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Master DSAI
Advanced Deep Learning
2024-2025

From Artificial Intelligence to a first neuron model

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Disclaimer

If any content in this presentation is yours but is not correctly referenced or if it should be removed, please contact me and I will correct it.

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Overview

- **Context & Vocabulary**
- Math Basics
- Simple Models

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Overview

- **Context & Vocabulary**
  - ***What is Artificial Intelligence?***
  - ***Machine Learning without Maths***
  - ***Machine Learning & Statistics?***
- Math Basics
- Simple Models

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CONTEXT & VOCABULARY

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What is Artificial intelligence?

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We want to believe it, and not from "yesterday"

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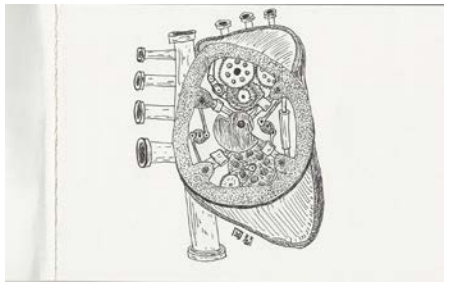
Artificial Intelligence

Artificial intelligence, as a field of research, is considered to have been created at the conference held on the campus of **Dartmouth College** in the summer of **1956**, even though this notion has been present since antiquity: Hephaestus built metal automatons to work for himself or protect others (Talos protecting the goddess Europa) and created Pandora, the first human woman in Greek mythology, from clay; the Golem, in Jewish folklore, is also made of clay, Yan Shi built humanoid automatons in the 10th century BC. during the Zhou Dynasty.



Maria dans Metropolis 1927 De Fritz Lang

Sources :

- *Wikipedia, https://www.greeklegendsandmyths.com/automatons.html*
- *http://www.alanturing.net/turing_archive/pages/Reference%20Articles/what_is_AI/What%20is%20AI02.html*
- *Stanford Encyclopedia of Philosophy: https://plato.stanford.edu/entries/artificial-intelligence/*

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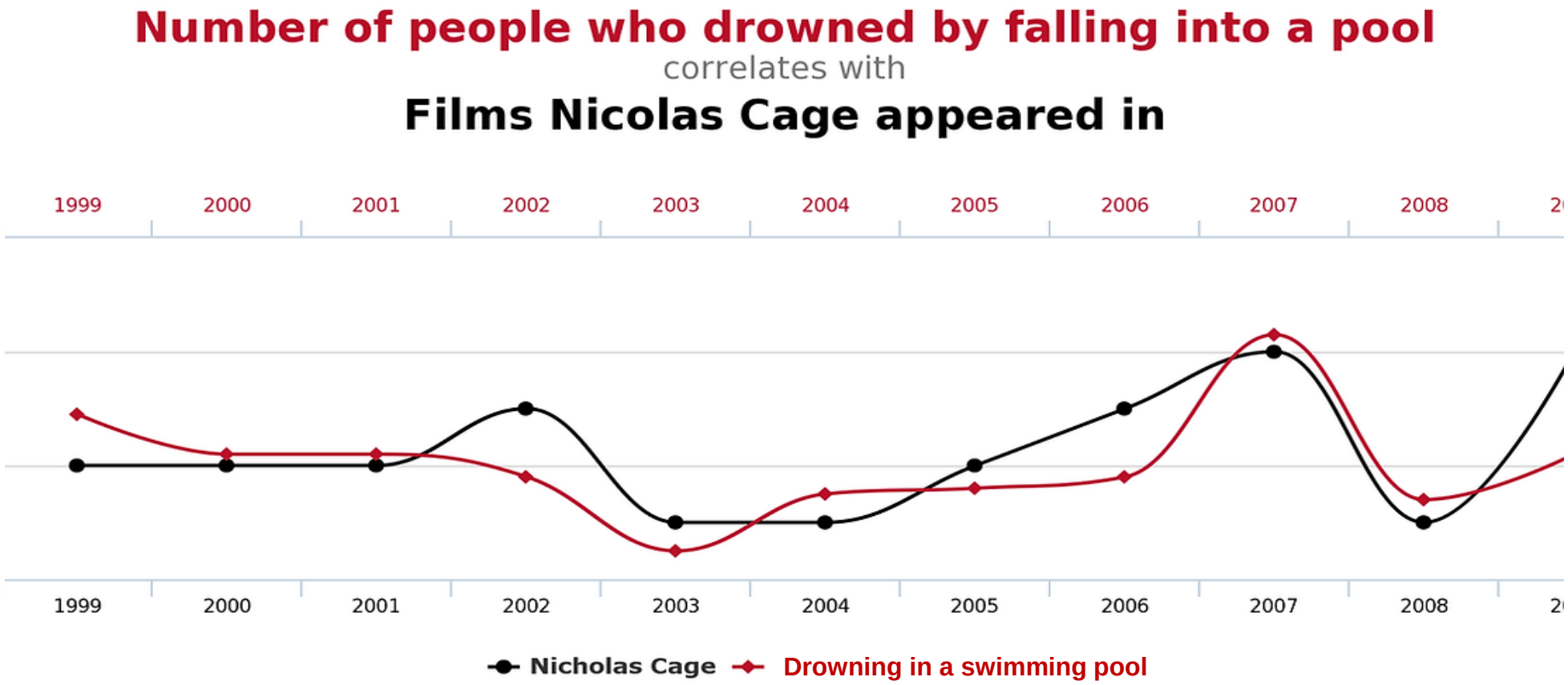
We confuse too easily correlation and causality



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How is Artificial intelligence defined?

- Closer to the Dartmouth conference but still before, the first manifesto on Artificial Intelligence, an unpublished report ***"Intelligent Machinery"***, written by Alan Turing in **1948**. He already distinguished two different approaches to AI, which may be termed ***"top-down"*** and ***"bottom-up"*** *(now more commonly called knowledge-driven AI and data-driven AI respectively).*

- ***Go to read (at least from 20th Century), it is very informative on the different branches of AI****: https://en.wikipedia.org/wiki/History_of_artificial_intelligence*

(sources: Wikipedia, https://www.greeklegendsandmyths.com/automatons.html ,
http://www.alanturing.net/turing_archive/pages/Reference%20Articles/what_is_AI/What%20is%20AI02.html
Stanford Encyclopedia of Philosophy: https://plato.stanford.edu/entries/artificial-intelligence/*)*

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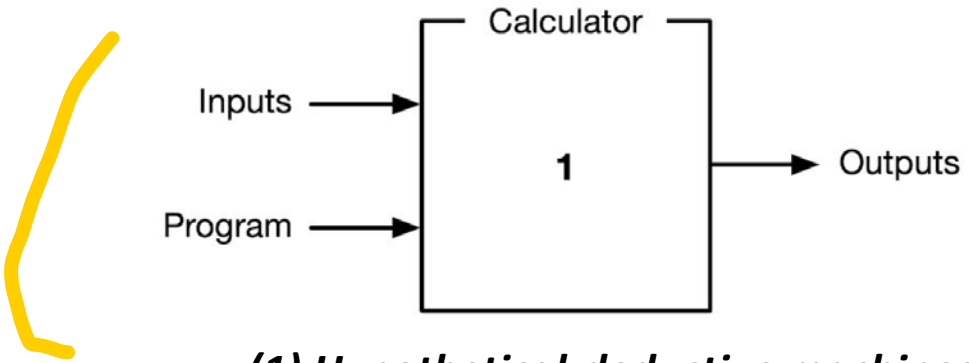
How is Artificial intelligence defined?

- ***"top-down"*** or ***knowledge-driven AI***
  - cognition = high-level phenomenon, independent of low-level details of implementation mechanism
  - Evolutionary Algorithms (1954,1957, 1960), Knowledge Representation, Reasoning (1959,1970), Expert Systems (1970), Logic, Automata, Intelligent Agent Systems (1990)…



(1) Hypothetical-deductive machines

(Figure from: Neurons spike back The invention of inductive machines and the artificial intelligence controversy", D. Cardon, J.-P. Cointet, A. Mazières, Translated by Elizabeth Libbrecht In Réseaux Volume 211, Issue 5, 2018, pages 173 to 220)

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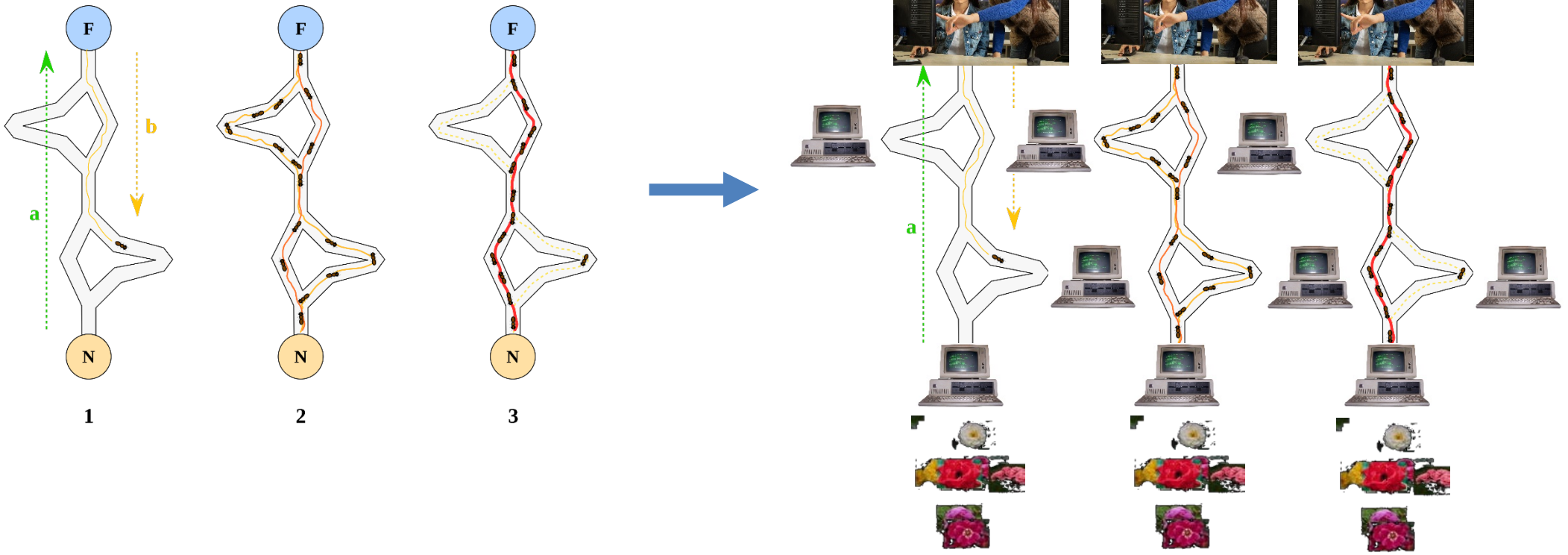
Artificial Intelligence, Top-Down

- **Example of a Multi-Agent System:** the Ant Colony Algorithm



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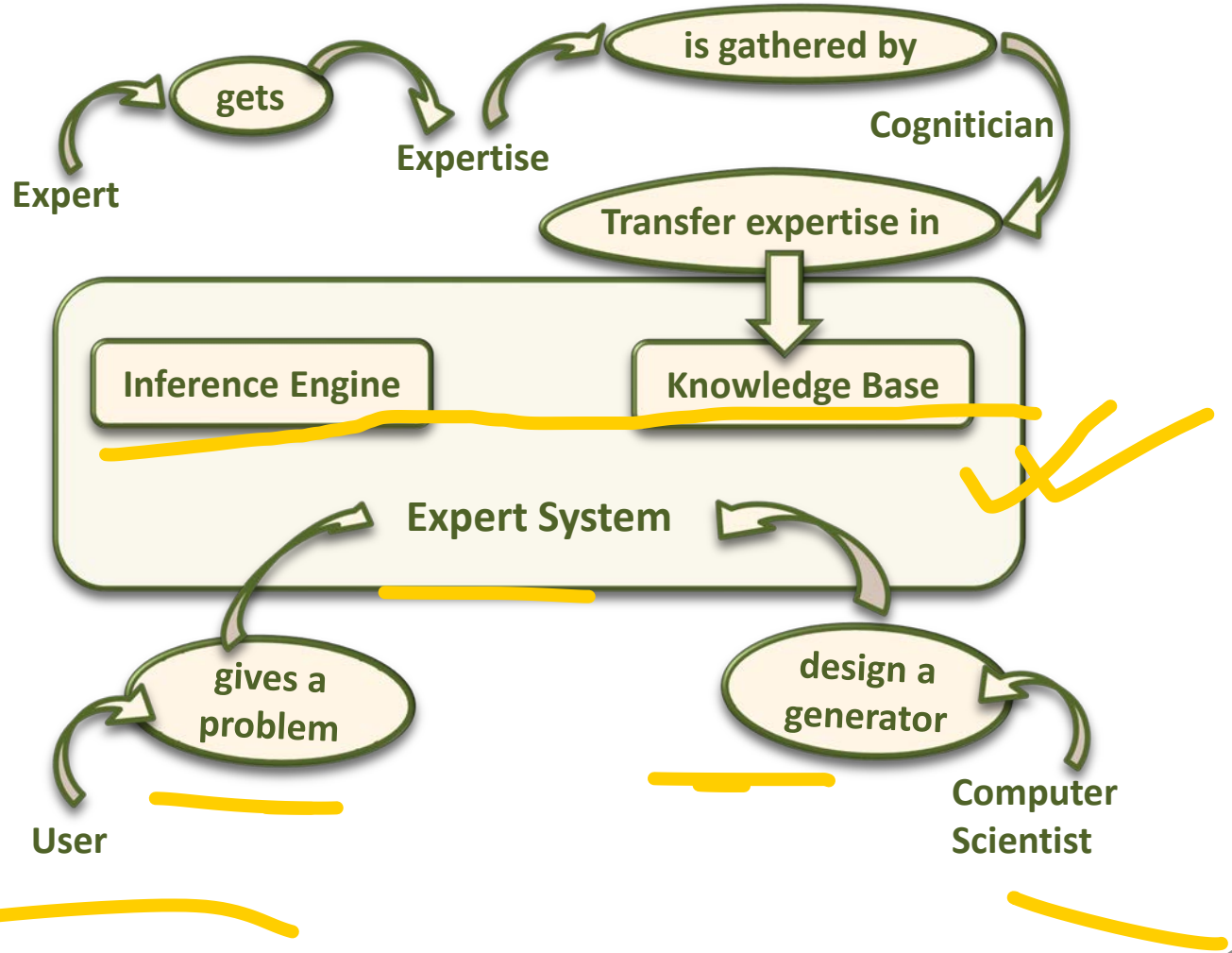
Artificial Intelligence, Top-Down

- **Example of an expert system:**



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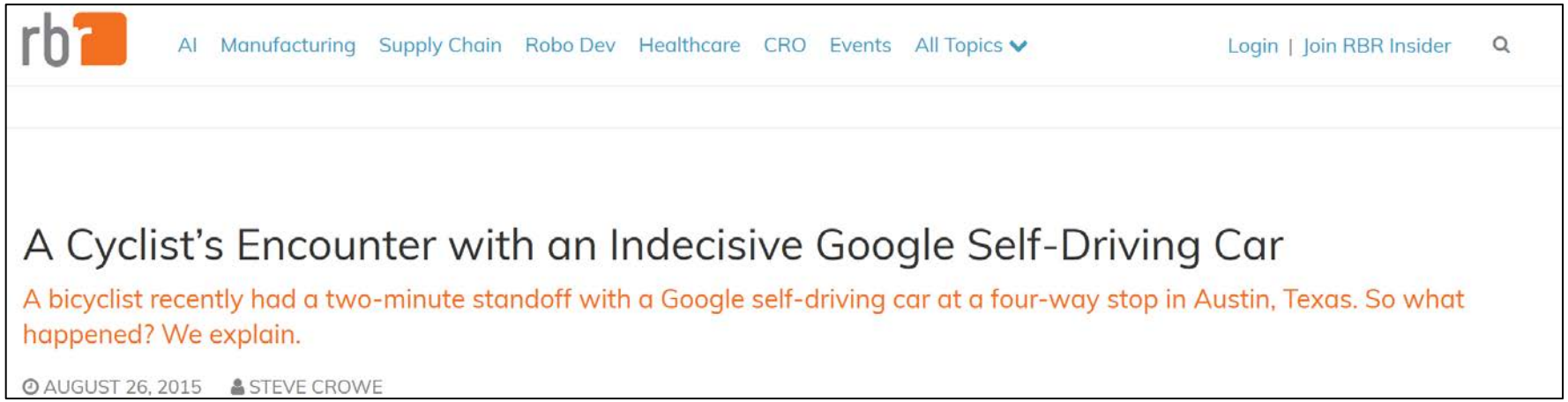
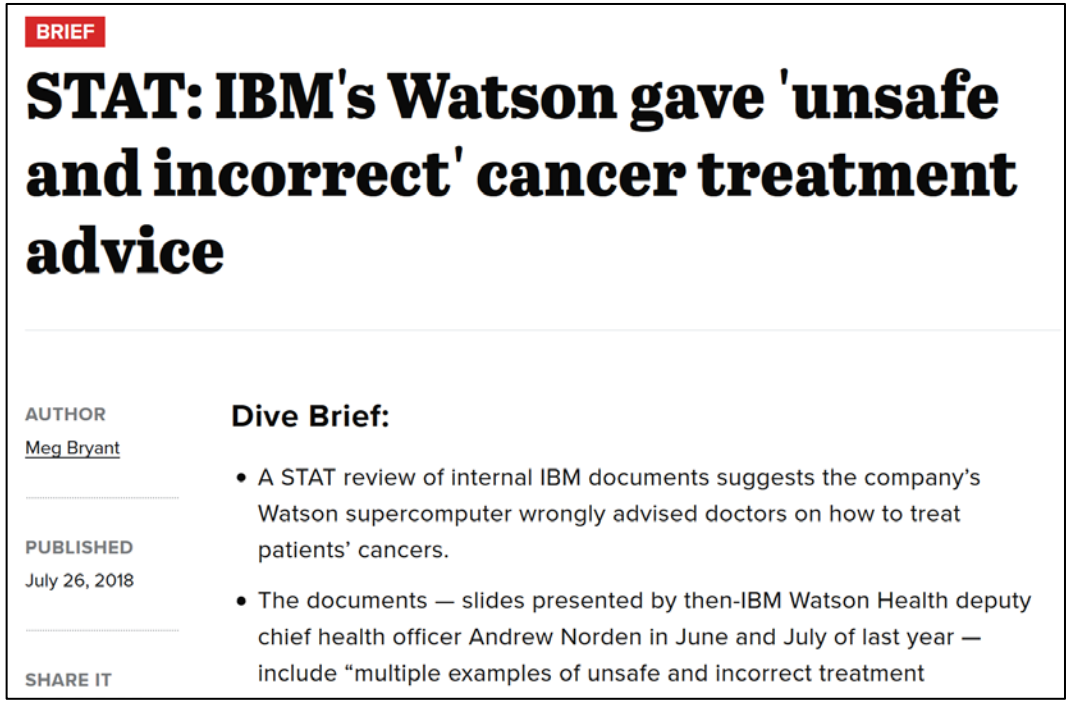
Artificial Intelligence, Top-Down

- **Expert system:**





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AI Timeline

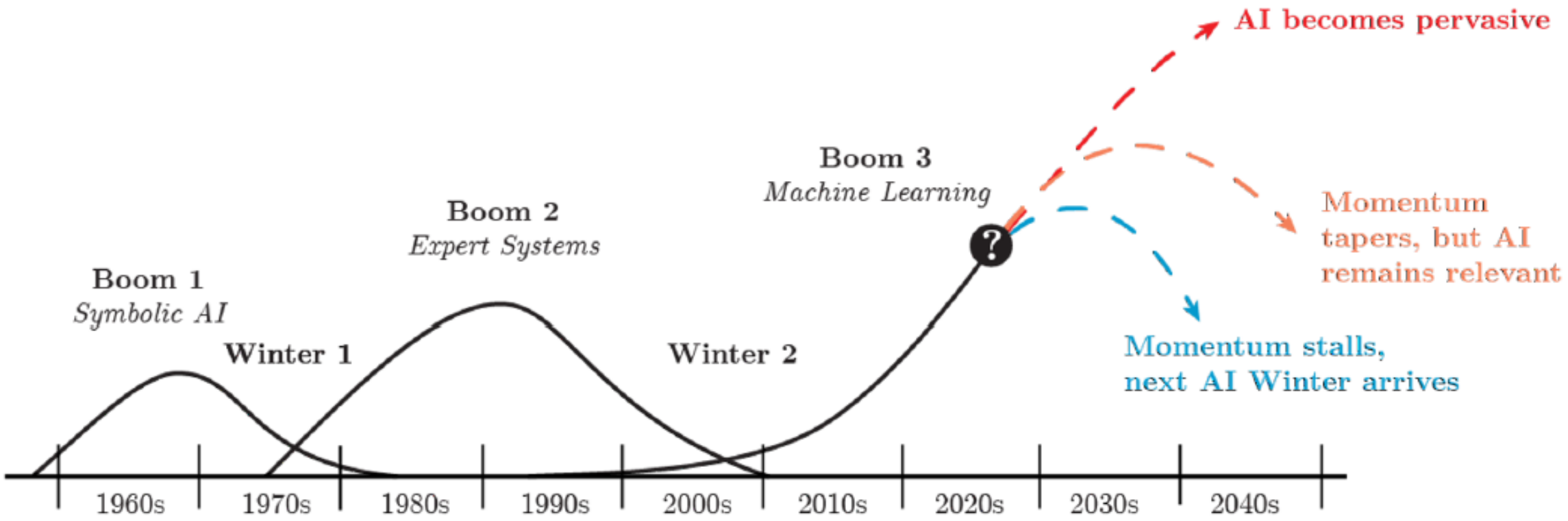

Fig. 1: Past AI Winters: What does the future hold?

