Unit step function

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

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(Logistic) sigmoid

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

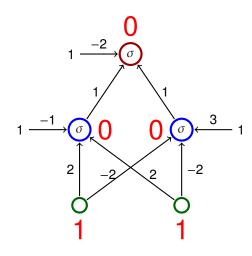
here $\lambda \in \mathbb{R}$ is a steepness parameter.

Hyperbolic tangens

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

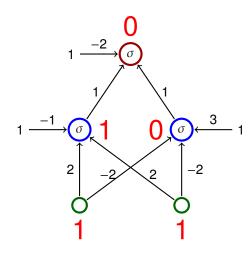
ReLU

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



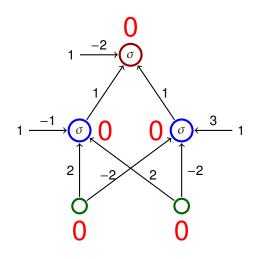
$$\sigma(\xi) = \begin{cases} 1 & \xi \ge 0; \\ 0 & \xi < 0. \end{cases}$$

$$\begin{array}{c|ccc} x_1 & x_2 & y \\ \hline 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{array}$$



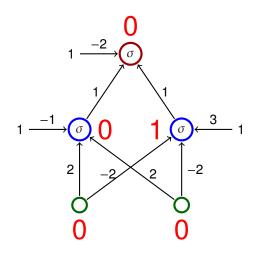
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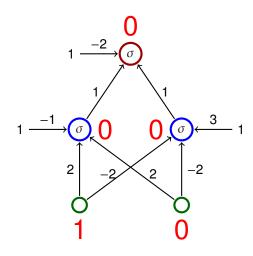
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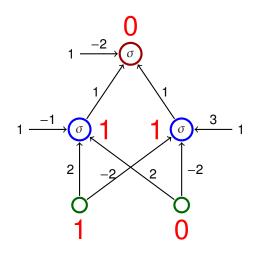
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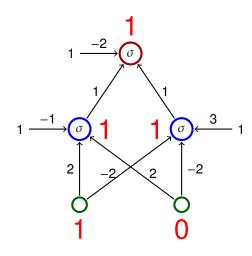
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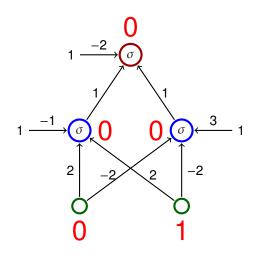
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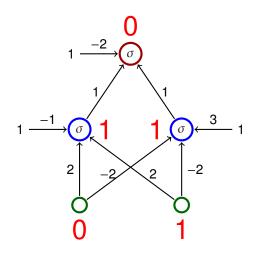
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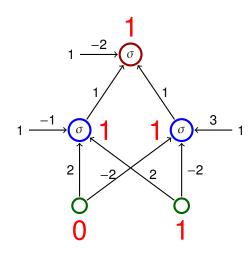
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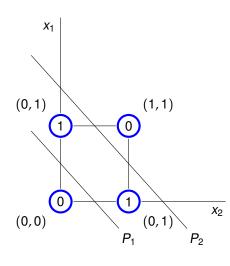
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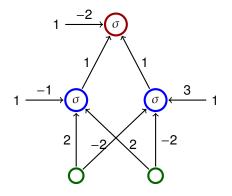


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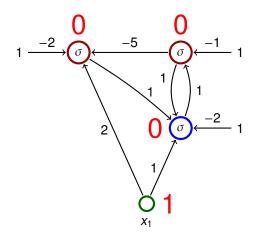
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Activity – MLP and linear separation



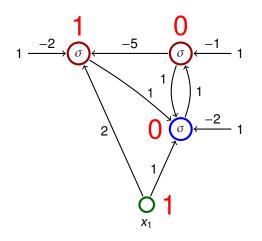


- The line P_1 is given by $-1 + 2x_1 + 2x_2 = 0$
- The line P_2 is given by $3-2x_1-2x_2=0$



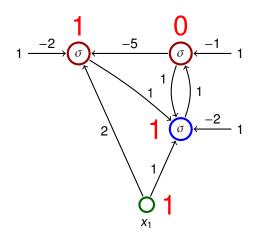
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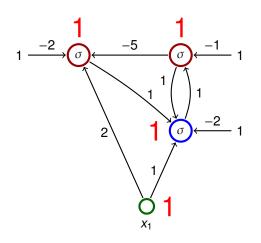
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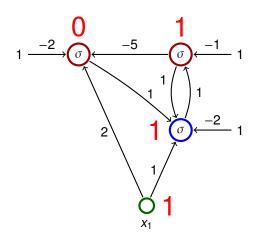
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initial configuration

weights can be initialized randomly or using some sophisticated algorithm

Learning rule for weight adaptation.

(the goal is to find a configuration in which the network computes a desired function)

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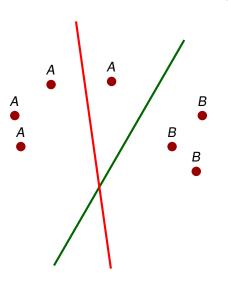
- Supervised learning
 - The desired function is described using *training examples* that are pairs of the form (input, output).
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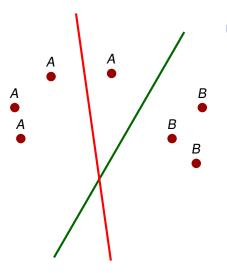
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- Unsupervised learning
 - The training set contains only inputs.
 - The goal is to determine distribution of the inputs (clustering, deep belief networks, etc.)

