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by Michael Nielsen http://neuralnetworksanddeeplearning.com/ (Extremely well written online textbook (a little outdated))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("Classical" overview of the theory of neural networks (a little outdated))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

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- Project (Dr. Tomáš Foltýnek)
- implementation of a selected model + analysis of given data
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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

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- 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 unusual exam system! You can repeat the oral exam as many times as needed (only the best grade goes into IS).
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


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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.



## Why artificial neural networks?

Modelling of biological neural networks (computational neuroscience).

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- ...


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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.
- You should learn
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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.
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- Afterwards, the output signal is transfered 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



## Formal neuron (without bias)



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\sigma(\xi)= \begin{cases}1 & \xi \geq h \\ 0 & \xi<h .\end{cases}
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where $h \in \mathbb{R}$ is a threshold.

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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


## Neuron and linear separation


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

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## Neuron and linear separation

$$
w_{0}+\sum_{i=1}^{n} w_{i} x_{i}=0
$$

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

- Otherwise it is acyclic (feed-forward)



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

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## Example 1

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


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here $\vec{x}=\left(x_{1}, \ldots, x_{n}\right)$ are inputs of the neuron and $\vec{w}=\left(w_{1}, \ldots, w_{n}\right)$ 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:

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

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

## Activity - inner potential and activation functions

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- (Logistic) sigmoid

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

- Hyperbolic tangens

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

$$
\sigma(\xi)=\max (\xi, 0)
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## Activity - XOR

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- The network computes $X O R\left(x_{1}, x_{2}\right)$

| $x_{1}$ | $x_{2}$ | $y$ |
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- The network computes $X O R\left(x_{1}, x_{2}\right)$

| $x_{1}$ | $x_{2}$ | $y$ |
| :---: | :---: | :---: |
| 1 | 1 | 0 |
| 1 | 0 | 1 |
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## Activity - MLP and linear separation



- The line $P_{1}$ is given by

$$
-1+2 x_{1}+2 x_{2}=0
$$

- The line $P_{2}$ is given by $3-2 x_{1}-2 x_{2}=0$


## Activity - example

The activation function is the unit step function

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


## Learning algorithms

Learning rule for weight adaptation.
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- Supervised learning
- The desired function is described using training examples that are pairs of the form (input, output).
- Learning algorithm searches for a configuration which "corresponds" to the training examples, typically by minimizing an error function.
- 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



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## Supervised learning - illustration

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- 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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- many sophisticated learning algorithms used to "program" neural networks
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- information is encoded in a distributed manner in weights
- "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
- $\xi$ is an inner potential; almost always $\xi=w_{0}+\sum_{i=1}^{n} w_{i} x_{i}$
- y is an output given by $\mathrm{y}=\sigma(\xi)$ where $\sigma$ is an activation function;
e.g. a unit step function

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

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

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

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## Proof.

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


$$
\begin{aligned}
& w_{0}=-\sum_{i=1}^{n} v_{i} \\
& w_{i}=\left\{\begin{array}{cc}
1 & v_{i}=1 \\
-1 & v_{i}=0
\end{array}\right.
\end{aligned}
$$

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


## Non-linear separation



- 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 ).


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


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- Each hypercube $K$ can be separated using a two layer network $N_{K}$ (i.e. a function computed by $N_{K}$ gives 1 for points in $K$ and 0 for the rest).


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- Each hypercube $K$ can be separated using a two layer network $N_{K}$ (i.e. a function computed by $N_{K}$ gives 1 for points in $K$ and 0 for the rest).
- Finally, connect outputs of the nets $N_{K}$ satisfying $K \cap A \neq \emptyset$ using a neuron implementing $O R$.


## Power of ReLU



Consider a two layer network

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


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For every continuous function $f:[0,1] \rightarrow[0,1]$ and $\varepsilon>0$ there is a network of the above type computing a function $F:[0,1] \rightarrow \mathbb{R}$ such that $|f(x)-F(x)| \leq \varepsilon$ for all $x \in[0,1]$.

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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.





$\qquad$


## Non-linear separation - sigmoid

## Theorem (Cybenko 1989 - informal version)

Let $\sigma$ be a continuous function which is sigmoidal, i.e. satisfies

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

For every "reasonable" set $A \subseteq[0,1]^{n}$, there is a two layer network where each hidden neuron has the activation function $\sigma$ (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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- ALVINN drives a car
- The net has $30 \times 32=960$ inputs (the input space is thus $\mathbb{R}^{960}$ )


## Non-linear separation - practical illustration



- ALVINN drives a car
- The net has $30 \times 32=960$ inputs (the input space is thus $\mathbb{R}^{960}$ )
- Input values correspond to shades of gray of pixels.