Harguess, J. Is the Next Winter Coming for AI? The Elements of Making Secure and Robust AI. In Workshop on Trustworthy and Socially Responsible Machine Learning, NeurIPS 2022.

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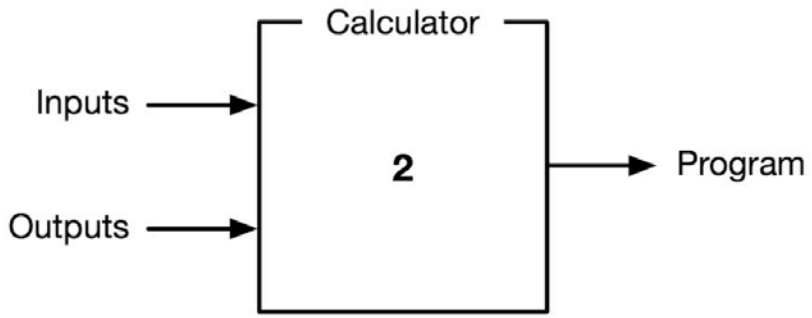
How is Artificial intelligence defined?

- ***"bottom-up" or data-driven AI***
  - opposite approach, start from data to build incrementally and mathematically mechanisms taking decisions
  - First neuron (1943), first neural network machine (1950), neucognitron (1975), Decision Trees (1983), Backpropagation (1984-1986), Random Forest (1995), Support Vector Machine (1995), Boosting (1995), Deep Learning (1998/2006)…



(2) inductive machines

(Figure from: Neurons spike back The invention of inductive machines and the artificial intelligence controversy", D. Cardon, J.-P. Cointet, A. Mazières, Translated by Elizabeth Libbrecht In Réseaux Volume 211, Issue 5, 2018, pages 173 to 220)

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How is Artificial intelligence defined?

- *AI is originally defined in 1956, by Marvin Lee Minsky:*

  *"The construction of computer programs doing tasks, that are, **for the moment**, accomplished **more satisfyingly** by human beings because they require **high level mental processes** such as: learning, perceptual organization of memory and critical reasoning".*

- There are so the "artificial" side with the usage of computers or sophisticated electronic processes and the side "intelligence" associated with its goal to imitate the (human) behavior.

(sources: Wikipedia & http://www.alanturing.net & Stanford Encyclopedia of Philosophy)

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Why Artificial Intelligence is so difficult to grasp?

- Frequently, when a technique reaches **mainstream use**, it is **no longer considered as artificial intelligence**; this phenomenon is described as the ***AI effect***: "AI is whatever hasn't been done yet.“ (***Larry Tesler's Theorem***)
- “As soon as it works, no one calls it AI any more.” (John McCarthy)
- -> e.g. Path Finding (GPS), Chess electronic game, Alpha Go…
- Consequently, AI domain is continuously evolving and so very difficult to grasp.

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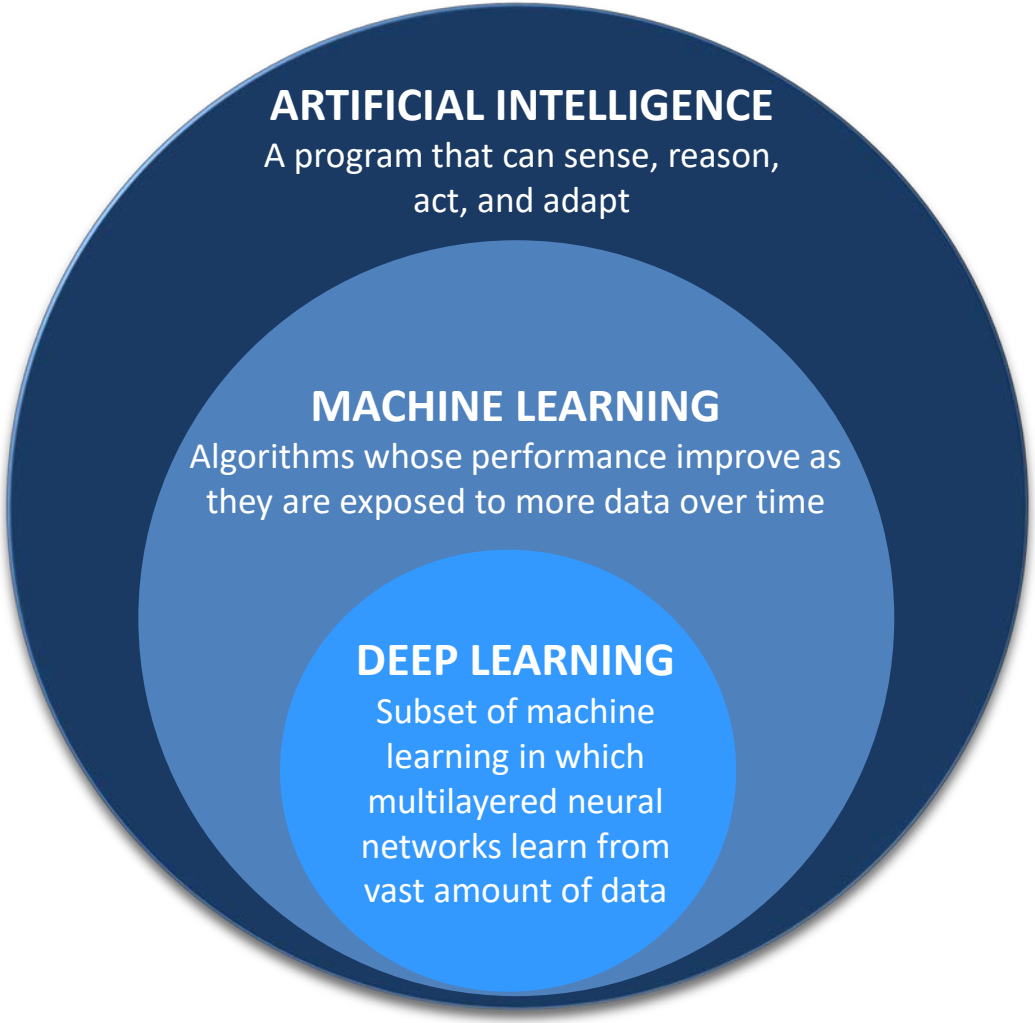
AI vs Machine Learning vs Deep Learning



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But what is Machine Learning?

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Machine Learning

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\boldsymbol{\alpha})\ ?} y$$

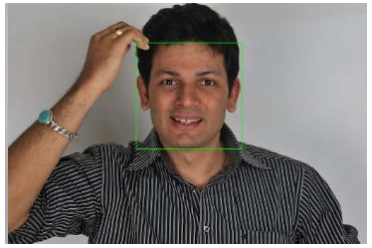
$\left(\mathbf{x}\right)$

Face detection

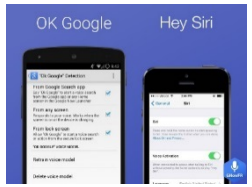
Scores prediction

Voice recognition

y



Sport bets



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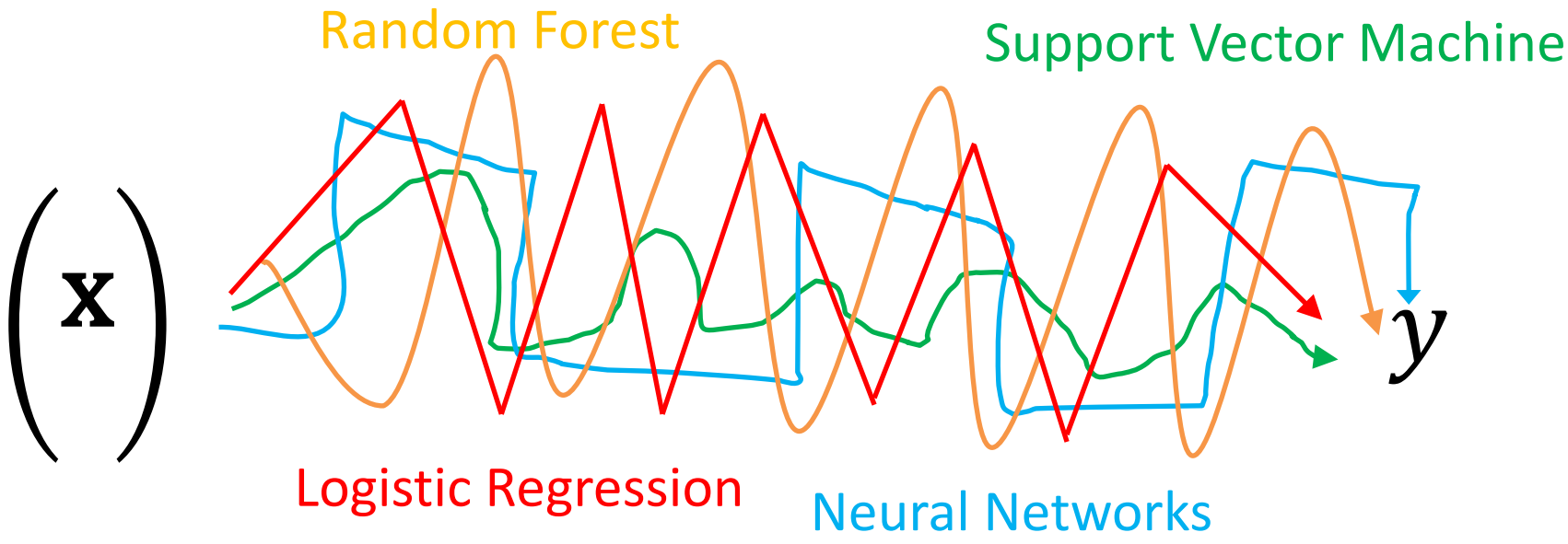
Machine Learning

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\alpha)\ ?} y$$



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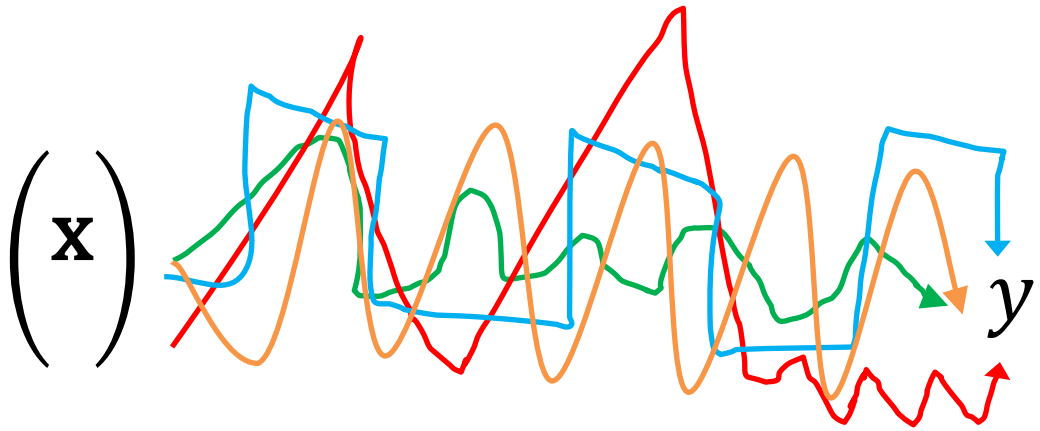
Machine Learning

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\alpha)\ ?} y$$



ML

$\Leftrightarrow$ "Weather Forcasting"

Cf. Question trolley dilemma

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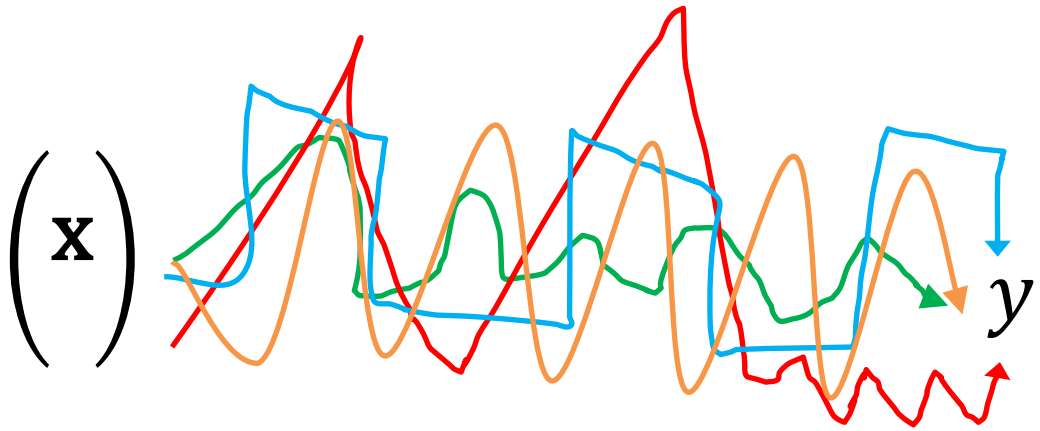
Machine Learning

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\alpha)\ ?} y$$



ML

$\neq$

AI

Francis Bach at *Frontier Research and Artificial Intelligence Conference*: **"Machine Learning is not AI"**
(https://erc.europa.eu/sites/default/files/events/docs/Francis_Bach-SEQUOIA-Robust-algorithms-for-learning-from-modern-data.pdf
https://webcast.ec.europa.eu/erc-conference-frontier-research-and-artificial-intelligence-25#)

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Beware of the diversion!

Trolley dilemma

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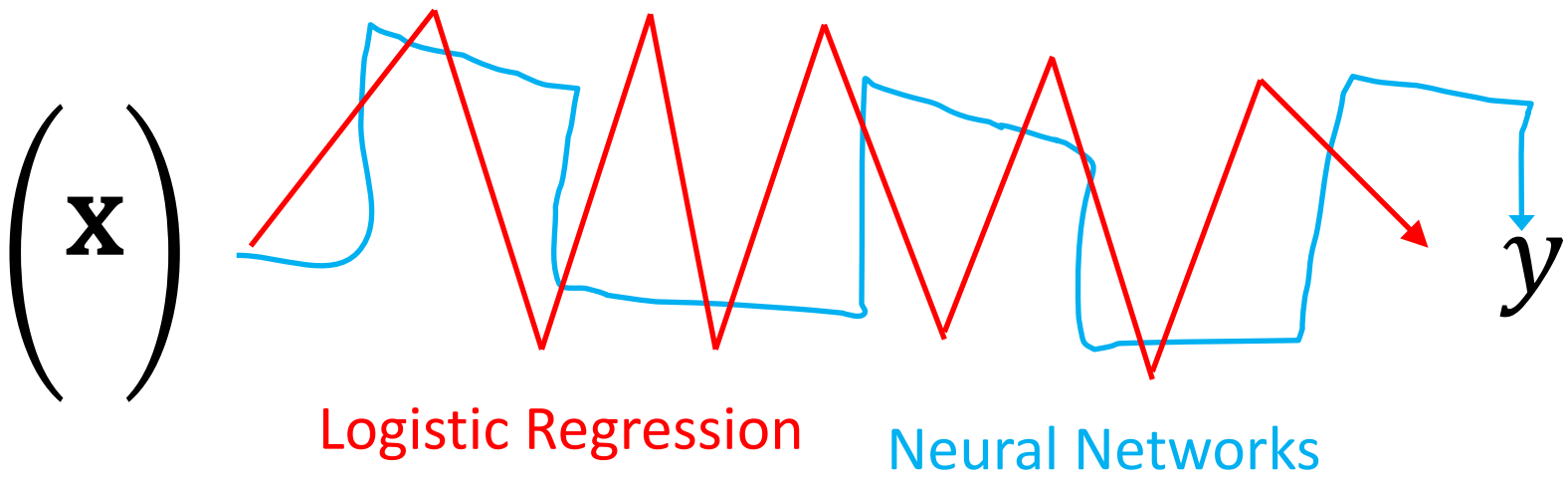
Machine Learning

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\alpha)\ ?} y$$



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Machine Learning is Statistics?

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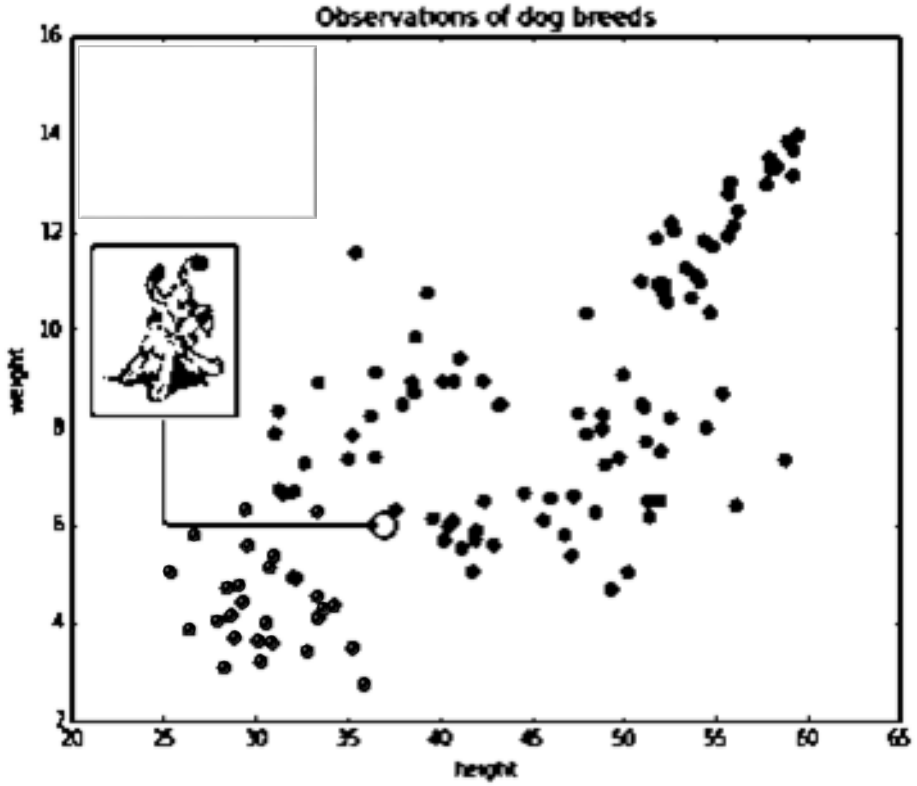
What breed is that Dogmatix (Idéfix)?



The illustrations of the slides in this section come from the blog "Bayesian Vitalstatistix: What Breed of Dog was Dogmatix?"

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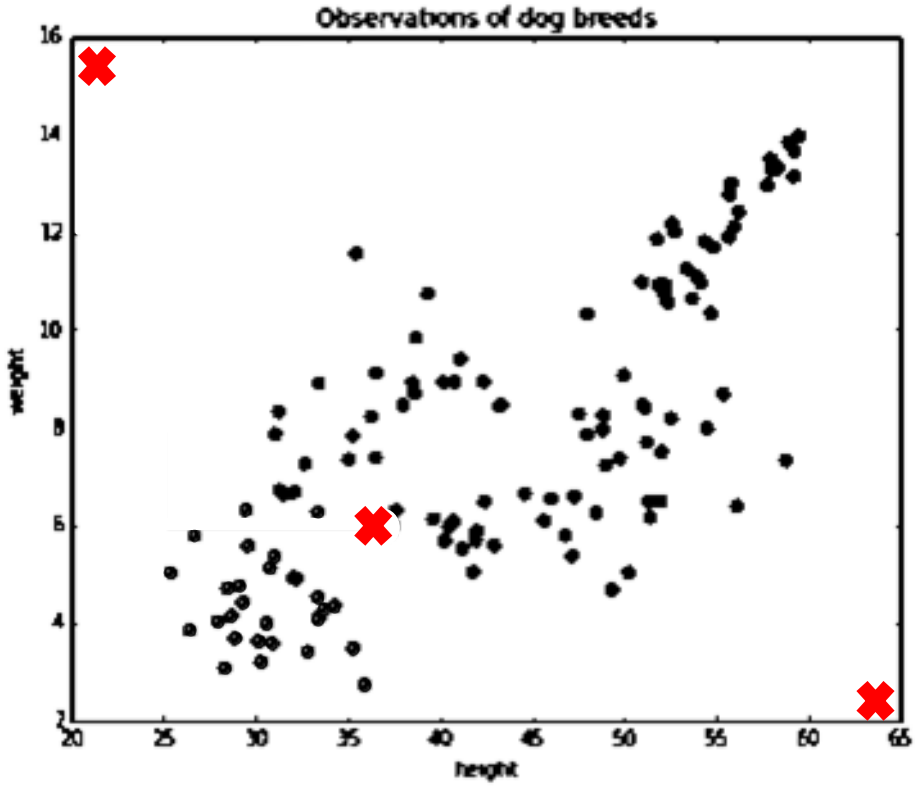
Does any real dog get this height and weight?