Supervised learning – illustration



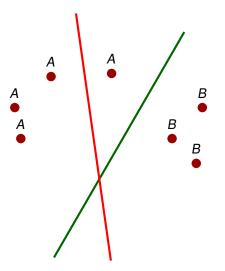
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- the algorithm considers examples one after another
- whenever an incorrectly classified point is considered, the learning algorithm turns the line in the direction of the point

Massive parallelism

neurons can be evaluated in parallel

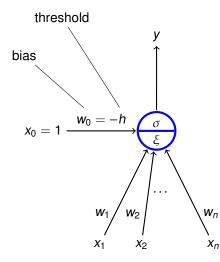
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- Graceful degradation
 - damage typically causes only a decrease in precision of results

Expressive power of neural networks

Formal neuron (with bias)



• $x_0 = 1, x_1, \dots, x_n \in \mathbb{R}$ are inputs

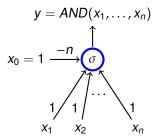
- $w_0, w_1, \ldots, w_n \in \mathbb{R}$ are weights
- ► ξ is an **inner potential**; almost always $\xi = w_0 + \sum_{i=1}^{n} w_i x_i$
- y is an output given by y = σ(ξ) where σ is an activation function;

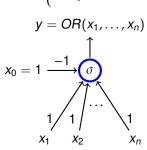
e.g. a unit step function

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

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

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$$y = NOT(x_1)$$

$$x_0 = 1 \xrightarrow[-1]{\sigma}$$

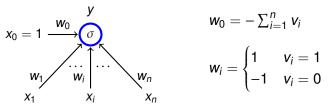
Theorem

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

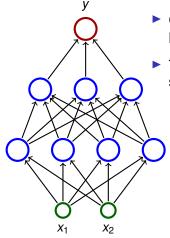
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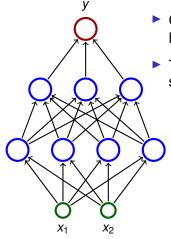
Proof.



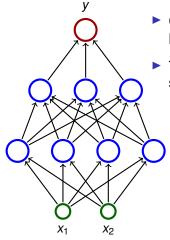
Now let us connect all outputs of all neurons $N_{\vec{v}}$ satisfying $F(\vec{v}) = 1$ using a neuron implementing *OR*.



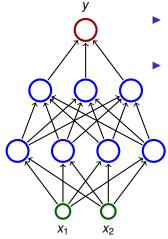
- Consider a three layer network; each neuron has the unit step activation function.
- The network divides the input space in two subspaces according to the output (0 or 1).



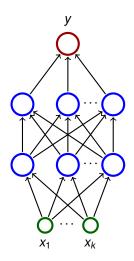
- Consider a three layer network; each neuron has the unit step activation function.
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 - The first (hidden) layer divides the input space into half-spaces.



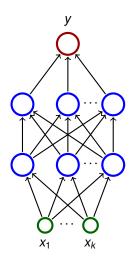
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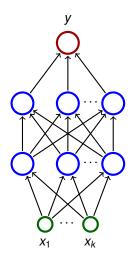
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 - The third layer may e.g. make unions of some convex sets.



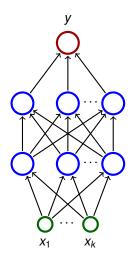
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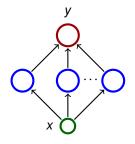


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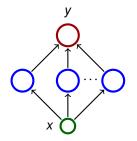
Power of ReLU



Consider a two layer network

- with a single input and single output;
- hidden neurons with the ReLU activation:
 σ(ξ) = max(ξ, 0);
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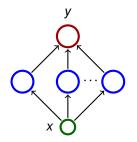