## Non-linear separation - practical illustration



## Function approximation - two-layer networks

## Theorem (Cybenko 1989)

Let $\sigma$ 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 $\sigma$ (output neurons are linear), that satisfies the following

$$
|f(\vec{v})-F(\vec{v})|<\varepsilon \quad \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 $F: A \rightarrow \mathbb{R}(A \subseteq \mathbb{R})$ such that

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\omega \in L \text { iff } \delta(\omega) \in A \text { and } F(\delta(\omega))>0
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- Recurrent networks with rational weights are equivalent to Turing machines
- For every recursively enumerable language $L \subseteq\{0,1\}^{+}$ there is a recurrent network with rational weights and less than 1000 neurons, which recognizes $L$.
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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.
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- 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 <br> \& damage | changing one bit may <br> completely crash the <br> computation |
| Precision | imprecise, network recalls a <br> training example "similar" to <br> 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 $20 \times 20$ 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

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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 shapt
# here, 20-dimensional vectors.
model.add(Dense(64, input_dim=20, init='uniform'))
model.add(Activation('tan\overline{h'))}
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,
    n\overline{b}_epoch=2\overline{0},
    ba\overline{tch size=16)}
score = model.e\overline{valuate(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

```
# tf Graph input
X = tf.placeholder("float", [None, n_input])
Y = tf.placeholder("float", [None, n_classes])
# Store layers weight & bias
weights = {
    'h1': tf.Variable(tf.random_normal([n_input, n_hidden_1])),
    'h2': tf.Variable(tf.random_normal([n_hidden_1, n_hidden_2])),
    'out': tf.Variable(tf.random_normal([n_hidden_2, n_classes]))
}
biases = {
    'b1': tf.Variable(tf.random_normal([n_hidden_1])),
    'b2': tf.Variable(tf.random_normal([n_hidden_2])),
    'out': tf.Variable(tf.random_normal([n_classes]))
}
```


## Current software - TensorFlow

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


## Current software - PyTorch

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


## Other software implementations

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

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

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

## Training linear models

## Linear regression (ADALINE)

## Architecture:


$\vec{w}=\left(w_{0}, w_{1}, \ldots, w_{n}\right)$ and $\vec{x}=\left(x_{0}, x_{1}, \ldots, x_{n}\right)$ 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 $\vec{x}_{k}=\left(x_{k 0}, x_{k 1} \ldots, x_{k n}\right) \in \mathbb{R}^{n+1}, x_{k 0}=1$, 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 <br> (years) | DBH <br> (inch) |
| ---: | ---: | ---: |
| 97 | 12.5 |
| 93 | 12.5 |
| 88 | 8.0 |
| 21 | 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:

$$
E(\vec{w})=\frac{1}{2} \sum_{k=1}^{p}\left(\vec{w} \cdot \vec{x}_{k}-d_{k}\right)^{2}=\frac{1}{2} \sum_{k=1}^{p}\left(\sum_{i=0}^{n} w_{i} x_{k i}-d_{k}\right)^{2}
$$



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


## Error function

Error Surface of a Linear Neuron with Two Input Weights


## 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 $\nabla E(\vec{w})=\overrightarrow{0}=(0, \ldots, 0)$, 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

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

## Gradient of the error function

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

Thus

$$
\nabla E(\vec{w})=\left(\frac{\partial E}{\partial w_{0}}(\vec{w}), \ldots, \frac{\partial E}{\partial w_{n}}(\vec{w})\right)=\sum_{k=1}^{p}\left(\vec{w} \cdot \vec{x}_{k}-d_{k}\right) \vec{x}_{k}
$$

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

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Here $k=(t \bmod p)+1$ 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 $\nabla E(\vec{w})=\overrightarrow{0})$.

## Linear regression - animation

Linear regression by gradient descent
Error function


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## MLP training - theory

## Architecture - Multilayer Perceptron (MLP)



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


## MLP - architecture

## Notation:

- Denote
- $X$ a set of input neurons
- Y a set of output neurons
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- $w_{j i}$ is the weight of the connection from $i$ to $j$
(in particular, $w_{j 0}$ is the weight of the connection from the formal unit input, i.e. $w_{j 0}=-b_{j}$ where $b_{j}$ is the bias of the neuron $j$ )


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(i.e. there is an arc from $j$ to $i$ )


## MLP - activity

## Activity:

- inner potential of neuron $j$ :

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

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


## MLP - learning

## Learning:

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

$$
\left\{\left(\vec{x}_{k}, \vec{d}_{k}\right) \quad \mid \quad k=1, \ldots, p\right\}
$$