- Let us consider ***x***, vectors independently generated in $\boldsymbol{R}^d$ (here $\boldsymbol{R}^2$), following a probability distribution fixed but ***unknown*** $P(\boldsymbol{x})$.

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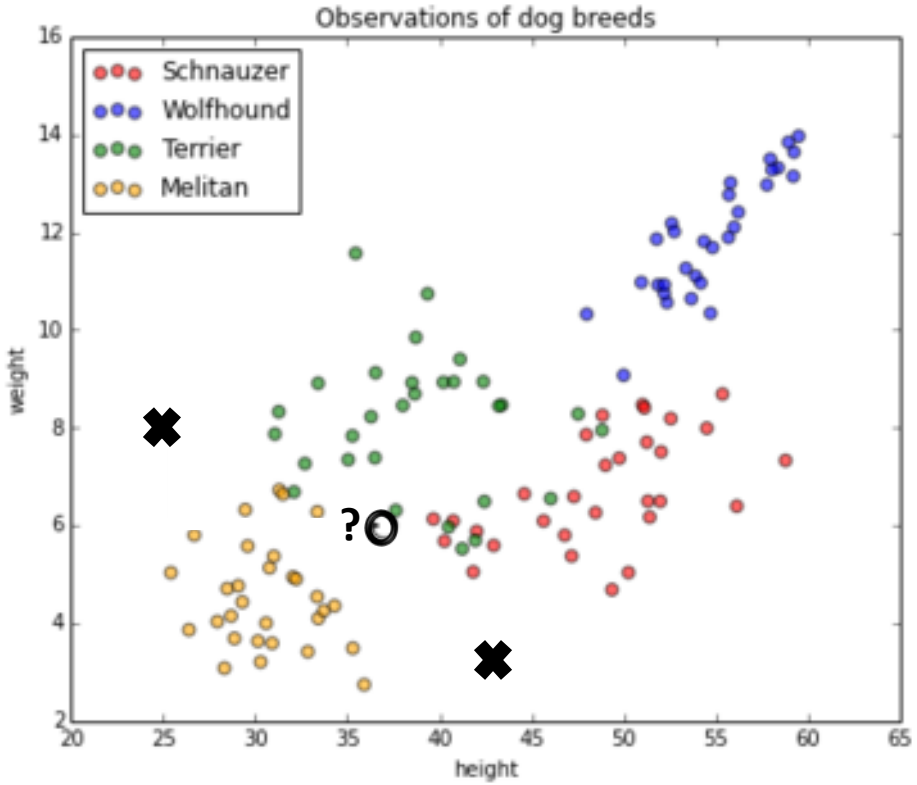
What should be the breed of these dogs?



- An Oracle assigns a value *y* to each vector ***x*** following a probability distribution *P(y|**x**)* also fixed but ***unknown***.

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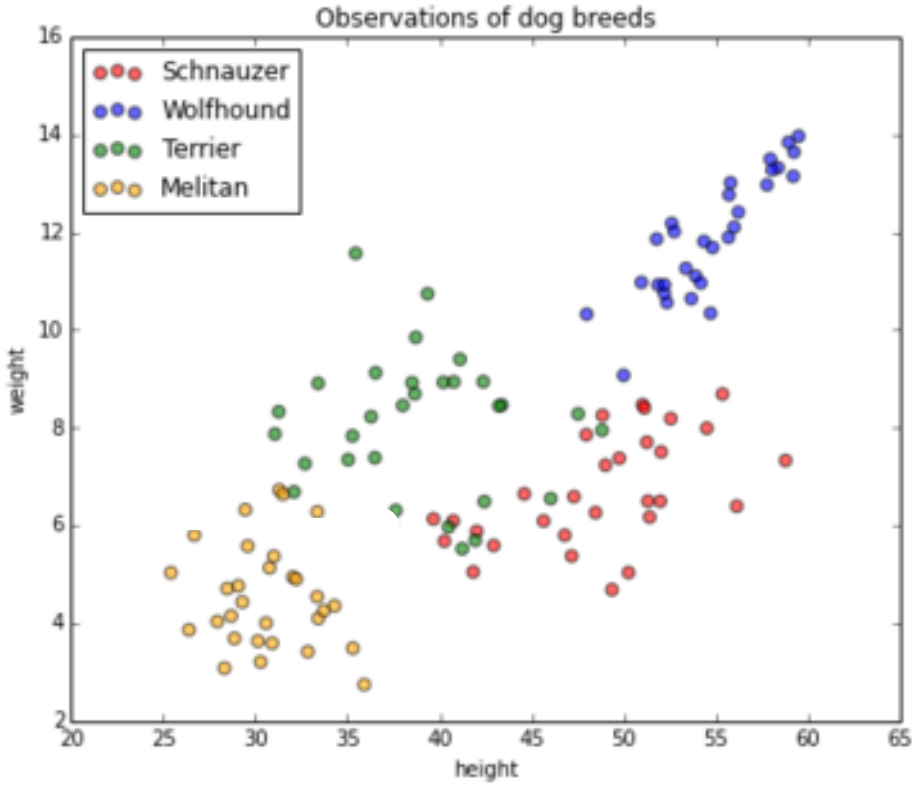
An oracle provides me with examples?



- Let S be a training set $S = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_m, y_m)\}$, with m **training samples i.i.d.** which follow the **joint probability** $P(\boldsymbol{x}, y) = P(\boldsymbol{x})P(y|\boldsymbol{x})$.

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Machine Learning vs Statistics

- **Statistical path**

- Machine learning path

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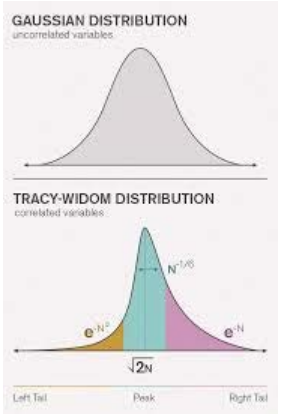
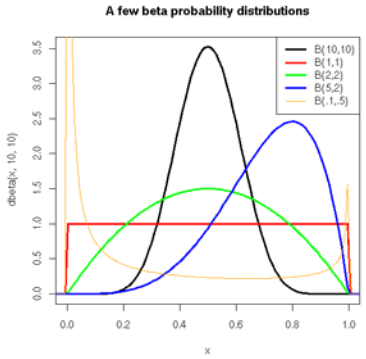
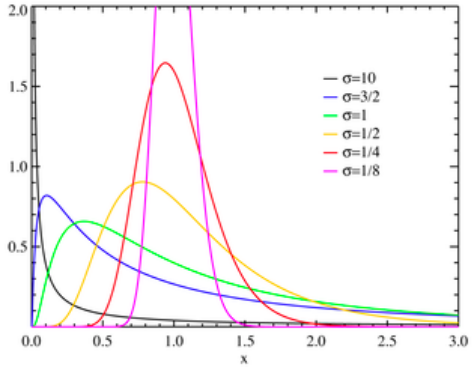
Statistical solution: Models, Hypotheses…







Statisticians make asumptions on the models of $P(X)$ and $P(Y)$.

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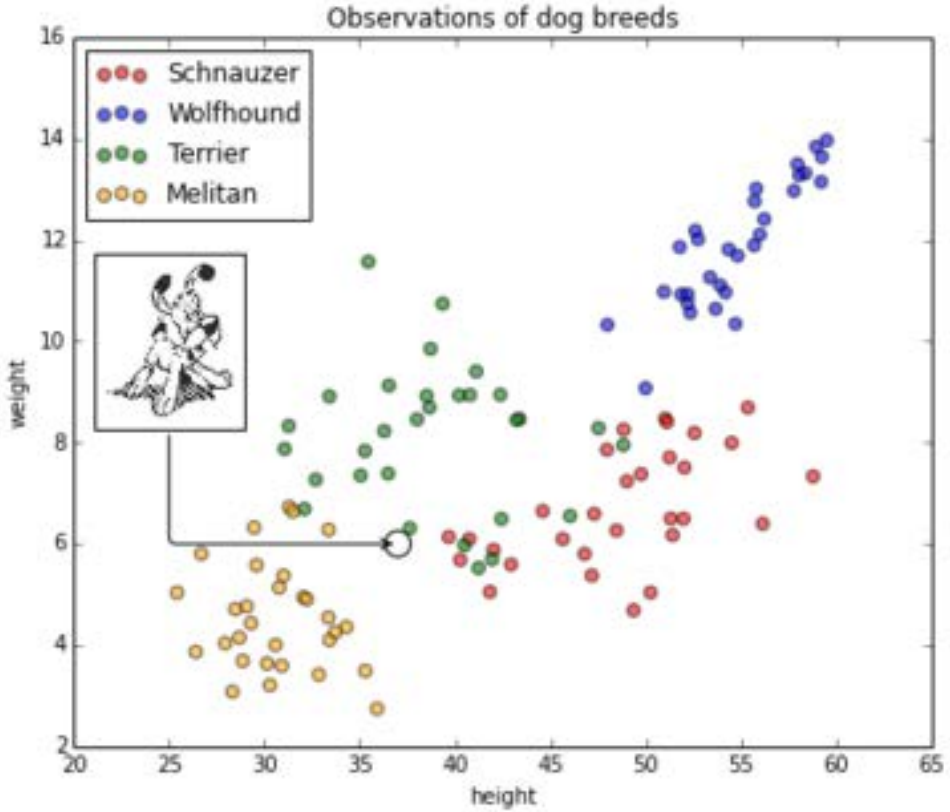
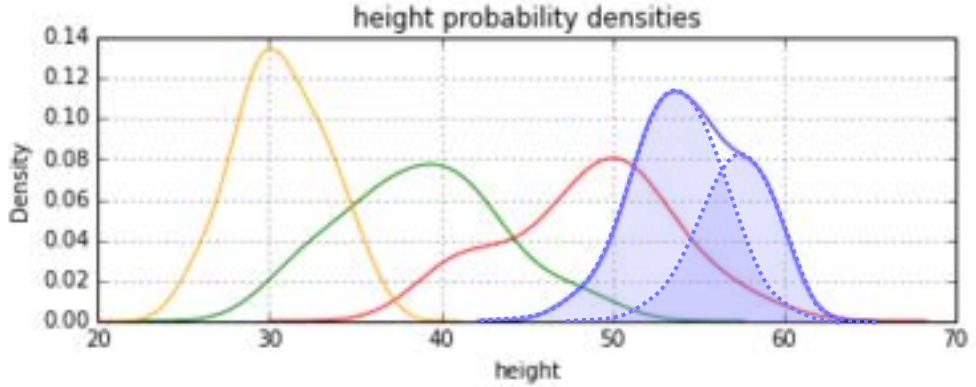
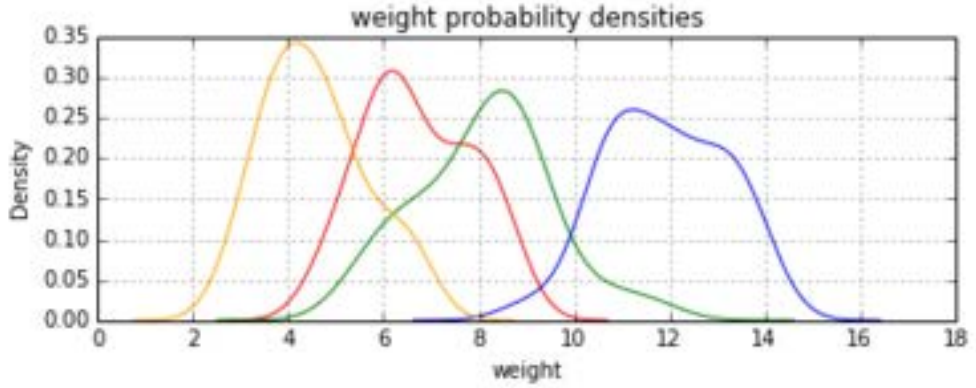
Statistical solution P(height, weight|breed)…







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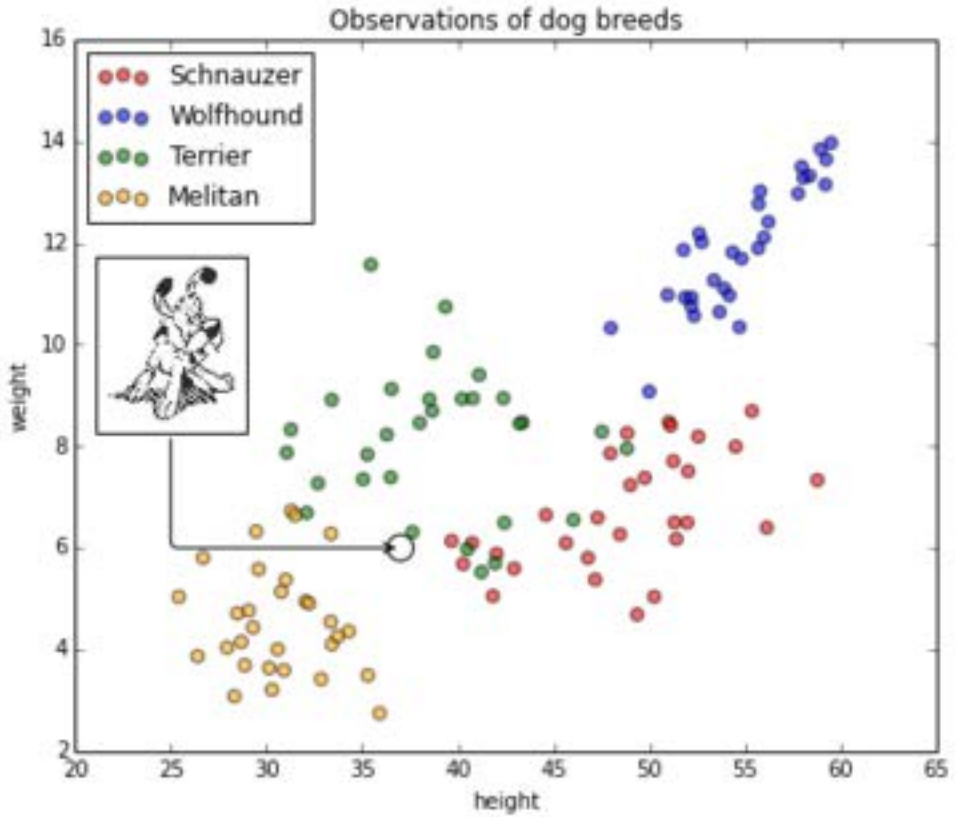

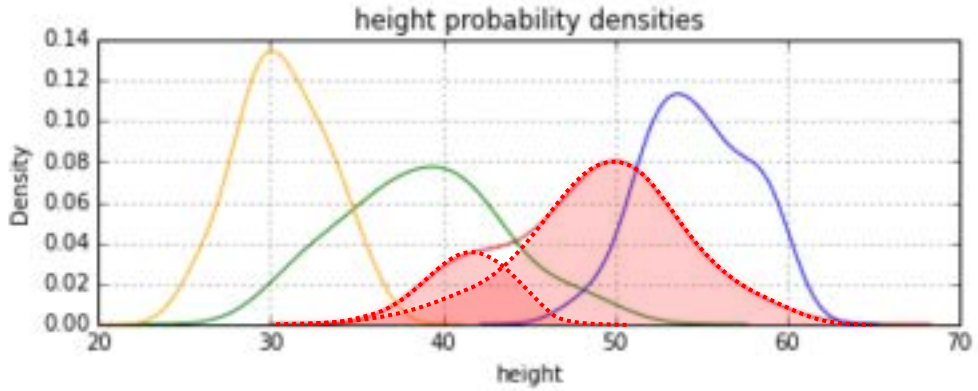

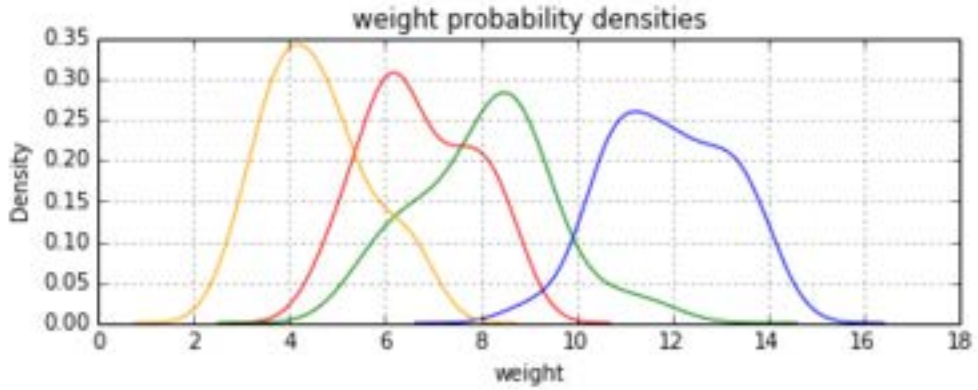

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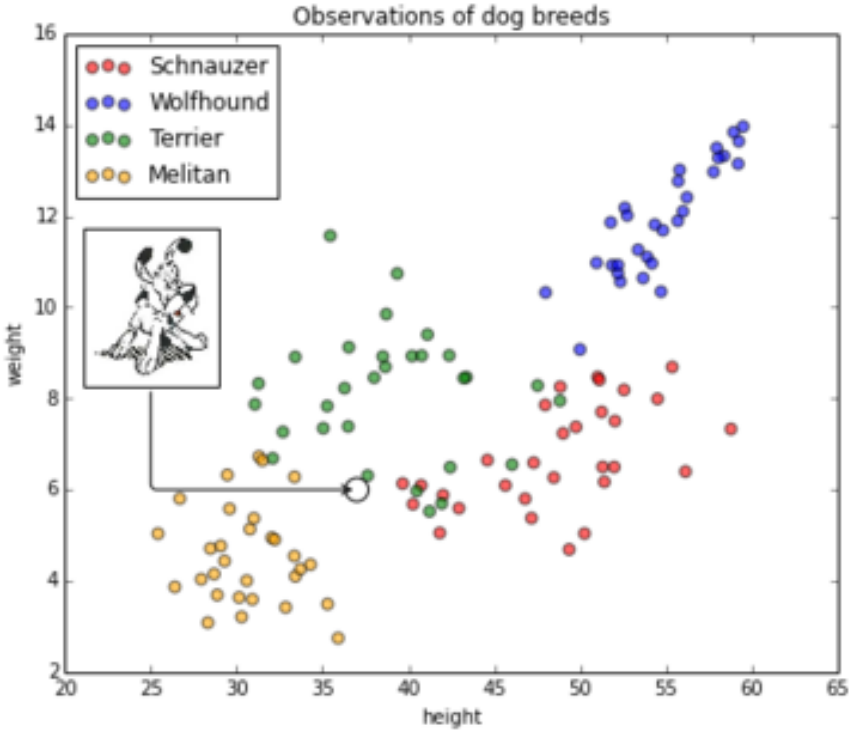
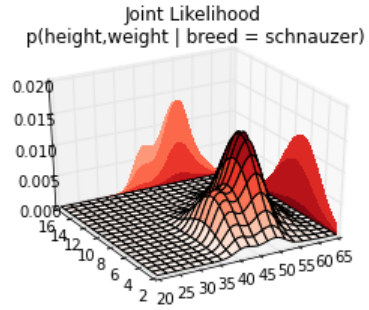
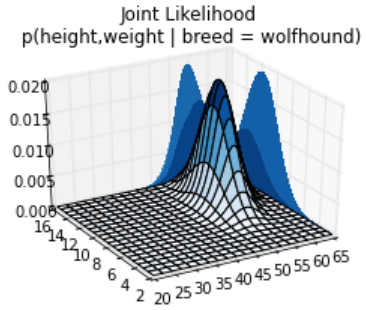
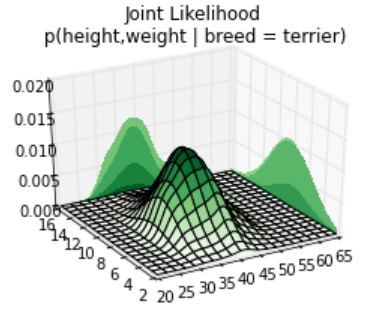
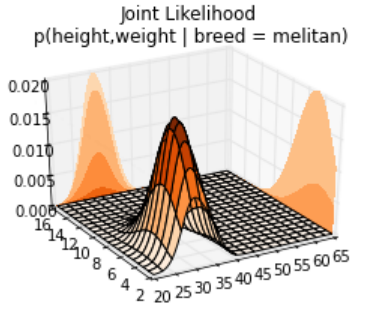
Statistical solution P(height, weight|breed)…