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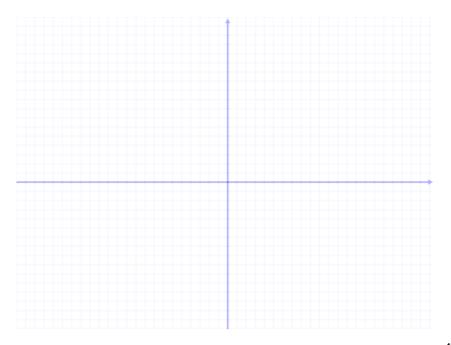
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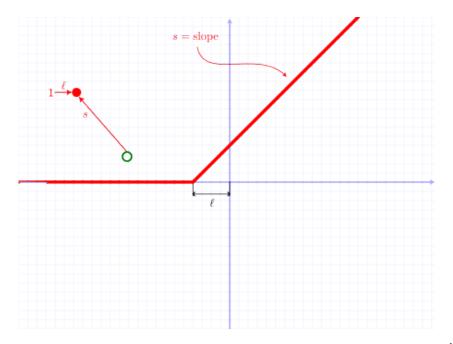
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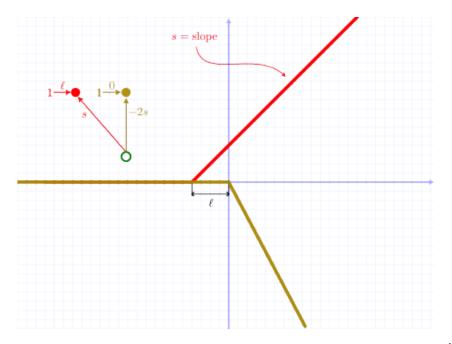
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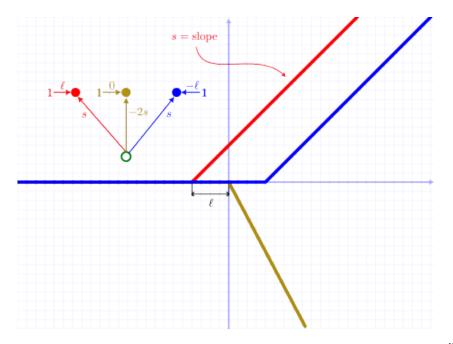
For every open subset $A \subseteq [0, 1]$ there is a network of the above type such that for "most" $x \in [0, 1]$ we have that $x \in A$ iff the network's output is > 0 for the input x.

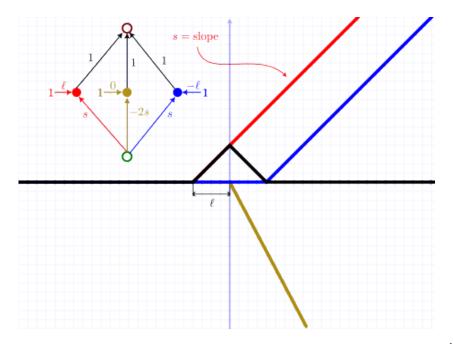
Just consider a continuous function f where f(x) is the minimum difference between x and a point on the boundary of A. Then uniformly approximate fusing the networks.

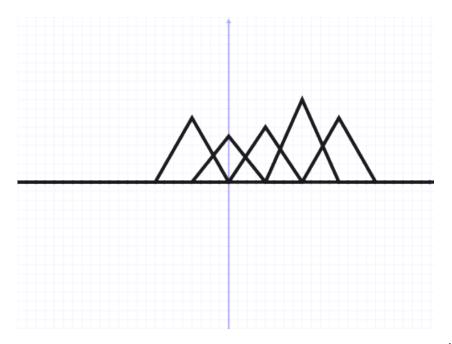


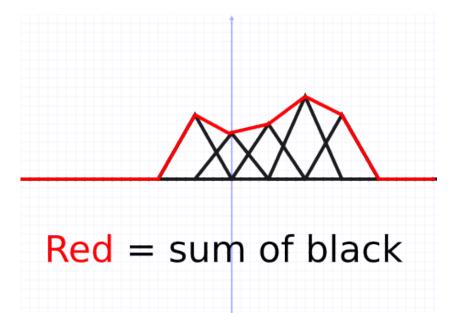












Theorem (Cybenko 1989 - informal version)

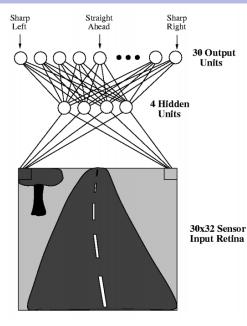
Let σ be a continuous function which is sigmoidal, i.e. satisfies

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

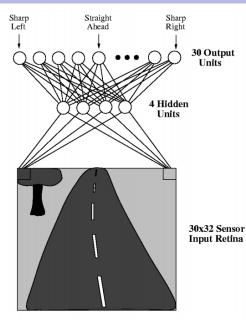
For every "reasonable" set $A \subseteq [0, 1]^n$, there is a **two layer network** where each hidden neuron has the activation function σ (output neurons are linear), that satisfies the following: For "most" vectors $\vec{v} \in [0, 1]^n$ we have that $\vec{v} \in A$ iff the network output is > 0 for the input \vec{v} .

For mathematically oriented:

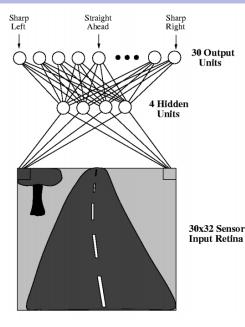
- "reasonable" means Lebesgue measurable
- "most" means that the set of incorrectly classified vectors has the Lebesgue measure smaller than a given ε > 0



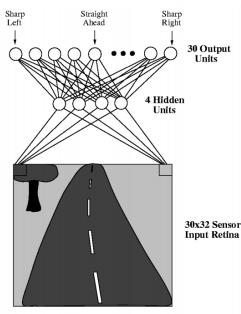
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- The net has 30×32 = 960 inputs (the input space is thus R⁹⁶⁰)
- Input values correspond to shades of gray of pixels.
- Output neurons "classify" images of the road based on their "curvature".

Image source: http://jmvidal.cse.sc.edu/talks/ann/alvin.html

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

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

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

- Consider recurrent networks (i.e., containing cycles)
 - with real weights (in general);
 - one input neuron and one output neuron (the network computes a function *F* : *A* → ℝ where *A* ⊆ ℝ contains all inputs on which the network stops);
 - parallel activity rule (output values of all neurons are recomputed in every step);
 - activation function

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

• 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).