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

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- Error function:

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

where

$$
E_{k}(\vec{w})=\frac{1}{2} \sum_{j \in Y}\left(y_{j}\left(\vec{w}, \vec{x}_{k}\right)-d_{k j}\right)^{2}
$$

## MLP - learning algorithm

## Batch algorithm (gradient descent):

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

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
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\Delta w_{j i}^{(t)}=-\varepsilon(t) \cdot \frac{\partial E}{\partial w_{j i}}\left(\vec{w}^{(t)}\right)
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is a weight update of $w_{j i}$ in step $t+1$ and $0<\varepsilon(t) \leq 1$ is a learning rate in step $t+1$.

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

## MLP - error function gradient

For every $w_{j i}$ we have

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\frac{\partial E}{\partial w_{j i}}=\sum_{k=1}^{p} \frac{\partial E_{k}}{\partial w_{j i}}
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where for every $k=1, \ldots, p$ holds

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\frac{\partial E_{k}}{\partial w_{j i}}=\frac{\partial E_{k}}{\partial y_{j}} \cdot \sigma_{j}^{\prime}\left(\xi_{j}\right) \cdot y_{i}
$$

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

$$
\frac{\partial E_{k}}{\partial y_{j}}=y_{j}-d_{k j}
$$

$$
\text { for } j \in Y
$$

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$$

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

$$
\begin{array}{ll}
\frac{\partial E_{k}}{\partial y_{j}}=y_{j}-d_{k j} & \text { for } j \in Y \\
\frac{\partial E_{k}}{\partial y_{j}}=\sum_{r \in j \rightarrow} \frac{\partial E_{k}}{\partial y_{r}} \cdot \sigma_{r}^{\prime}\left(\xi_{r}\right) \cdot w_{r j} & \text { for } j \in Z \backslash(Y \cup X)
\end{array}
$$

(Here all $y_{j}$ are in fact $\left.y_{j}\left(\vec{w}, \vec{x}_{k}\right)\right)$.

## MLP - error function gradient (history)

- If $y_{j}=\sigma_{j}\left(\xi_{j}\right)=\frac{1}{1+e^{-\varepsilon_{j}}}$ for all $j \in Z$, then

$$
\sigma_{j}^{\prime}\left(\xi_{j}\right)=y_{j}\left(1-y_{j}\right)
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$$

and thus for all $j \in Z \backslash X$ :

$$
\begin{array}{ll}
\frac{\partial E_{k}}{\partial y_{j}}=y_{j}-d_{k j} & \text { for } j \in Y \\
\frac{\partial E_{k}}{\partial y_{j}}=\sum_{r \in j \rightarrow} \frac{\partial E_{k}}{\partial y_{r}} \cdot y_{r}\left(1-y_{r}\right) \cdot w_{r j} & \text { for } j \in Z \backslash(Y \cup X)
\end{array}
$$

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$$
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4. $\mathcal{E}_{j i}:=\mathcal{E}_{j i}+\frac{\partial E_{k}}{\partial w_{j i}}$

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

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- if $j \in Y$, then $\frac{\partial E_{k}}{\partial y_{j}}=y_{j}-d_{k j}$
- if $j \in Z \backslash Y \cup X$, then assuming that $j$ is in the $\ell$-th layer and assuming that $\frac{\partial E_{k}}{\partial y_{t}}$ has already been computed for all neurons in the $\ell+1$-st layer, compute

$$
\frac{\partial E_{k}}{\partial y_{j}}=\sum_{r \in j} \frac{\partial E_{k}}{\partial y_{r}} \cdot \sigma_{r}^{\prime}\left(\xi_{r}\right) \cdot w_{r j}
$$

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

## Complexity of the batch algorithm

Computation of $\frac{\partial \mathrm{E}}{\partial w_{i}}\left(\vec{w}^{(t-1)}\right)$ stops in time linear in the size of the network plus the size of the training set. (assuming unit cost of operations including computation of $\sigma_{r}^{\prime}\left(\xi_{r}\right)$ for given $\xi_{r}$ )

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

## Illustration of the gradient descent - XOR



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

## MLP - learning algorithm

## Online algorithm:

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

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

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

where

$$
\Delta w_{j i}^{(t)}=-\varepsilon(t) \cdot \frac{\partial E_{k}}{\partial w_{j i}}\left(w_{j i}^{(t)}\right)
$$

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

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

## SGD

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

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

where

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

- $0<\varepsilon(t) \leq 1$ is a learning rate in step $t+1$
- $\nabla E_{k}\left(\vec{w}^{(t)}\right)$ 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.