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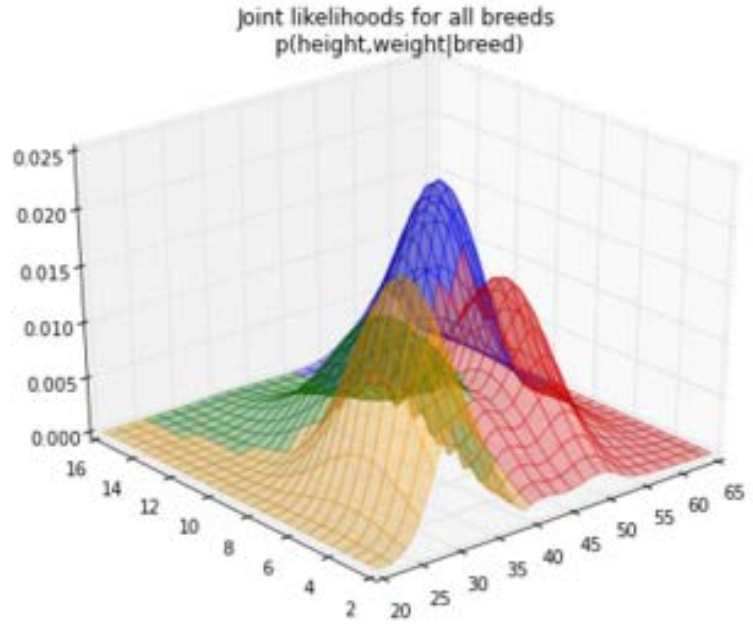
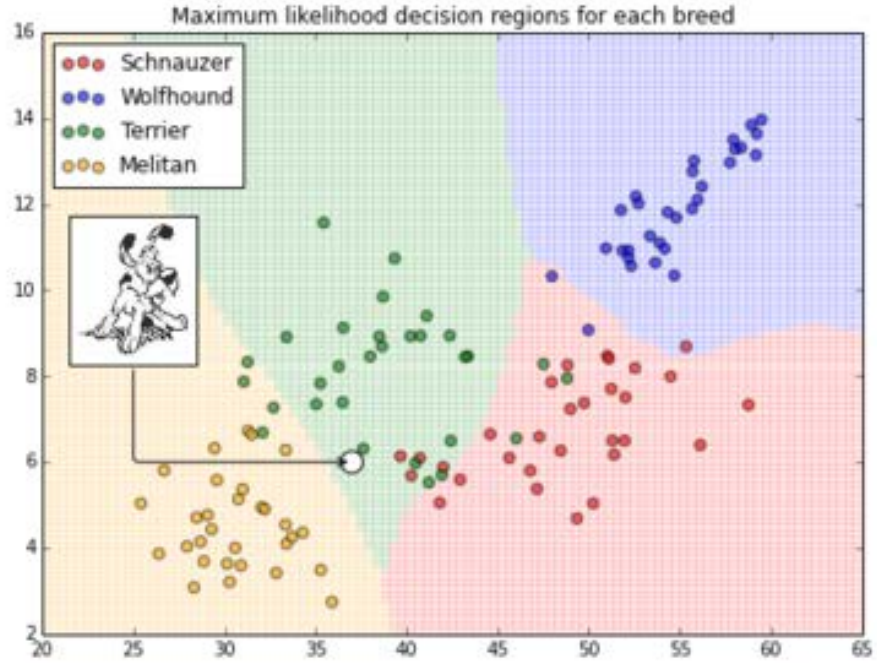
Statistical solution P(height,weight|breed)…





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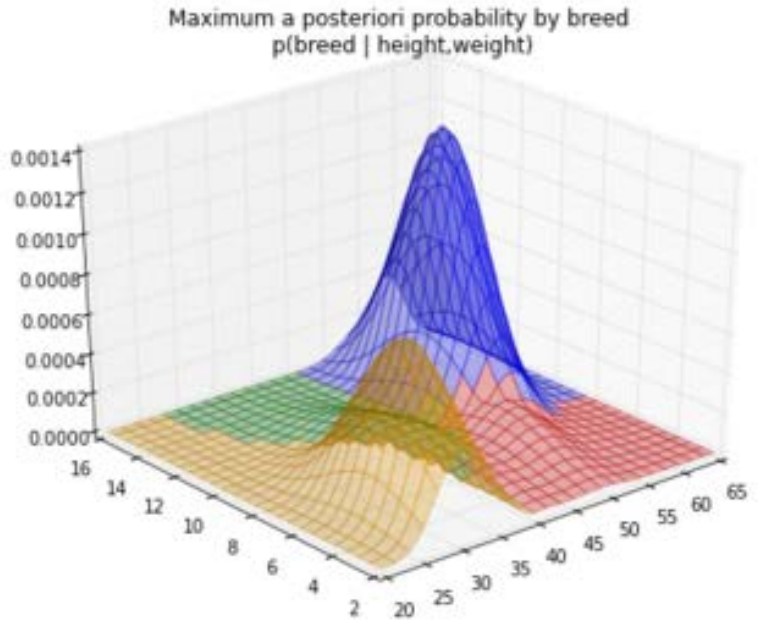
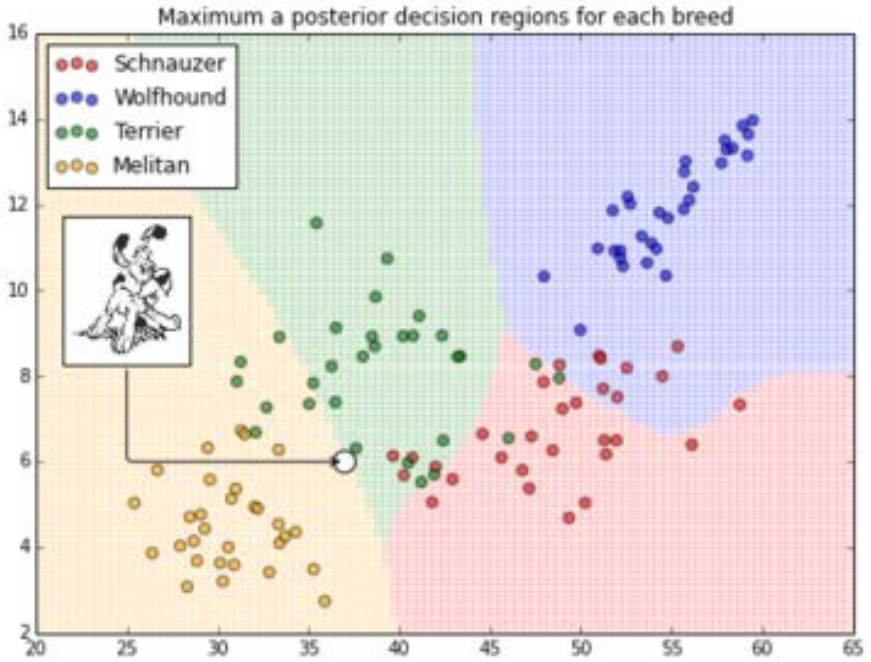
Statistical solution: Bayes, P(breed|height, weight)…

Reminder Bayes' Theorem:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$





$$P(breed|height, weight) = \frac{P(height, weight|breed)P(breed)}{P(height, weight)}$$

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Machine Learning vs Statistics

- Statistical path
- **Machine learning path**

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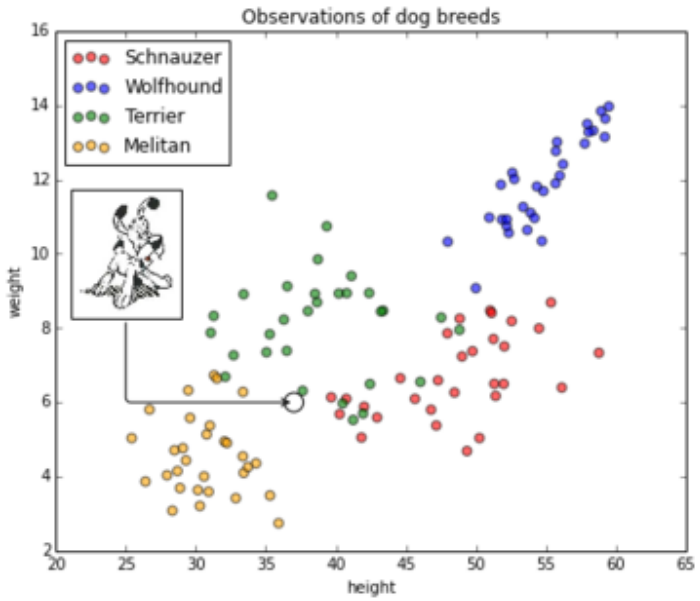
Machine Learning



- we have a learning machine (i.e. an algorithm) which can provide a family of functions *{f(**x**;α)}*, where α is a set of parameters.

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\boldsymbol{\alpha})\ ?} y$$

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The problem of (Machine) Learning

$$\left(\mathbf{x}\right) \xrightarrow{f(\mathbf{X},\boldsymbol{\alpha})\ ?} y$$

- The problem of learning consists in finding the function (among the $\{f(\boldsymbol{x};\alpha)\}$) which provides the best approximation $\hat{y}$ of the true label y given by the Oracle.

- "***best***" is defined in terms of minimizing a specific *error measure/cost/loss* ***related to your problem/objectives***

  $\boldsymbol{L}((\boldsymbol{x}, y), \alpha) \in [a; b]$.

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The problem of (Machine) Learning

- Thus, the objective is to minimize the *(real)* ***Risk***, i.e. the expectation of the error cost:

$$R(\alpha) = \int \boldsymbol{L}((\boldsymbol{x}, y), \alpha) dP(\boldsymbol{x}, y)$$

where $P(\boldsymbol{x}, y)$ is unknown.

- The training set $\mathbf{S} = \{(\boldsymbol{x}_i, y_i)\}_{i=1,\ldots,m}$ is built through an i.i.d. sampling according to $P(\boldsymbol{x}, y)$. Since we cannot compute $R(\alpha)$, we look for minimizing the ***Empirical Risk*** instead:

$$R_{emp}(\alpha) = \frac{1}{m} \sum_{k=1}^{m} \boldsymbol{L}((\boldsymbol{x}_i, y_i), \alpha)$$

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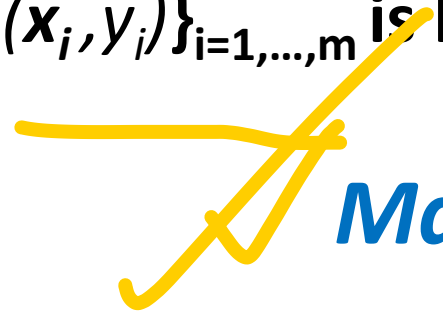
Machine Learning fundamental Hypothesis

$S = \{(x_i, y_i)\}_{i=1,\ldots,m}$ is built through an *i.i.d.* sampling according to $P(x, y)$.



Machine Learning ⇔ ***Statistics***

Train through Cross-Validation

Machine Learning ⇔ ***Statistics***

Training set & Test set have to be distributed according to the same law

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Vapnik learning theory (1995)

Vapnik had proven the following equation $\forall m$ with a probability at least equal to $1 - \eta$:

$$R(\alpha_m) \leq R_{emp}(\alpha_m) + (b - a)\sqrt{\frac{d_{VC}(ln(2m/d_{VC}) + 1) - ln(\eta/4)}{m}}$$

Training Error ***Generalization Error***

Thus minimizing the ***Risk*** depends on minimzing the ***Empirical Risk*** and the ***Generalization Error*** of the model which depends on *m* (the number of training sample), and d_{VC} (the complexity of the model family chosen, also called *Vapnik-Chervonenkis Dimension).*

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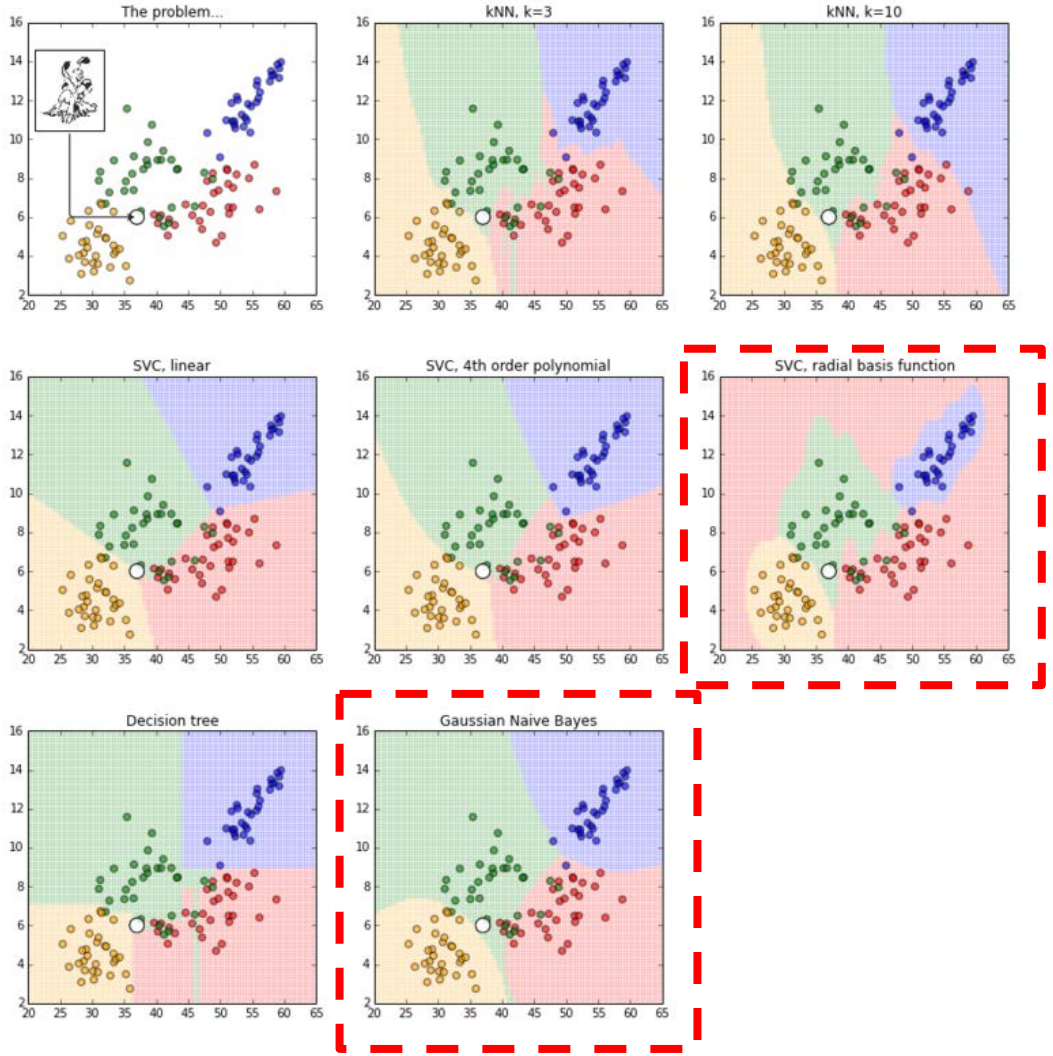
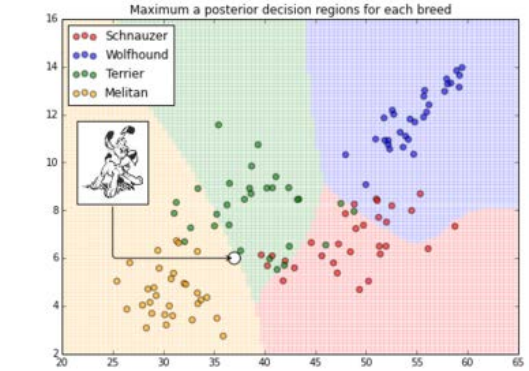
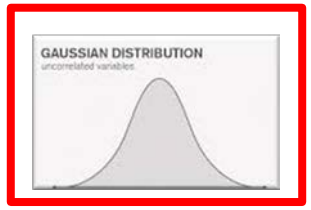
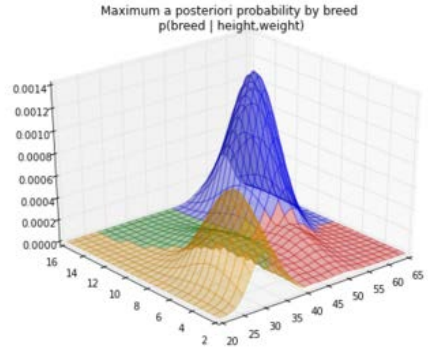
Machine Learning vs Statistics

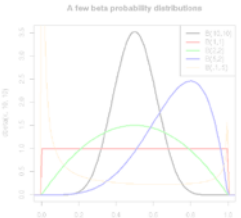


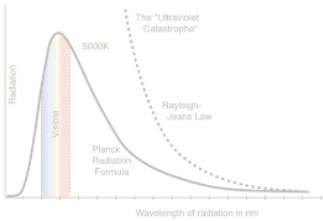
VS











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MATHEMATICAL BASICS

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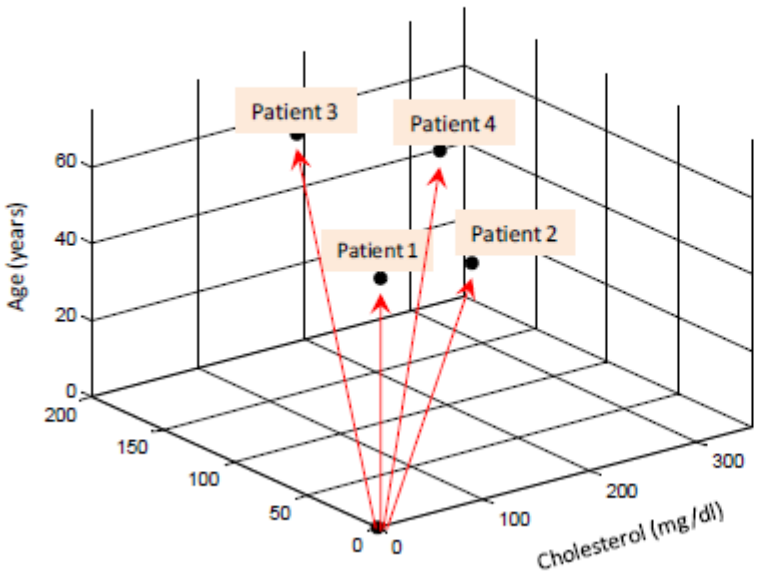
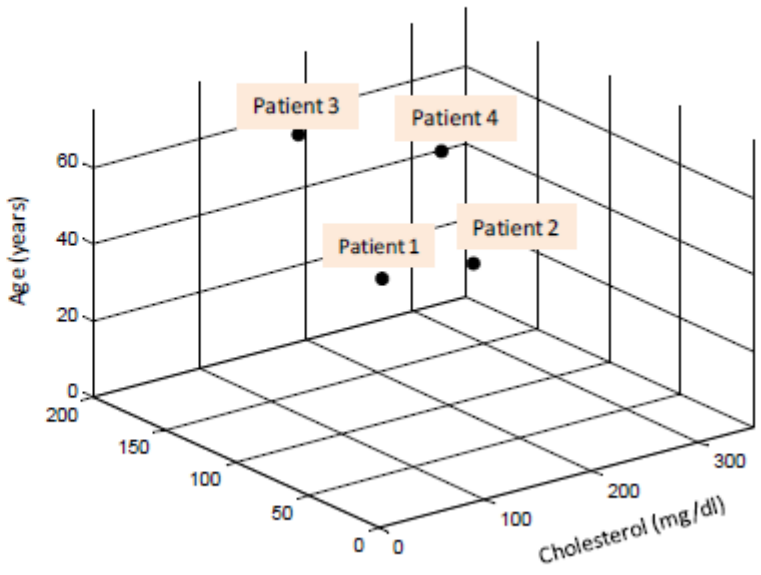
How to represent samples geometrically? Vectors & points in n-dimensional space (R^n)

Patient id	*Cholesterol* (mg/dl)	*Systolic BP* (mmHg)	*Age* (years)	**Tail of the vector**	**Arrow-head of the vector**
1	150	110	35	(0,0,0)	(150, 110, 35)
2	250	120	30	(0,0,0)	(250, 120, 30)
3	140	160	65	(0,0,0)	(140, 160, 65)
4	300	180	45	(0,0,0)	(300, 180, 45)

Vector representation



Point representation



From "A Gentle Introduction to Support Vector Machines in Biomedicine", A. Statnikov, et al, AMIA 2010.