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 - For every recursively enumerable language L ⊆ {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.

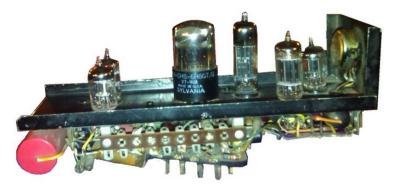
Summary of theoretical results

- Neural networks are very strong from the point of view of theory:
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 - 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	"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

- 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.)

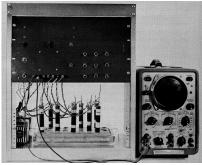


 1957: Mark I Perceptron (Rosenblatt et al) - the first successful network for image recognition



- 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

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.

- 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 ...

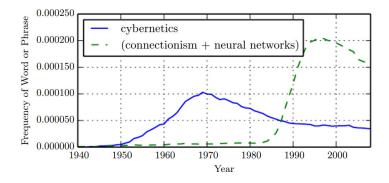
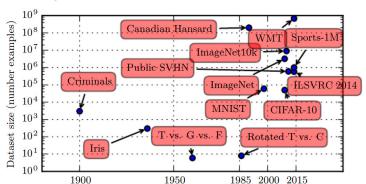


Figure: The figure shows two of the three historical waves of artificial neural nets research, as measured by the frequency of the phrases "cybernetics" and "connectionism" or "neural networks" according to Google Books (the third wave is too recent to appear).

Current hardware – What do we face?



Increasing dataset size ...

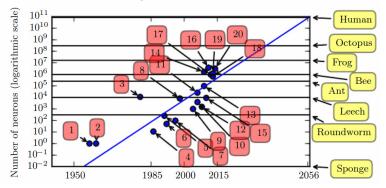
... weakly-supervised pre-training using hashtags from the Instagram uses $3.6 * 10^9$ images.

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

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

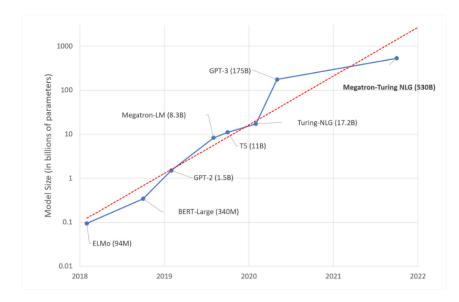
Current hardware – What do we face?

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



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 ...

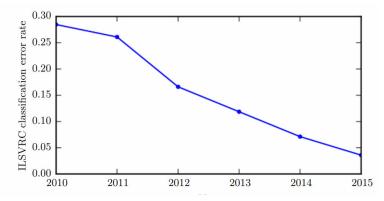


Figure: Since deep networks reached the scale necessary to compete in the ImageNetLarge Scale Visual Recognition Challenge, they have consistently won the competition every year, and yielded lower and lower error rates each time. Data from Russakovsky et al. (2014b) and He et al. (2015).

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.

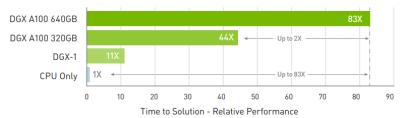


Current hardware – NVIDIA DGX Station

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



Up to 83X Higher Throughput than CPU, 2X Higher Throughput than DGX A100 320GB on Big Data Analytics Benchmark



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=sad,
              metrics=['accuracy'])
model.fit(X train, y train,
          n\overline{b} epoch=2\overline{0},
          batch size=16)
score = model.evaluate(X test, y test, batch size=16)
```

```
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 laver and three Dense lavers
model = Model(inputs=inputs, outputs=predictions)
model.compile(optimizer='rmsprop',
              loss='categorical_crossentropy',
              metrics=['accuracy'])
model.fit(data, labels) # starts training
```

Current software – TensorFlow

```
# tf Graph input
41
42
    X = tf.placeholder("float", [None, n_input])
    Y = tf.placeholder("float", [None, n classes])
    # Store layers weight & bias
    weights = {
         'h1': tf.Variable(tf.random_normal([n_input, n_hidden_1])),
47
         'h2': tf.Variable(tf.random normal([n hidden 1, n hidden 2])),
         'out': tf.Variable(tf.random_normal([n_hidden_2, n_classes]))
    3
    biases = {
         'b1': tf.Variable(tf.random normal([n hidden 1])),
         'b2': tf.Variable(tf.random_normal([n_hidden_2])),
         'out': tf.Variable(tf.random_normal([n_classes]))
    }
```

```
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

```
class Net(nn.Module):
         def __init__(self, input_size, hidden_size, num_classes):
             super(Net, self).__init__()
             self.fc1 = nn.Linear(input_size, hidden_size)
40
             self.relu = nn.ReLU()
             self.fc2 = nn.Linear(hidden_size, num_classes)
41
42
43
         def forward(self, x):
             out = self.fc1(x)
             out = self.relu(out)
             out = self.fc2(out)
             return out
47
    net = Net(input_size, hidden_size, num_classes)
```

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

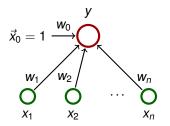
- MATLAB
- ► R
- STATISTICA
- Weka
- ► ...