## Output activations and error functions

## Regression:

- The output activation is typically the identity $y_{i}=\sigma\left(\xi_{i}\right)=\xi_{i}$.


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$$
\left\{\left(\vec{x}_{k}, \vec{d}_{k}\right) \quad \mid \quad k=1, \ldots, p\right\}
$$

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

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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

$$
E_{k}(\vec{w})=\frac{1}{2} \sum_{i \in Y}\left(y_{i}\left(\vec{w}, \vec{x}_{k}\right)-d_{k i}\right)^{2}
$$

## Output activations and error functions

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- The output activation function softmax:

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y_{i}=\sigma_{i}\left(\xi_{i}\right)=\frac{e^{\xi_{i}}}{\sum_{j \in Y} e^{\xi_{j}}}
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- The error function (categorical) cross entropy:

$$
E(\vec{w})=-\frac{1}{p} \sum_{k=1}^{p} \sum_{i \in Y} d_{k i} \log \left(y_{i}\left(\vec{w}, \vec{x}_{k}\right)\right)
$$

## Gradient with Softmax \& Cross-Entropy

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

$$
\begin{aligned}
E(\vec{w}) & =-\frac{1}{p} \sum_{k=1}^{p} \sum_{i \in Y} d_{k i} \log \left(y_{i}\left(\vec{w}, \vec{x}_{k}\right)\right) \\
& =-\frac{1}{p} \sum_{k=1}^{p} \sum_{i \in Y} d_{k i} \log \left(\frac{e^{\xi_{i}}}{\sum_{j \in Y} e^{\xi_{j}}}\right) \\
& =-\frac{1}{p} \sum_{k=1}^{p} \sum_{i \in Y} d_{k i}\left(\xi_{i}-\log \left(\sum_{j \in Y} e^{\xi_{j}}\right)\right) \\
& =-\frac{1}{p} \sum_{k=1}^{p} \sum_{i \in Y} d_{k i}\left(\sum_{\ell \in V} w_{i \ell} y_{\ell}-\log \left(\sum_{j \in Y} e^{\sum_{\ell \in V} w_{j e y} y_{\ell}}\right)\right)
\end{aligned}
$$

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

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## Binary classification

Assume a single output neuron $o \in Y=\{0\}$.

- The output activation function logistic sigmoid:

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\sigma_{0}\left(\xi_{0}\right)=\frac{e^{\xi_{0}}}{e^{\xi_{0}}+1}=\frac{1}{1+e^{-\xi_{0}}}
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- The error function (Binary) cross-entropy:

$$
E(\vec{w})=\sum_{k=1}^{p}-\left(d_{k} \log \left(y_{o}\left(\vec{w}, \vec{x}_{k}\right)\right)+\left(1-d_{k}\right) \log \left(1-y_{o}\left(\vec{w}, \vec{x}_{k}\right)\right)\right)
$$

## But what is the meaning of the sigmoid?

The model gives a probability $y_{o}$ of the class 1 given an input $\vec{x}$. But why do we model such a probability using $1 /\left(1+e^{-\xi_{0}}\right) ? ?$

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


... stretches from 0 to $\infty$

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$$
\operatorname{logit}(\bar{y})=\log (\bar{y} /(1-\bar{y}))
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... stretches from $-\infty$ to $\infty$

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

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and

$$
\bar{y}=\frac{1}{1+e^{-\xi_{0}}}
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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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Answer: The one that generates the data with maximum probability!

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$$
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$$

But then

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

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

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The likelihood:

$$
L(\vec{w})=\prod_{k=1}^{p}\left(y_{o}\left(\vec{w}, \vec{x}_{k}\right)\right)^{d_{k}} \cdot\left(1-y_{o}\left(\vec{w}, \vec{x}_{k}\right)\right)^{\left(1-d_{k}\right)}
$$

$\log (L)=$
$\sum_{k=1}^{p}\left(d_{k} \cdot \log \left(y_{o}\left(\vec{w}, \vec{x}_{k}\right)\right)+\left(1-d_{k}\right) \cdot \log \left(1-y_{o}\left(\vec{w}, \vec{x}_{k}\right)\right)\right)$
and thus $-\log (L)=$ the cross-entropy.
Minimizing the cross-netropy maximizes the log-likelihood (and vice versa).

## Squared Error vs Logistic Output Activation

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

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Thus

- If $d=1$ and $y \approx 0$, then $\frac{\delta E}{\delta w} \approx 0$
- If $d=0$ and $y \approx 1$, then $\frac{\delta E}{\delta w} \approx 0$

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

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For $d=1$

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

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For $d=0$

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

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