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Basic operation on vectors in R^n

1. Multiplication by a scalar

Consider a vector $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ and a scalar c

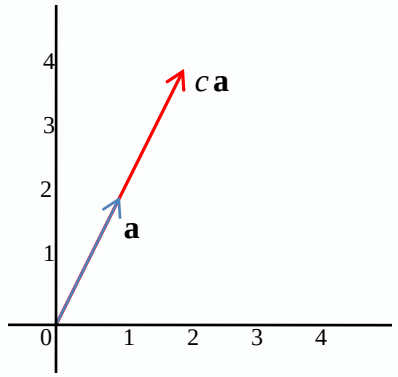
Define: $c\,\mathbf{a} = (ca_1, ca_2, \ldots, ca_n)$

When you multiply a vector by a scalar, you "stretch" it in the same or opposite direction depending on whether the scalar is positive or negative.

$\mathbf{a} = (1, 2)$

$c = 2$

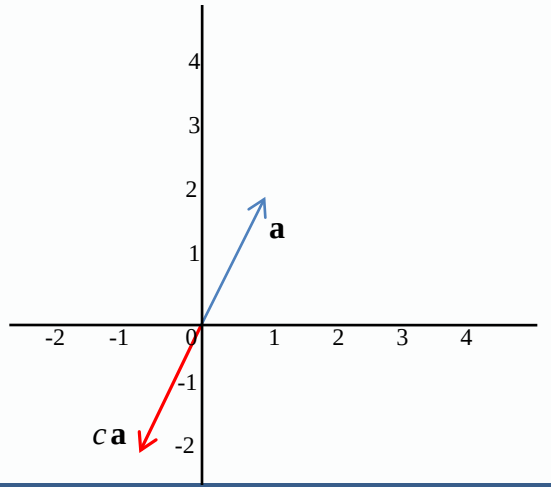
$c\,\mathbf{a} = (2, 4)$



$\mathbf{a} = (1, 2)$

$c = -1$

$c\,\mathbf{a} = (-1, -2)$



Basic operation on vectors in R^n

2. Addition

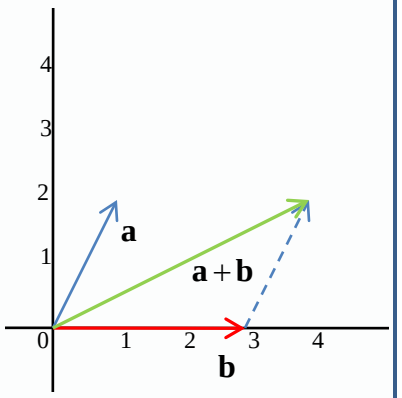
Consider vectors $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ and $\mathbf{b} = (b_1, b_2, \ldots, b_n)$

Define: $\mathbf{a} + \mathbf{b} = (a_1 + b_1, a_2 + b_2, \ldots, a_n + b_n)$

$\mathbf{a} = (1, 2)$

$\mathbf{b} = (3, 0)$

$\mathbf{a} + \mathbf{b} = (4, 2)$



Recall addition of forces in classical mechanics.

From "A Gentle Introduction to Support Vector Machines in Biomedicine", A. Statnikov, et al, AMIA 2010.

Basic operation on vectors in R^n

3. Subtraction

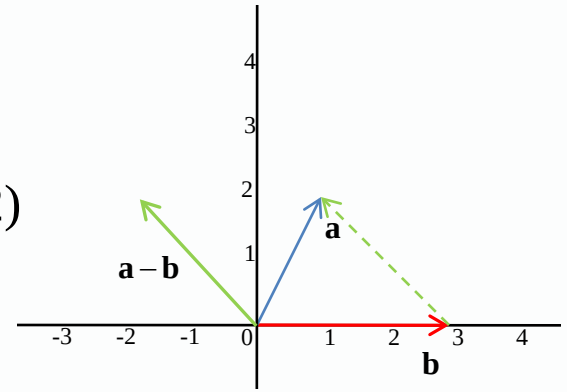
Consider vectors $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ and $\mathbf{b} = (b_1, b_2, \ldots, b_n)$

Define: $\mathbf{a} - \mathbf{b} = (a_1 - b_1, a_2 - b_2, \ldots, a_n - b_n)$

$\mathbf{a} = (1, 2)$

$\mathbf{b} = (3, 0)$

$\mathbf{a} - \mathbf{b} = (-2, 2)$



What vector do we need to add to $\vec{b}$ to get $\vec{a}$? I.e., similar to subtraction of real numbers.

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Basic operation on vectors in R^n

4. Euclidian length or L2-norm

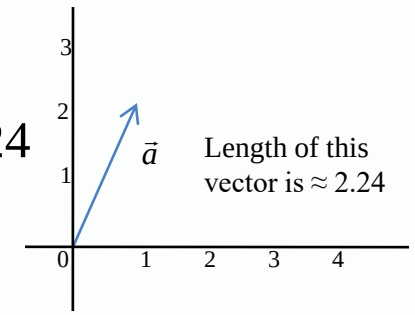
Consider a vector $\mathbf{a} = (a_1, a_2, ..., a_n)$

Define the L2-norm: $\|\mathbf{a}\|_2 = \sqrt{a_1^2 + a_2^2 + ... + a_n^2}$

We often denote the L2-norm without subscript, i.e. $\|\mathbf{a}\|$

$\mathbf{a} = (1, 2)$

$\|\mathbf{a}\|_2 = \sqrt{5} \approx 2.24$



L2-norm is a typical way to measure length of a vector; other methods to measure length also exist.

From "A Gentle Introduction to Support Vector Machines in Biomedicine", A. Statnikov, et al, AMIA 2010.

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Basic operation on vectors in R^n

5. Dot product

Consider vectors $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ and $\mathbf{b} = (b_1, b_2, \ldots, b_n)$

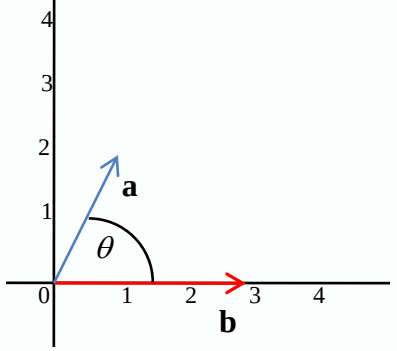
Define dot product: $\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + \ldots + a_n b_n = \sum_{i=1}^{n} a_i b_i$

The law of cosines says that $\mathbf{a} \cdot \mathbf{b} = \| \mathbf{a} \|_2 \| \mathbf{b} \|_2 \cos\theta$ where θ is the angle between $\mathbf{a}$ and $\mathbf{b}$. Therefore, when the vectors are perpendicular $\mathbf{a} \cdot \mathbf{b} = 0$.

$\mathbf{a} = (1, 2)$

$\mathbf{b} = (3, 0)$

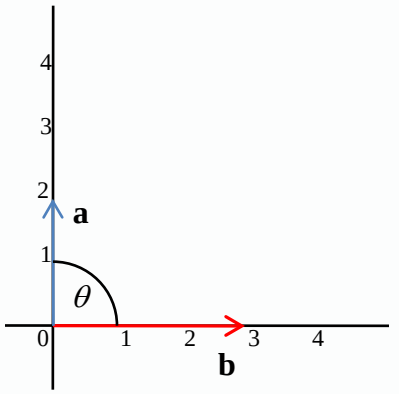
$\mathbf{a} \cdot \mathbf{b} = 3$



$\mathbf{a} = (0, 2)$

$\mathbf{b} = (3, 0)$

$\mathbf{a} \cdot \mathbf{b} = 0$



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Basic operation on vectors in R^n

5. Dot product (continued)

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + \ldots + a_n b_n = \sum_{i=1}^{n} a_i b_i$$

- Property: $\mathbf{a} \cdot \mathbf{a} = a_1 a_1 + a_2 a_2 + \ldots + a_n a_n = \|\mathbf{a}\|_2^2$
- In the classical regression equation $y = \mathbf{w} \cdot \mathbf{x} + b$

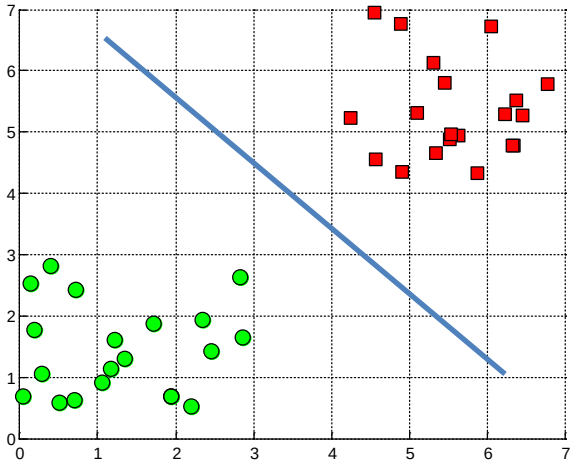
  the response variable *y* is just a dot product of the vector representing patient characteristics ($\mathbf{x}$) and the regression weights vector ($\mathbf{w}$) which is common across all patients plus an offset b.

From "A Gentle Introduction to Support Vector Machines in Biomedicine", A. Statnikov, et al, AMIA 2010.

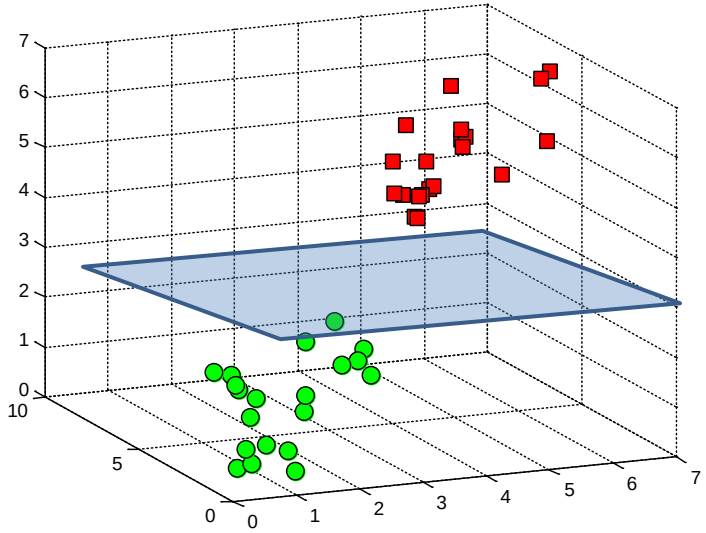
Hyperplanes as decision surfaces

- A hyperplane is a linear decision surface that splits the space into two parts;
- It is obvious that a hyperplane is a binary classifier.

A hyperplane in $\mathbb{R}^2$ is a line



A hyperplane in $\mathbb{R}^3$ is a plane



A hyperplane in $\mathbb{R}^n$ is an n-1 dimensional subspace

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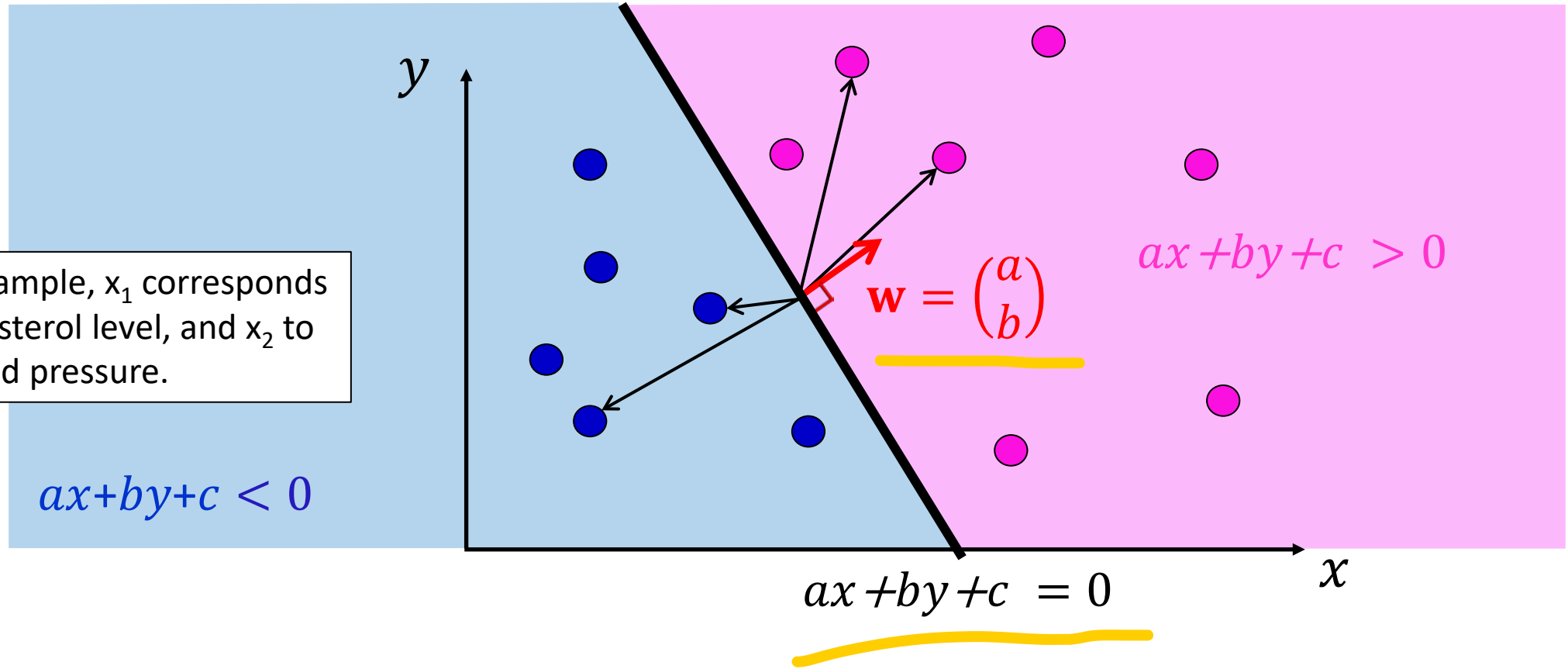
Binary classification in 2D = defining a straight line

Reminder of the equation of a straight line in the plane (in 2D), and of the equations of the two semiplanes that it defines by cutting the space in 2.



Here, for example, x_1 corresponds to the cholesterol level, and x_2 to systolic blood pressure.

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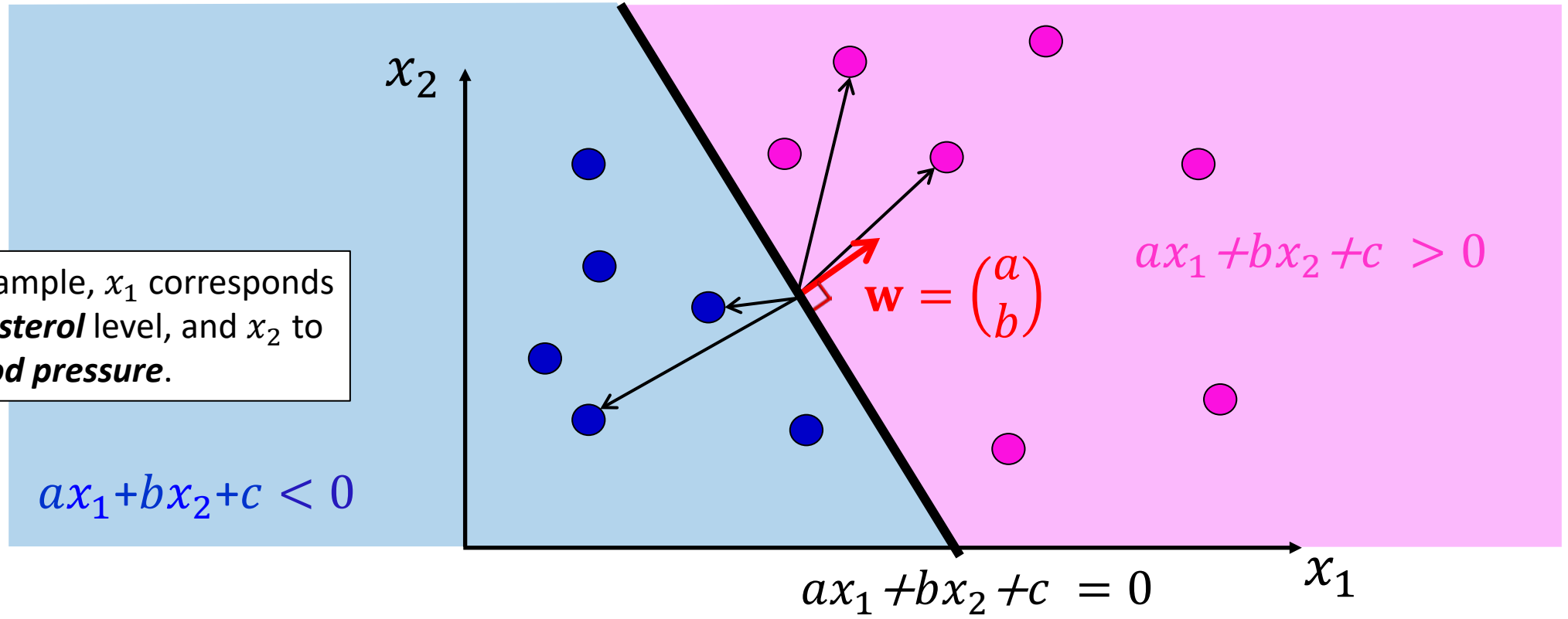
Binary classification in 2D = defining a straight line

Reminder of the equation of a straight line in the plane (in 2D), and of the equations of the two semiplanes that it defines by cutting the space in 2.



Here, for example, x_1 corresponds to the ***cholesterol*** level, and x_2 to ***systolic blood pressure***.

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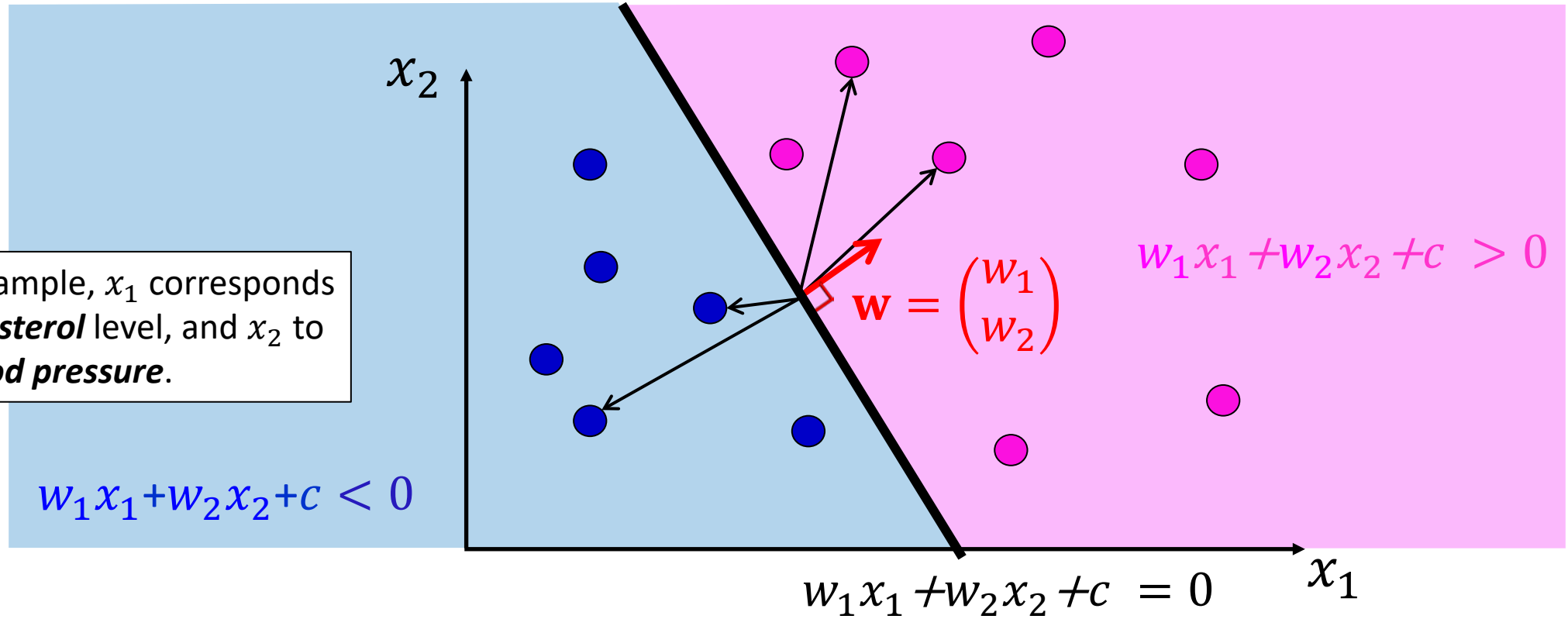
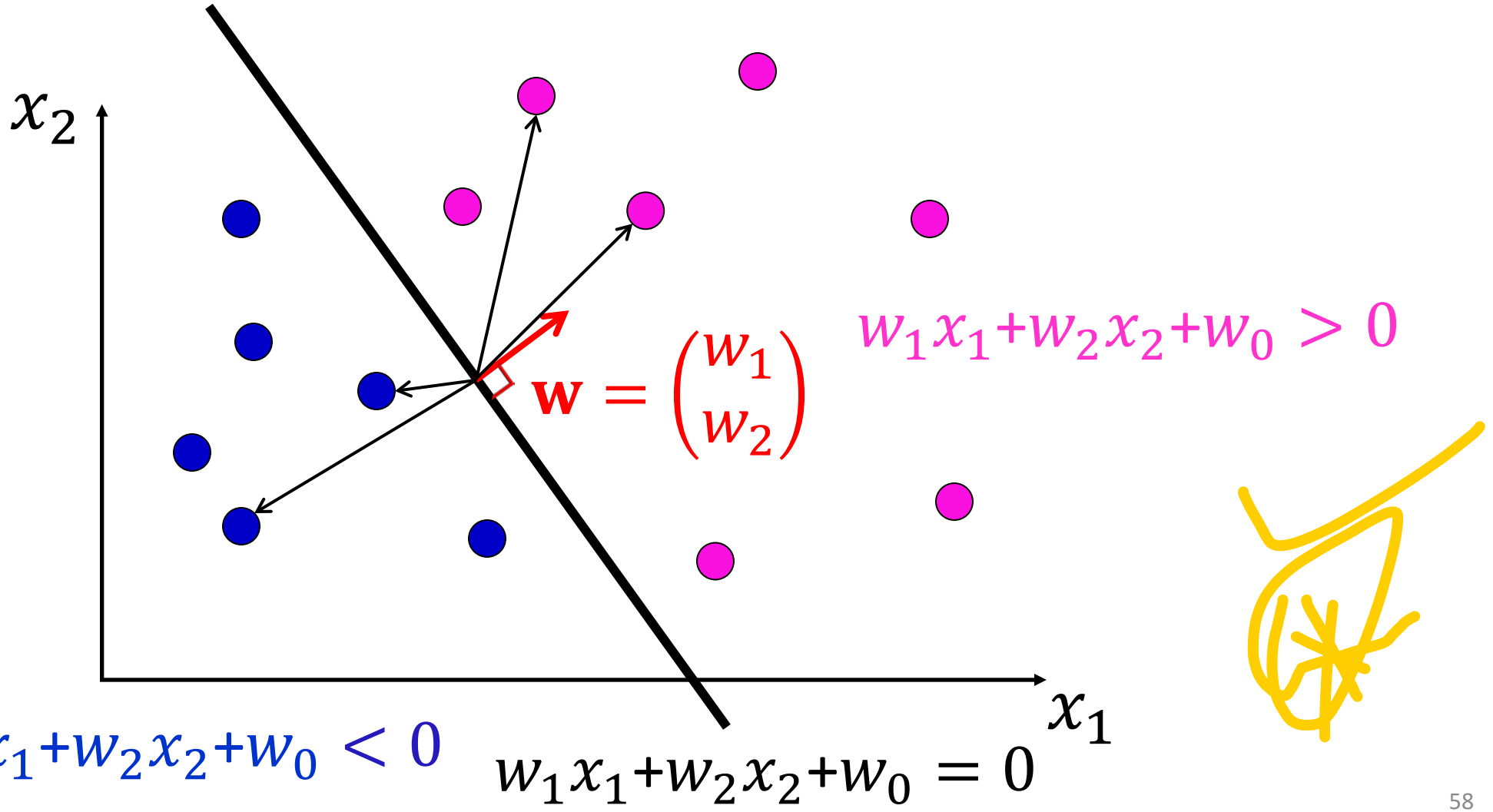
Binary classification in 2D = defining a straight line