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

Training linear models

Linear regression (ADALINE)

Architecture:



 $\vec{w} = (w_0, w_1, \dots, w_n)$ and $\vec{x} = (x_0, x_1, \dots, x_n)$ 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: $y[\vec{w}](\vec{x}) = \sigma(\xi) = \vec{w} \cdot \vec{x}$

Learning:

Given a training dataset

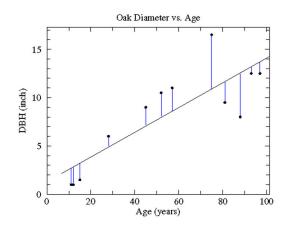
$$\mathcal{T} = \left\{ \left(\vec{x}_1, d_1 \right), \left(\vec{x}_2, d_2 \right), \dots, \left(\vec{x}_p, d_p \right) \right\}$$

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

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

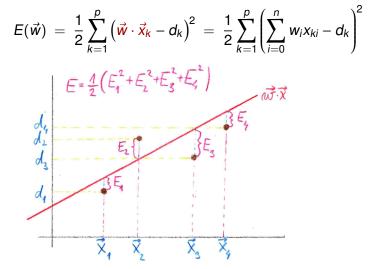
Oaks in Wisconsin

Age	DBH
(years)	(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



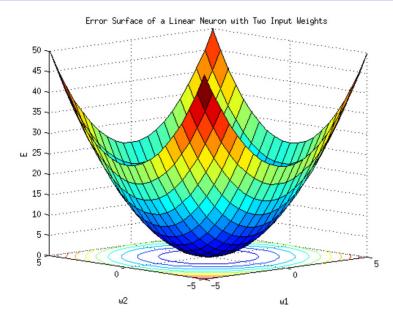
Linear regression (ADALINE)

Error function:



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

Error function



82

Consider gradient of the error function:

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

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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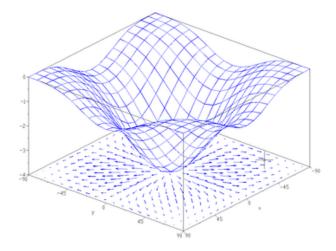
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Fact

If $\nabla E(\vec{w}) = \vec{0} = (0, \dots, 0)$, 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 $E(\vec{w})$!

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

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Thus

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

Batch algorithm (gradient descent):

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

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

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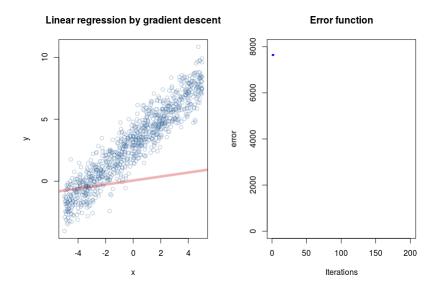
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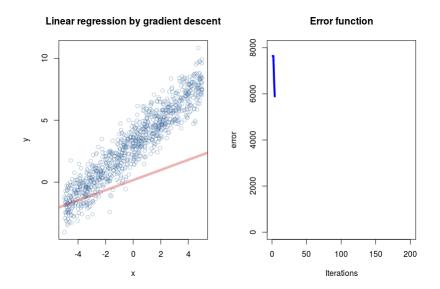
$$= W^{(1)} - \varepsilon \cdot \sum_{k=1}^{\infty} (W^{(1)} \cdot x_k - a_k) \cdot x_k$$

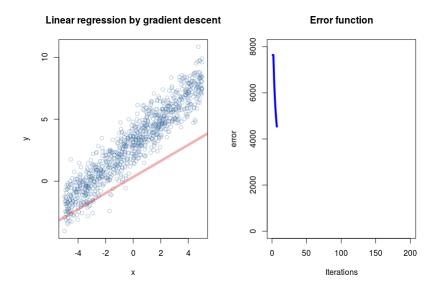
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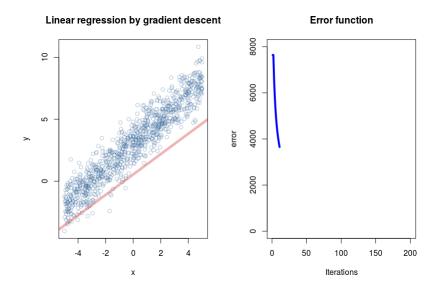
Proposition

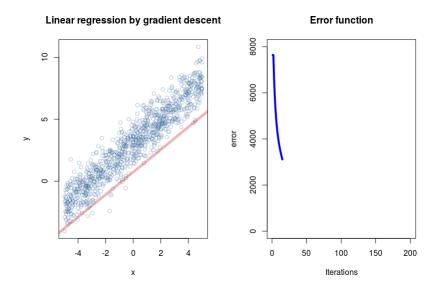
For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \dots$ converges (componentwise) to the global minimum of E (i.e. to the vector \vec{w} satisfying $\nabla E(\vec{w}) = \vec{0}$).