Usually weights of a neuron are called w_i.

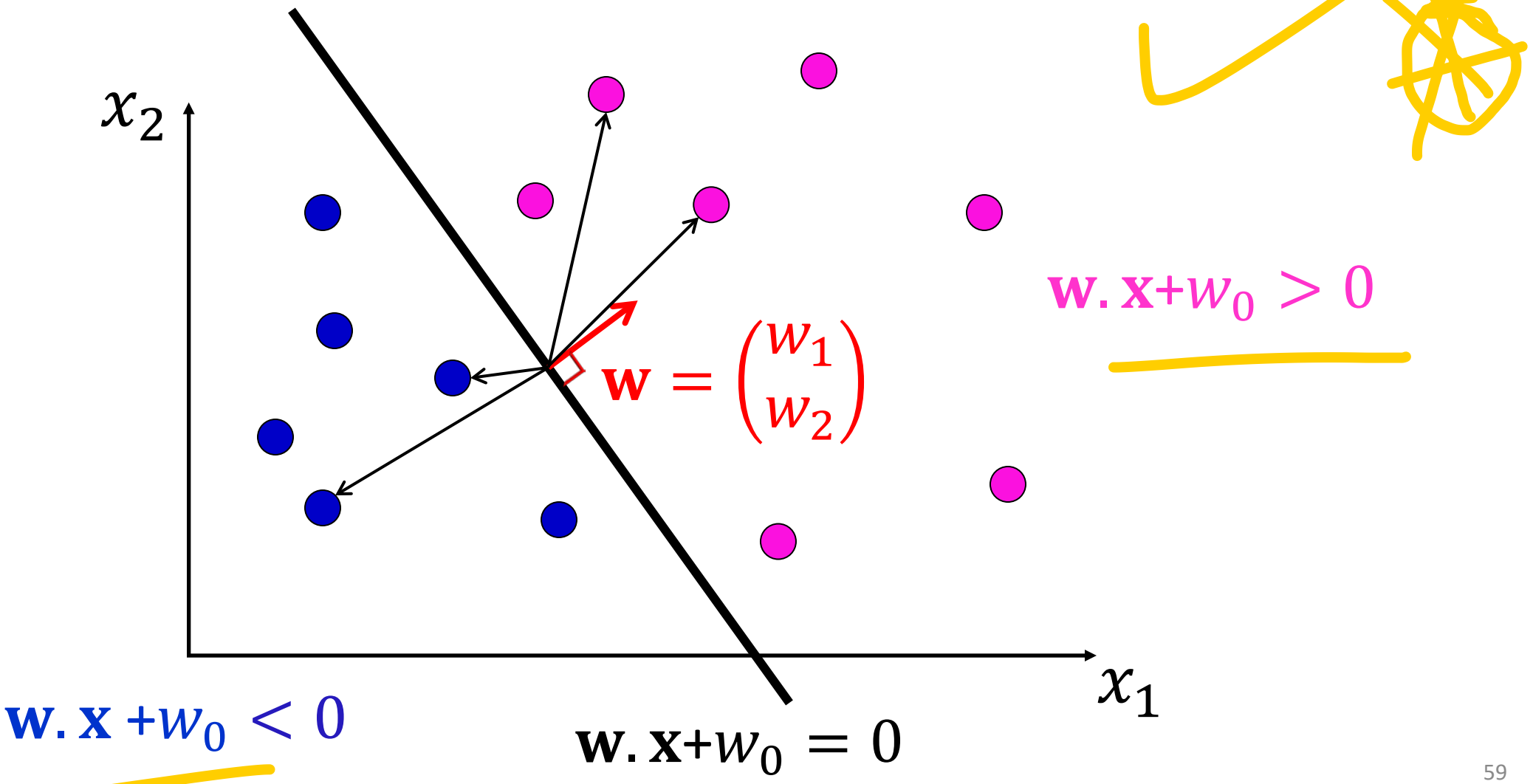


Here, for example, x_1 corresponds to the ***cholesterol*** level, and x_2 to ***systolic blood pressure***.

Geometry and Algebra



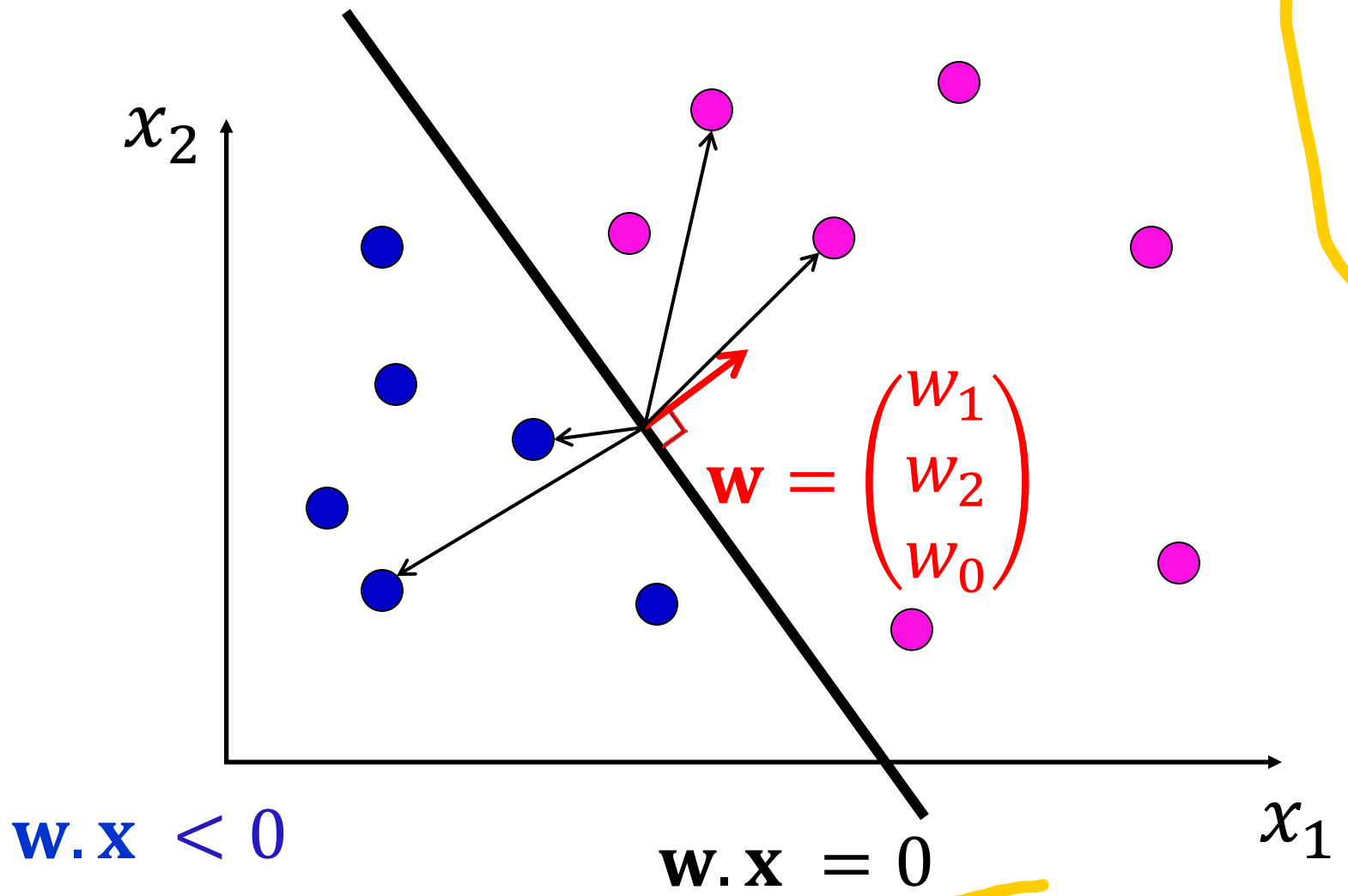
Geometry and Algebra



Simplification

$$\begin{pmatrix} w_1 \\ w_2 \\ w_0 \end{pmatrix} . \begin{pmatrix} x_1 \\ x_2 \\ 1 \end{pmatrix} > 0$$

$$\mathbf{w}.\mathbf{x} > 0$$



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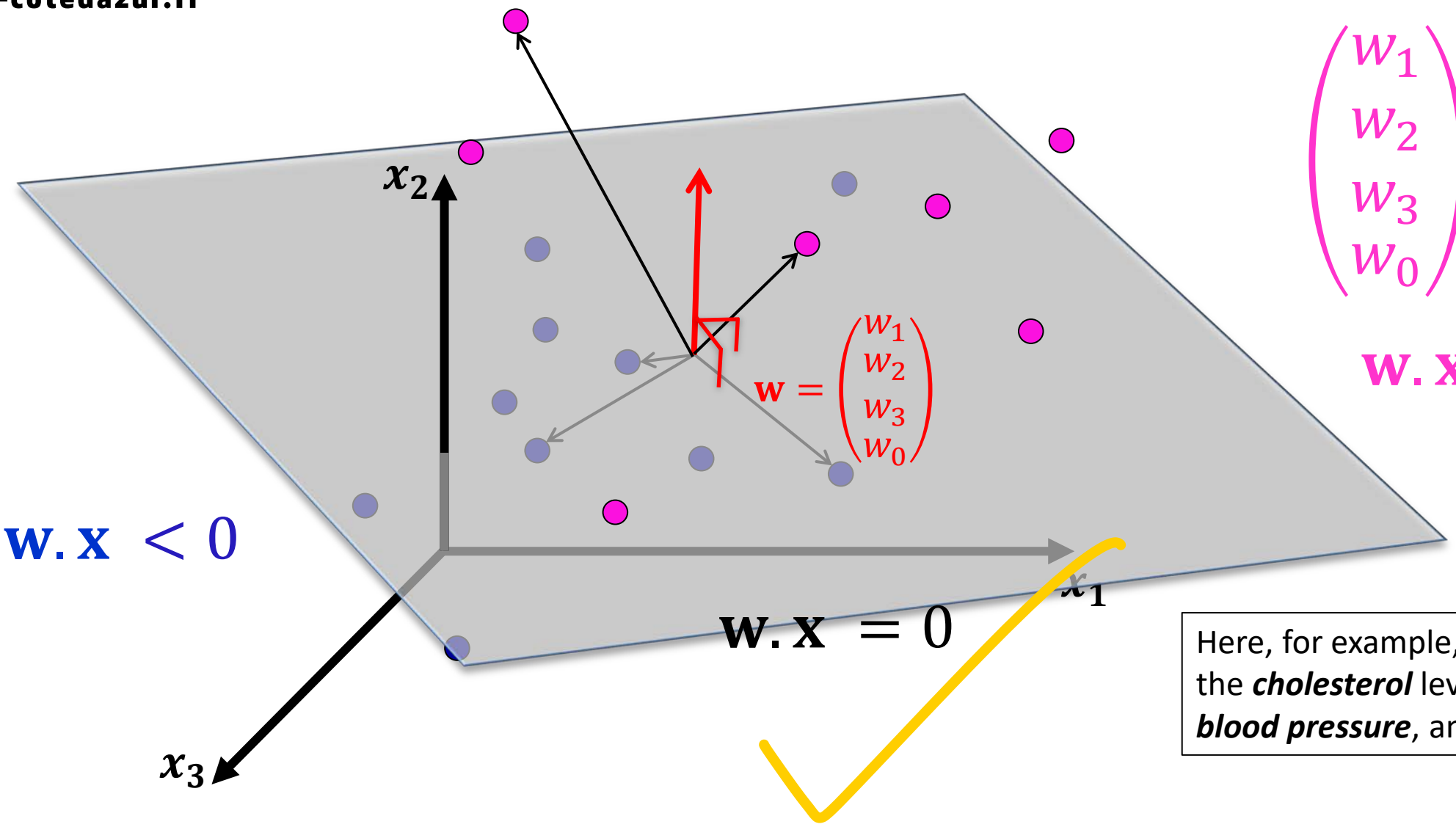
Geometry and Algebra



$$\begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_0 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ 1 \end{pmatrix} > 0$$

$$\mathbf{w}.\mathbf{x} > 0$$

Here, for example, x_1 corresponds to the ***cholesterol*** level, x_2 to ***systolic blood pressure***, and x_3 to ***age.***

Derivative

- Derivative of a scalar function (of one variable)
  - $(ax)' = a$
  - $(ax + b)' = a$
  - $(\mathrm{g}(\mathrm{f}(\mathrm{x})))' = \mathrm{g}'(\mathrm{f}(\mathrm{x}))\mathrm{f}'(\mathrm{x})$ **Chain rule**

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Gradient operator

- Gradient of a multivariate function ($\mathbf{x}$ is a vector)
  - $\nabla_{\mathbf{x}}(\boldsymbol{a}\mathbf{x}) = \boldsymbol{a}$
  - $\nabla_{\mathbf{x}}(\boldsymbol{a}\mathbf{x} + b) = \boldsymbol{a}$
  - $\nabla_{\mathbf{x}}(\mathrm{g}(\mathrm{f}(\mathbf{x}))) = \nabla_{\mathbf{x}}\mathrm{g}\,(\mathrm{f}(\mathbf{x}))\,\nabla_{\mathbf{x}}\mathrm{f}(\mathbf{x})$ **(Chain rule)**

  - $\nabla_{\mathbf{x_i}}(\mathbf{v}.\mathbf{x}) = \nabla_{\mathbf{x_i}}(v_1.x_1 + v_2.x_2 + \cdots + v_n.xn) = v_i$

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Overview

- Machine Learning vs Statistics
- Math Basics
- **Simple Model**
- From Simple to Complex

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SIMPLE MODEL

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Initial Model: Perceptron

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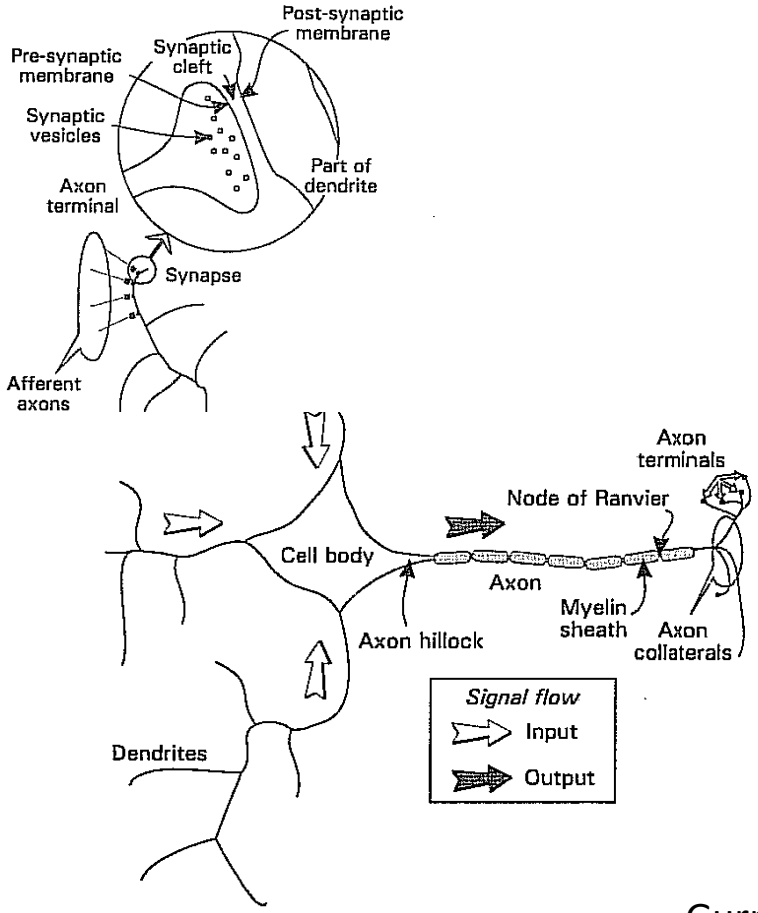
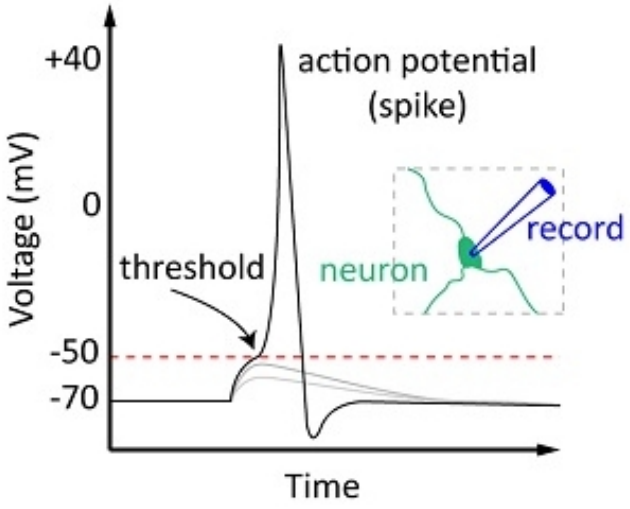
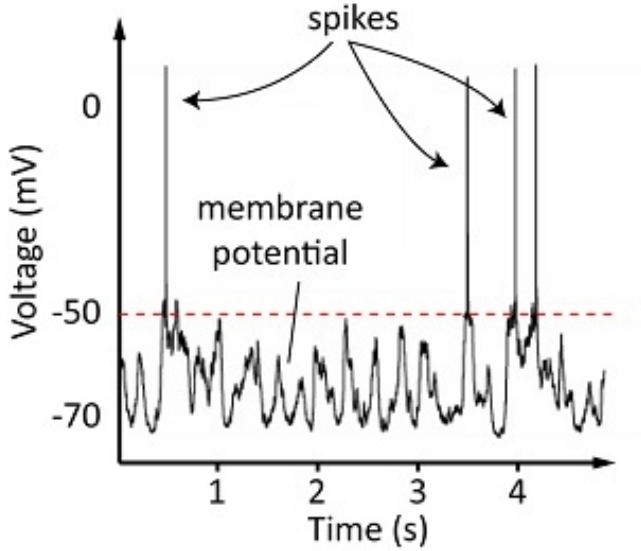
Biological neuron

- Before we study artificial neurons, let's look at a biological neuron







Gurney, K. (1997). *An introduction to neural networks*. CRC press.

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First, biological neurons

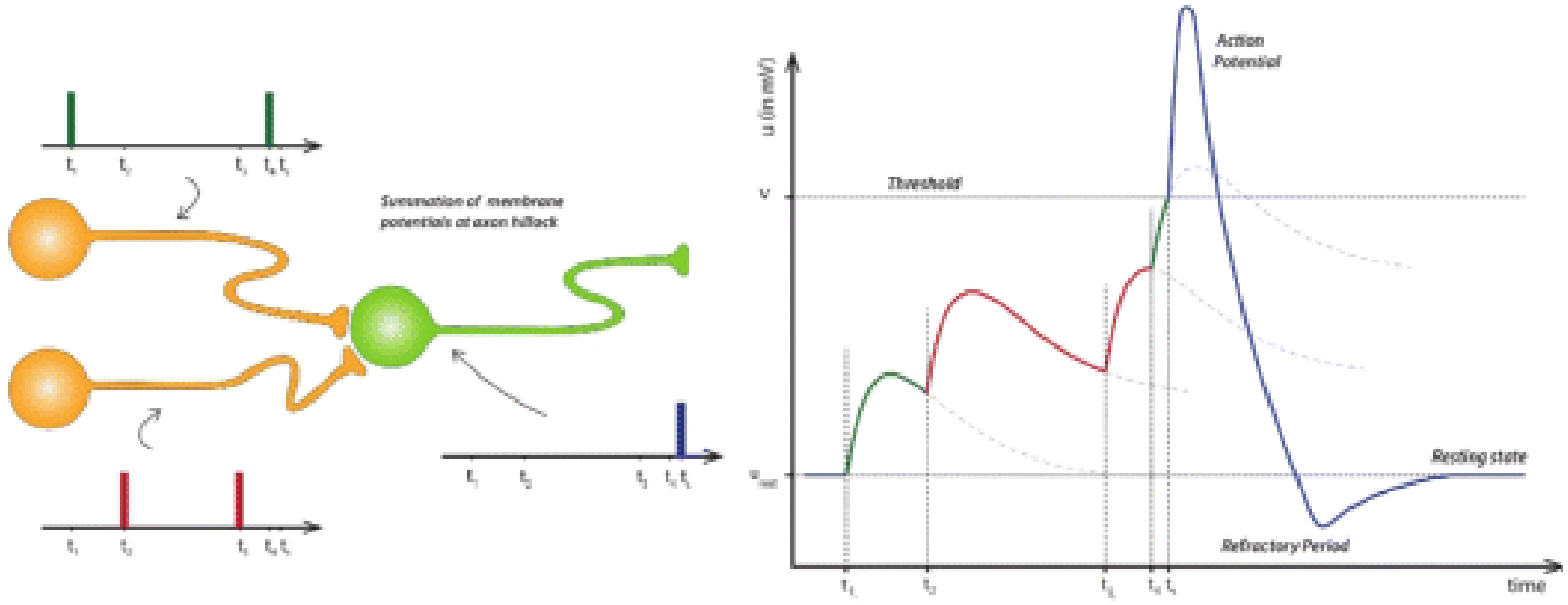

Figure from: Iakymchuk, T., et al. "Simplified spiking neural network architecture and STDP learning algorithm applied to image classification". In Journal of Image Video Proc. 2015, 4 (2015).

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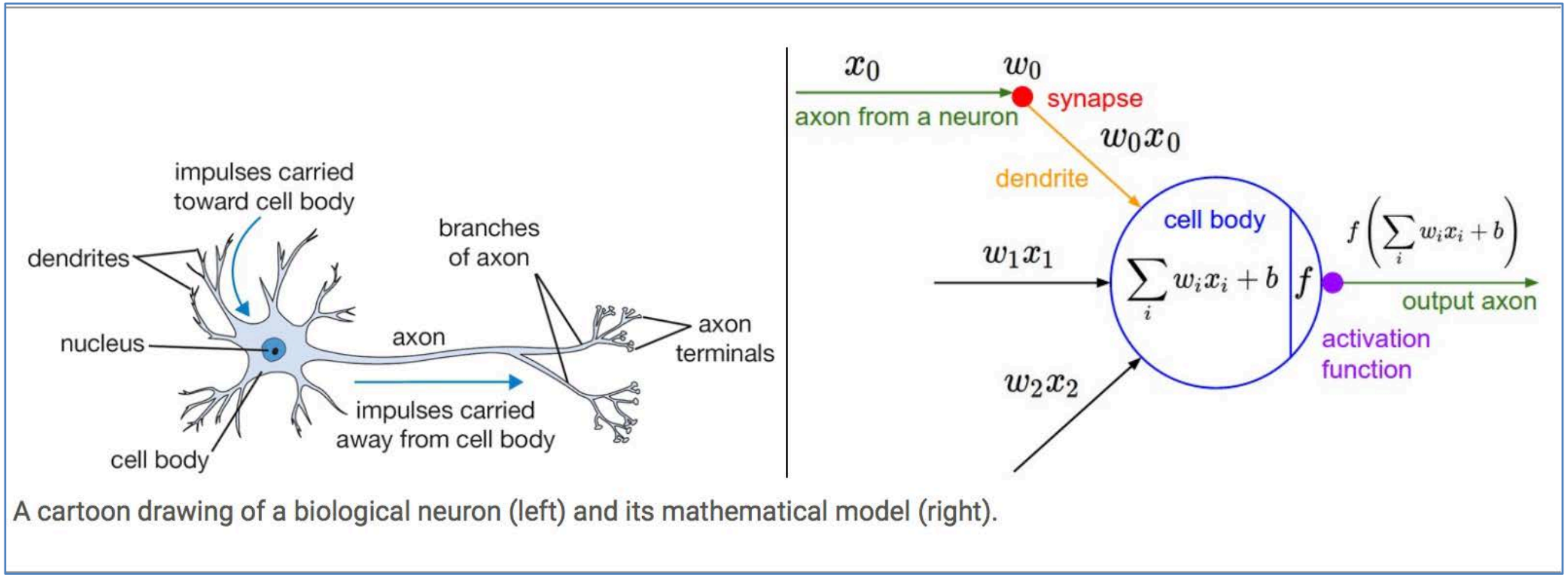
Then, artificial neurons



A cartoon drawing of a biological neuron (left) and its mathematical model (right).

Pitts & McCulloch (1943), binary inputs & activation function *f* thresholding

Rosenblatt (1956), real inputs & activation function *f* thresholding

(Schéma : Isaac Changhau)

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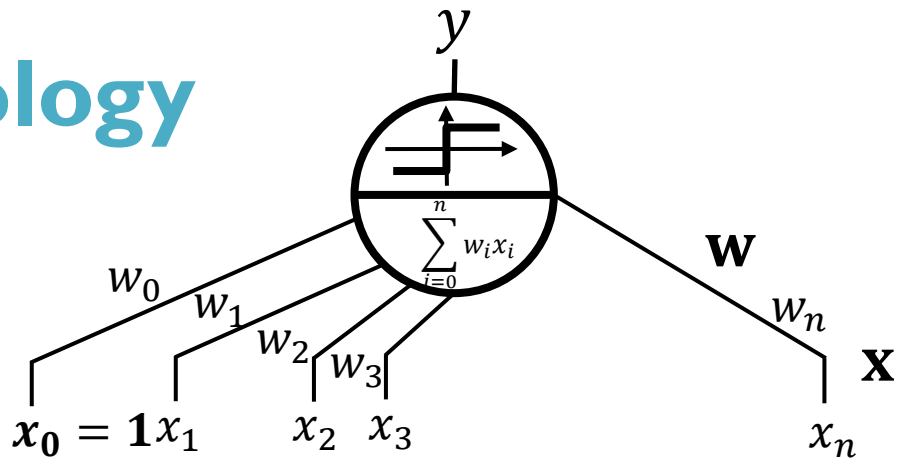
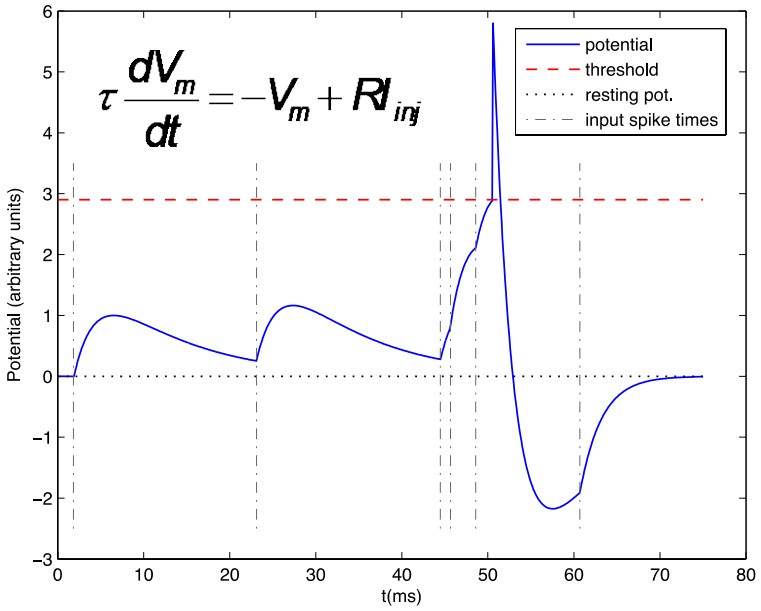
Artificial vs biology



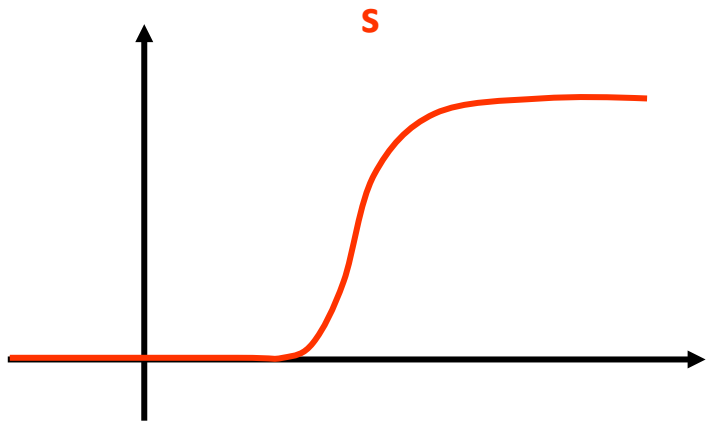
Spike-based description



Gradient descent: KO

Rate-based description

Steady regime



$y = s(\Sigma w_i x_i)$

Gradient descent: OK

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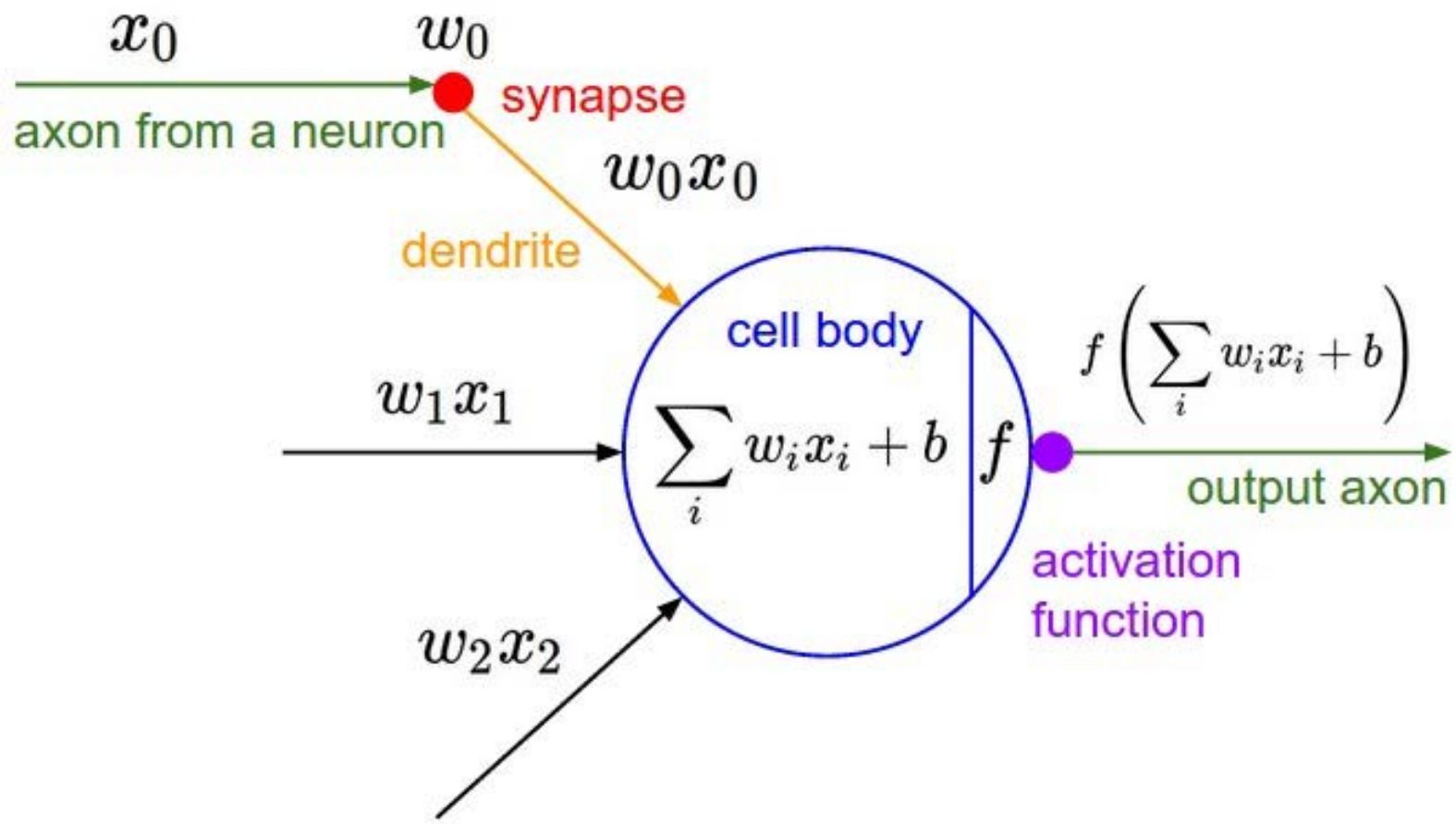
A single artificial neuron

- It is a **very simple abstract** of a biological neuron (McCulloch & Pitts, 1943)



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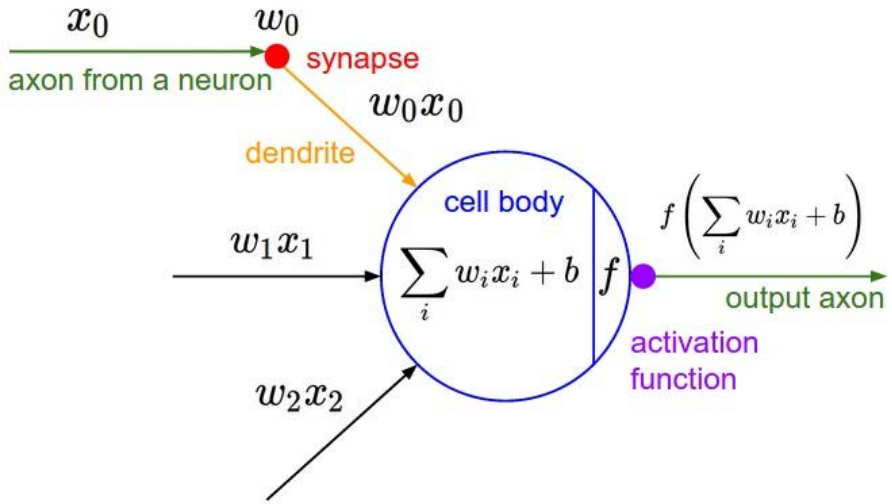
A single artificial neuron



- Each input *x* has an associated **weight *w*** which can be modified
- Inputs *x* corresponds to signals from other neuron axons
  - x_0 - Bias are 'special' inputs, with weight w_0
- Weights ***W*** corresponds to synaptic modulation (i.e. something like strength/amount of neurotransmitters)
- The summation corresponds to 'cell body'
- The activation function corresponds to axon hillock - computes some function *f* of the weighted sum of its inputs
- So, output *y=f(z)*, corresponds to axon signal

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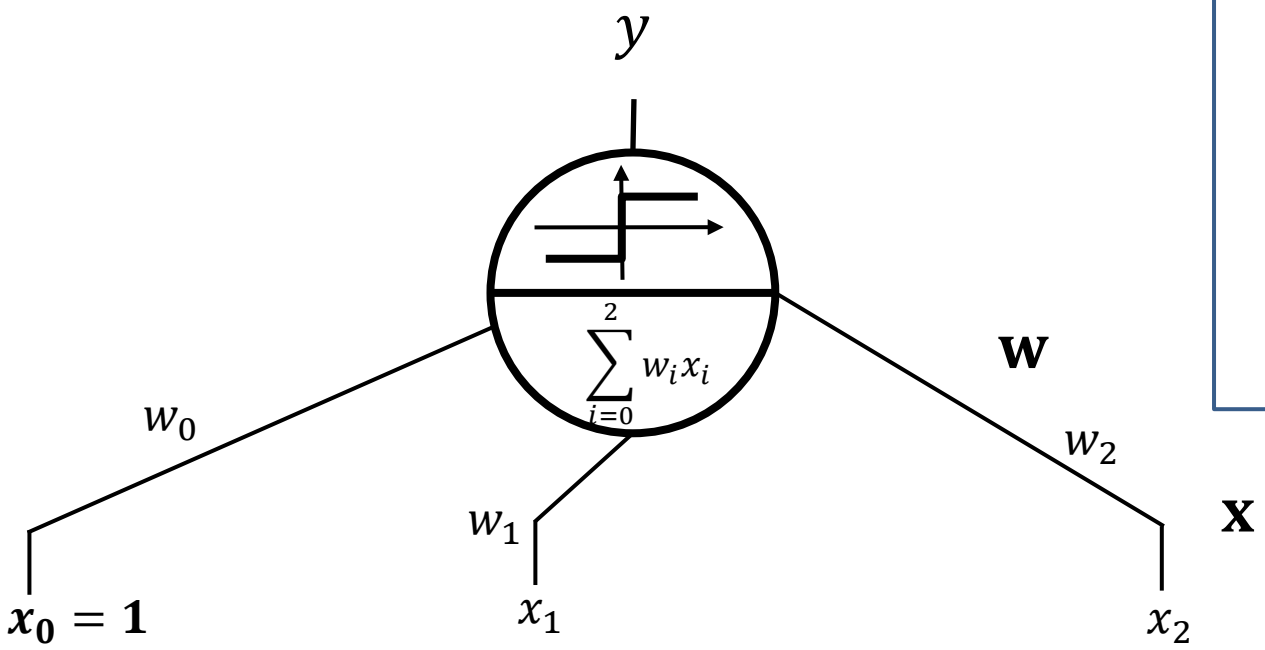
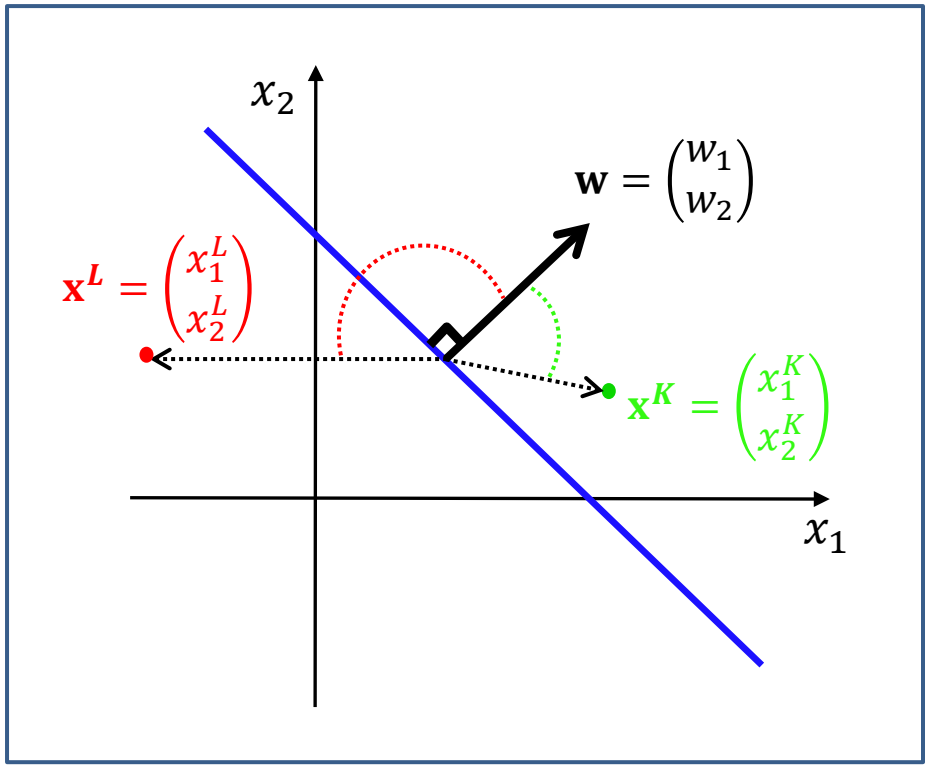
Artificial neuron = a linear classifier