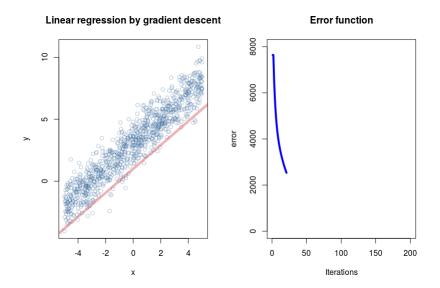


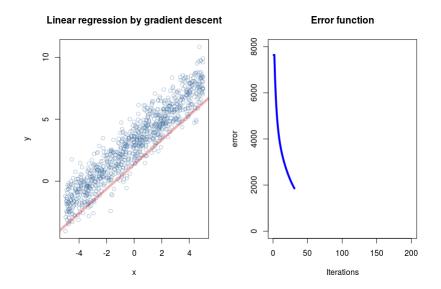


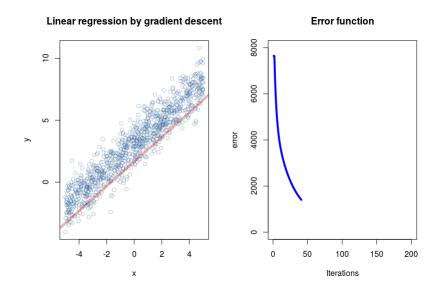


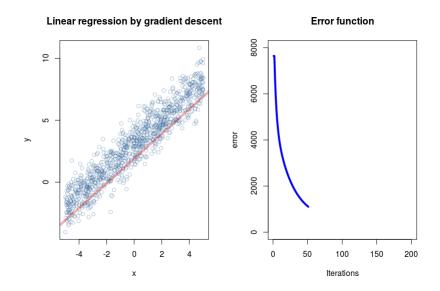


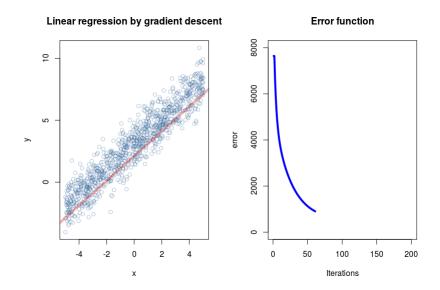


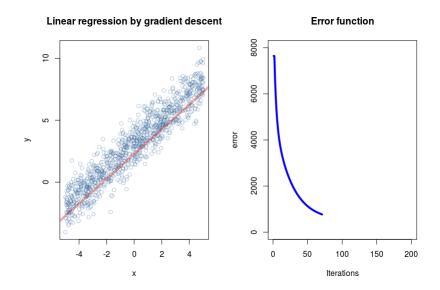


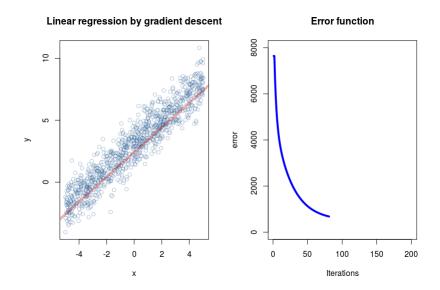


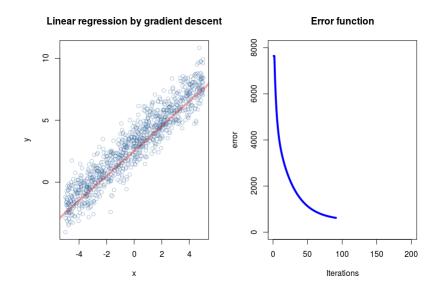


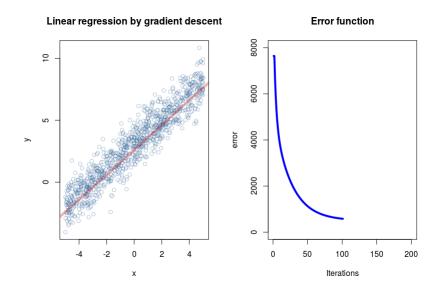


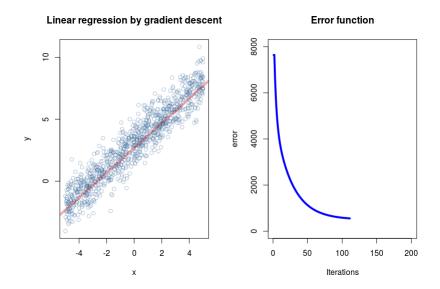


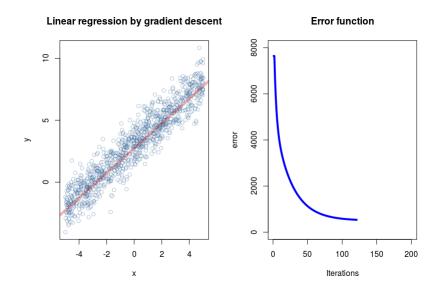


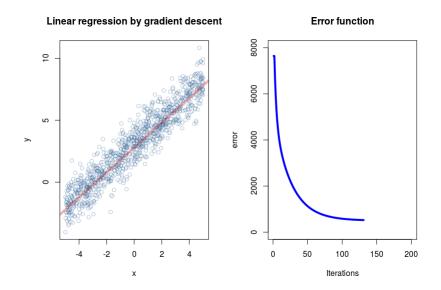


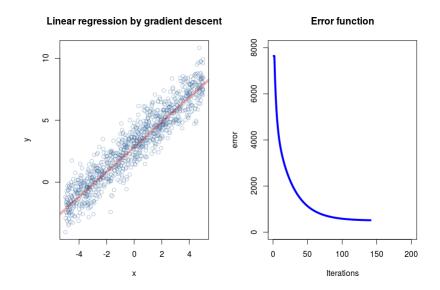


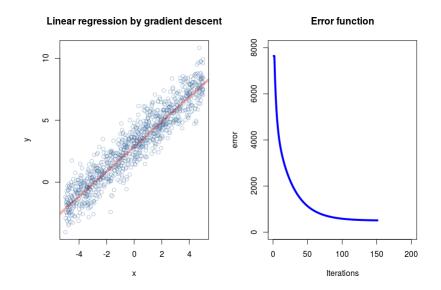


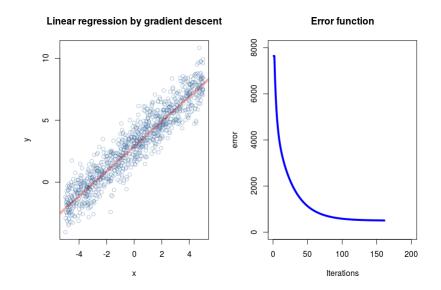


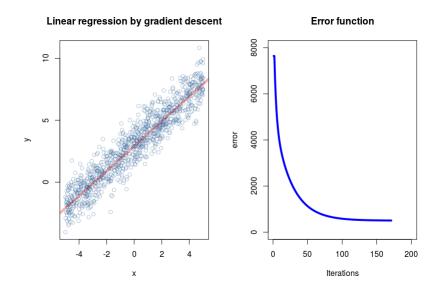


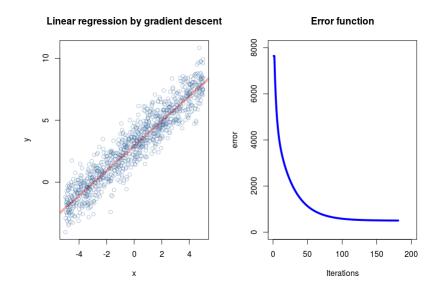


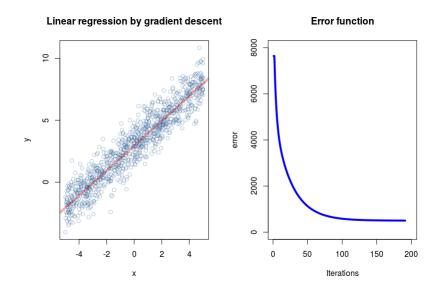


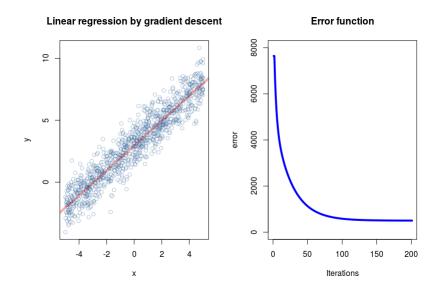






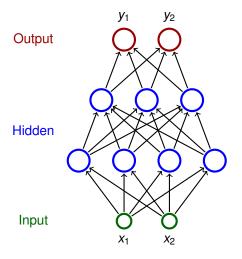






MLP training - theory

Architecture – Multilayer Perceptron (MLP)



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

Notation:

- Denote
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 - Y a set of *output* neurons
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inner potential of neuron j:

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The network computes a function R^{|X|} do 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 dataset \mathcal{T} of the form

$$\left\{ \left(\vec{x}_k, \vec{d}_k \right) \mid k = 1, \dots, p \right\}$$

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 $(d_{kj})_{i \in Y}$).

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Error function:

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

where

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

MLP – learning algorithm

Batch algorithm (gradient descent):

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

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
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is a weight update of w_{ji} in step t + 1 and $0 < \varepsilon(t) \le 1$ is a learning rate in step t + 1.

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

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

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

MLP – error function gradient (history)

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 for all $j \in Z$, then
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$$\mathcal{E}_{ji} := \mathcal{E}_{ji} + \frac{\partial E_k}{\partial w_{ji}}$$

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

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if j ∈ Z \ Y ∪ X, then assuming that j is in the ℓ-th layer and assuming that ∂E_k/∂y_r has already been computed for all neurons in the ℓ + 1-st layer, compute

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma'_r(\xi_r) \cdot \mathbf{w}_{rj}$$

(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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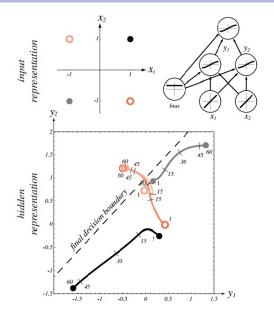
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The steps 1. - 3. take linear time.

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

Illustration of the gradient descent – XOR



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

MLP – learning algorithm

Online algorithm:

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

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

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

where

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

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

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

SGD

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

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

where

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

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

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

Regression:

• The output activation is typically the identity $y_i = \sigma(\xi_i) = \xi_i$.

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- A training dataset

$$\left\{ \left(\vec{x}_k, \vec{d}_k \right) \mid k = 1, \dots, p \right\}$$

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 $i \in Y$, denote by d_{ki} the desired output of the neuron *i* for a given network input \vec{x}_k (the vector \vec{d}_k can be written as $(d_{ki})_{i \in Y}$).

Regression:

- The output activation is typically the identity $y_i = \sigma(\xi_i) = \xi_i$.
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The error function mean squared error (mse):

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

where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{i \in Y} (y_i(\vec{w}, \vec{x}_k) - d_{ki})^2$$

Classification

The output activation function softmax:

$$\mathbf{y}_i = \sigma_i(\xi_i) = \frac{\mathbf{e}^{\xi_i}}{\sum_{j \in \mathbf{Y}} \mathbf{e}^{\xi_j}}$$

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► The error function (categorical) cross entropy:

$$E(\vec{w}) = -\frac{1}{p} \sum_{k=1}^{p} \sum_{i \in Y} d_{ki} \log(y_i(\vec{w}, \vec{x}_k))$$

Gradient with Softmax & Cross-Entropy

Assume that *V* is the layer just below the output layer *Y*.

$$\begin{split} E(\vec{w}) &= -\frac{1}{\rho} \sum_{k=1}^{\rho} \sum_{i \in Y} d_{ki} \log(y_i(\vec{w}, \vec{x}_k)) \\ &= -\frac{1}{\rho} \sum_{k=1}^{\rho} \sum_{i \in Y} d_{ki} \log\left(\frac{e^{\xi_i}}{\sum_{j \in Y} e^{\xi_j}}\right) \\ &= -\frac{1}{\rho} \sum_{k=1}^{\rho} \sum_{i \in Y} d_{ki} \left(\xi_i - \log\left(\sum_{j \in Y} e^{\xi_j}\right)\right) \\ &= -\frac{1}{\rho} \sum_{k=1}^{\rho} \sum_{i \in Y} d_{ki} \left(\sum_{\ell \in V} w_{i\ell} y_\ell - \log\left(\sum_{j \in Y} e^{\sum_{\ell \in V} w_{j\ell} y_\ell}\right)\right) \end{split}$$

Now compute the derivatives $\frac{\delta E}{\delta \gamma_{\ell}}$ for $\ell \in V$.

Binary classification

Assume a single output neuron $o \in Y = \{o\}$.

The output activation function logistic sigmoid:

$$\sigma_o(\xi_o) = \frac{e^{\xi_o}}{e^{\xi_o} + 1} = \frac{1}{1 + e^{-\xi_o}}$$

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The error function (Binary) cross-entropy:

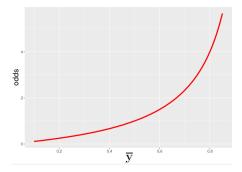
$$E(\vec{w}) = \sum_{k=1}^{p} -(d_k \log(y_o(\vec{w}, \vec{x}_k)) + (1 - d_k) \log(1 - y_o(\vec{w}, \vec{x}_k)))$$

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

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

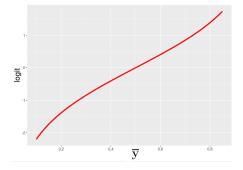


... stretches from 0 to ∞

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Let \bar{y} be the "true" probability of the class 1 to be modeled. What about log odds (aka logit) of the class 1?

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



... stretches from $-\infty$ to ∞

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

 $\log(\bar{y}/(1-\bar{y})) = \xi_o$

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and

$$\bar{y} = \frac{1}{1 + e^{-\xi_o}}$$

That is, modeling the probability using the *classification model* (with the logistic output activation) corresponds to modeling log-odds using the *regression model* (with the identity output activation).

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• What is the best model y of \overline{y} based on the data? **Answer:** The one that generates the data with maximum probability!

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

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

But then

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

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

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The likelihood:

$$L(\vec{w}) = \prod_{k=1}^{p} \left(y_o(\vec{w}, \vec{x}_k) \right)^{d_k} \cdot \left(1 - y_o(\vec{w}, \vec{x}_k) \right)^{(1-d_k)}$$

 $\log(L) = \sum_{k=1}^{p} \left(d_k \cdot \log(y_o(\vec{w}, \vec{x}_k)) + (1 - d_k) \cdot \log(1 - y_o(\vec{w}, \vec{x}_k)) \right)$ and thus $-\log(L) =$ the cross-entropy.

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

Consider a single neuron model $y = \sigma(w \cdot x) = 1/(1 + e^{-w \cdot x})$ where $w \in \mathbb{R}$ is the weight (ignore the bias).

A training dataset $\mathcal{T} = \{(x, d)\}$ where $x \in \mathbb{R}$ and $d \in \{0, 1\}$.

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Squared error $E(w) = \frac{1}{2}(y - d)^2$.

$$\frac{\delta E}{\delta w} = (y - d) \cdot y \cdot (1 - y) \cdot x$$

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Thus

The gradient of E is small even though the model is wrong!

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Cross-entropy error $E(w) = -d \cdot \log(y) - (1 - d) \cdot \log(1 - y)$. For d = 1 $\frac{\delta E}{\delta w} = -\frac{1}{v} \cdot y \cdot (1 - y) \cdot x = -(1 - y) \cdot x$

which is close to -x for $y \approx 0$.

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$$d = 0$$

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which is close to *x* for $y \approx 1$.