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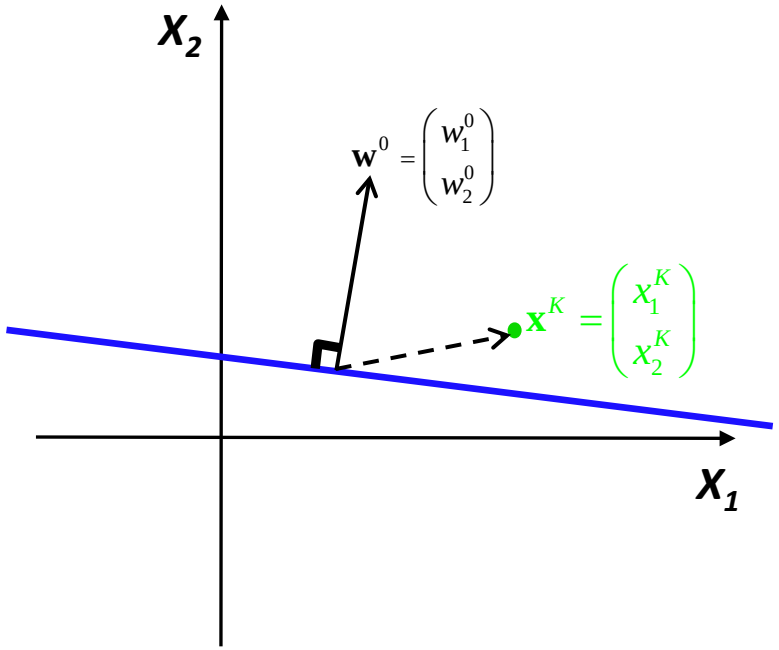
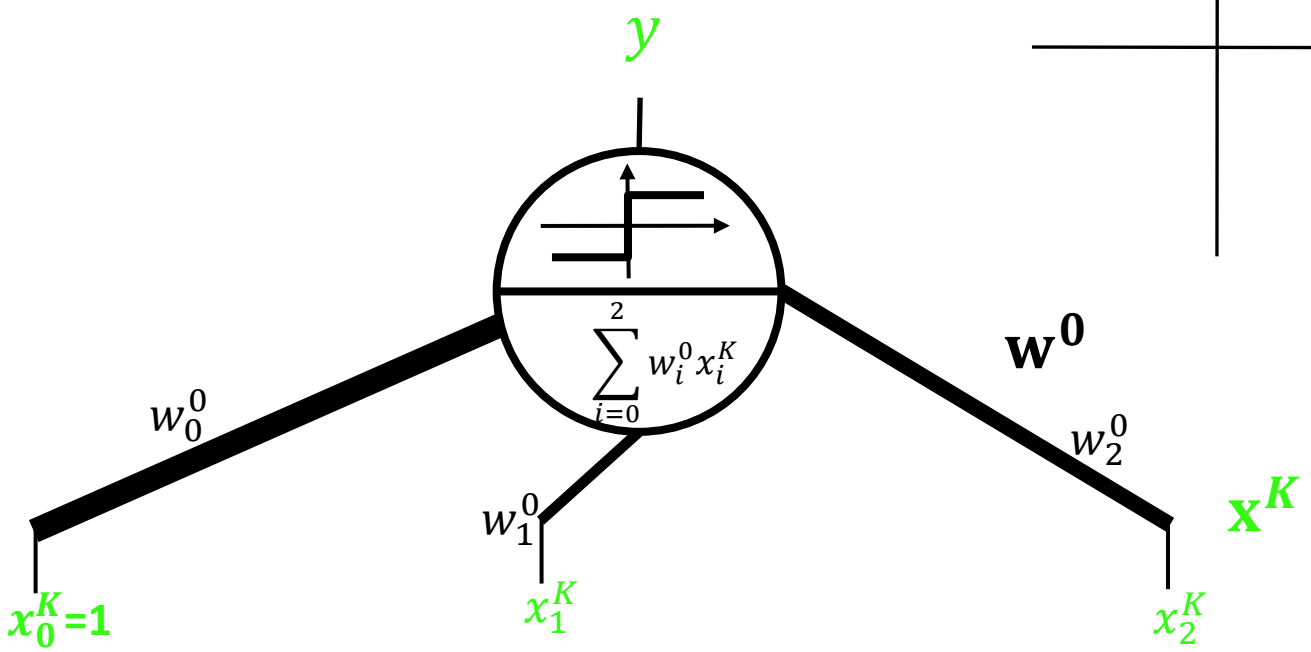
One artificial neuron (perceptron)

At training you want to set the weights,
so that your training samples are correctly classified:





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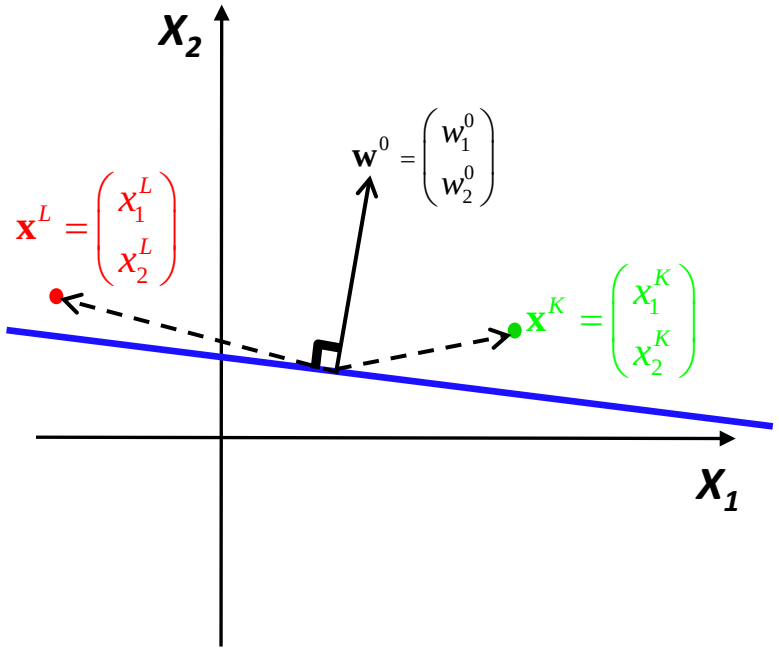

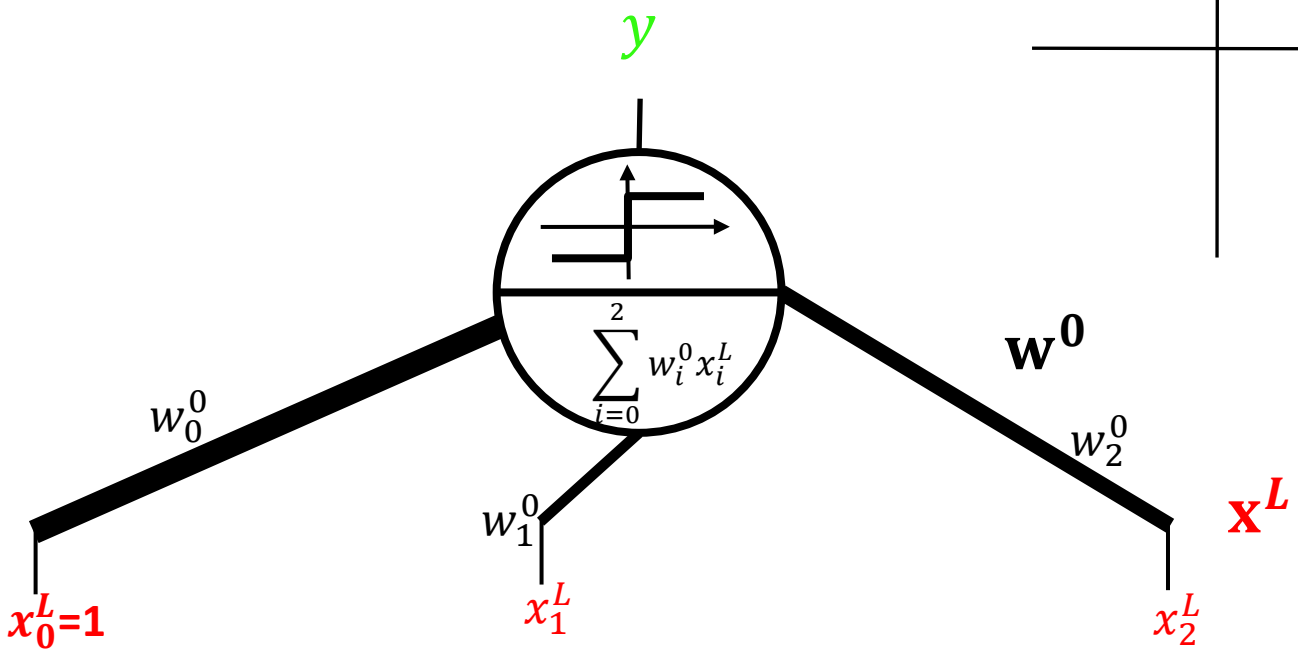

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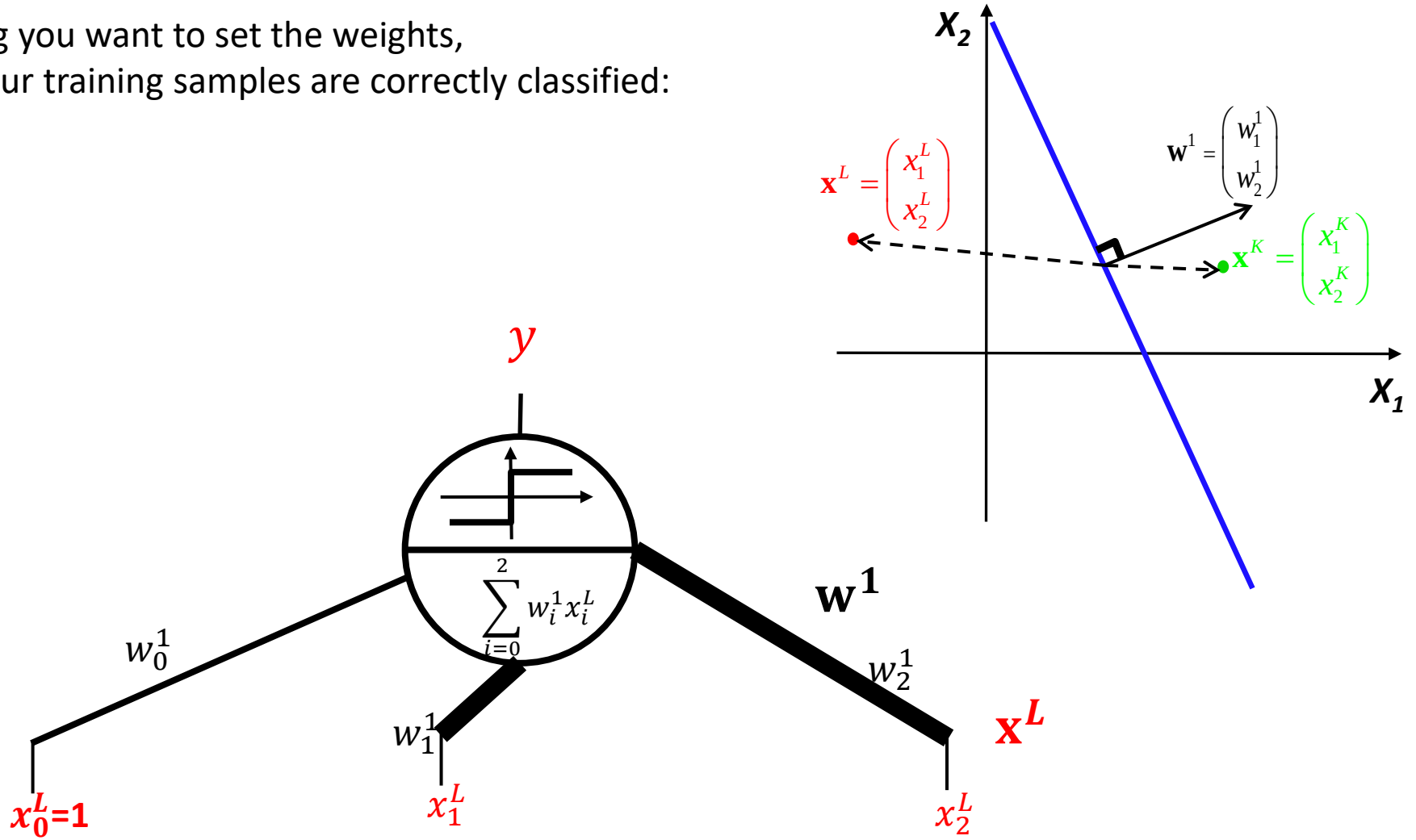

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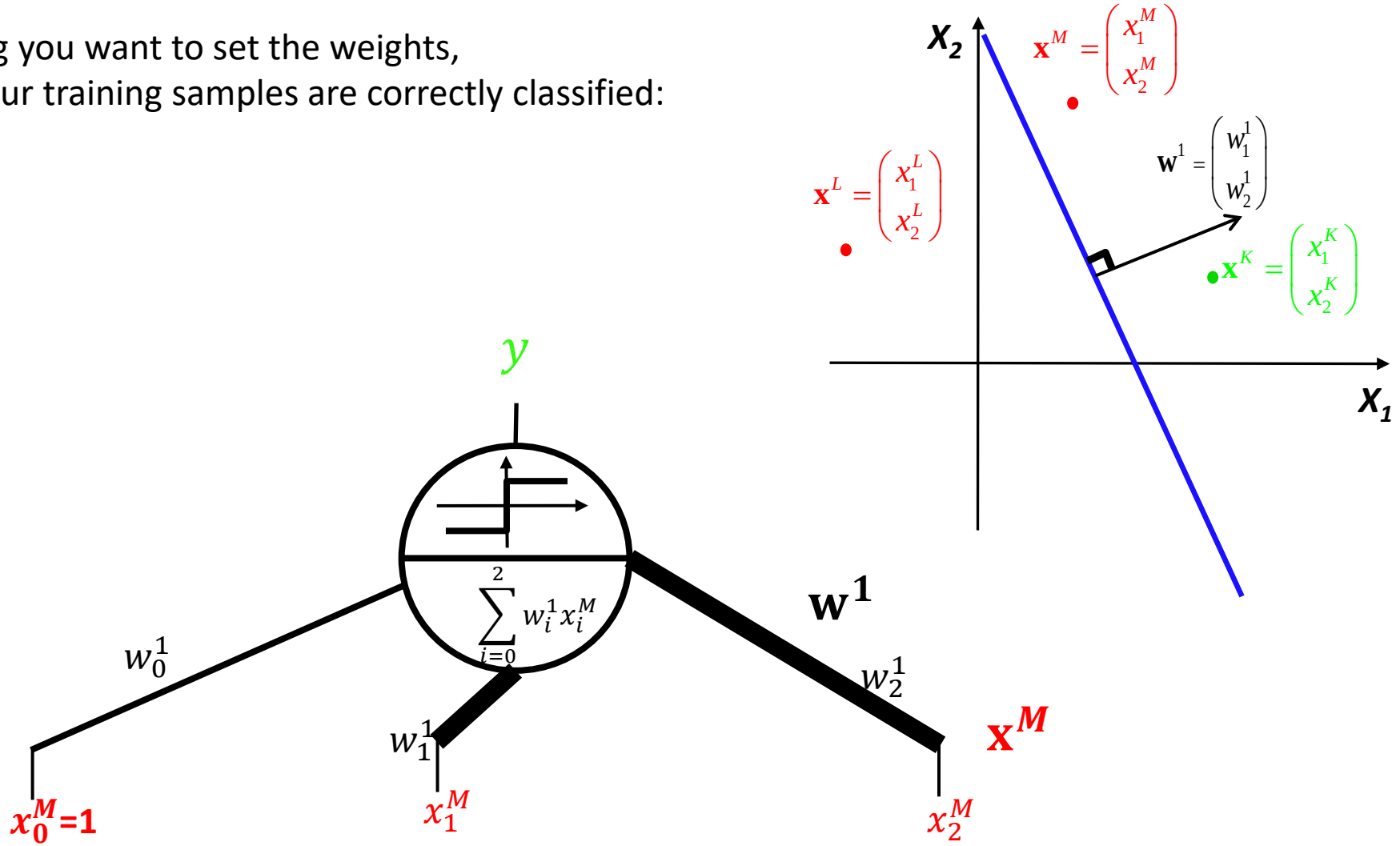

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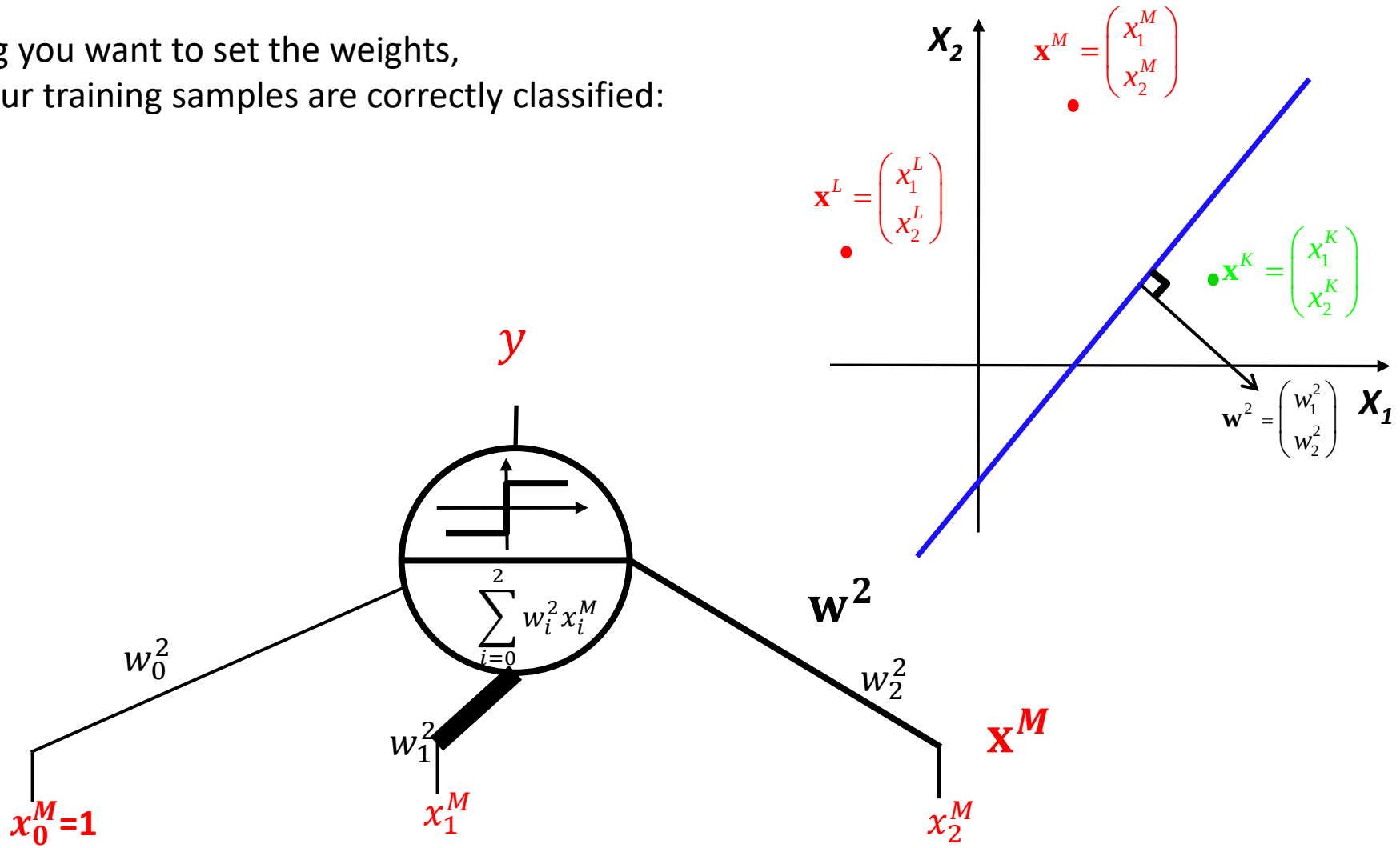

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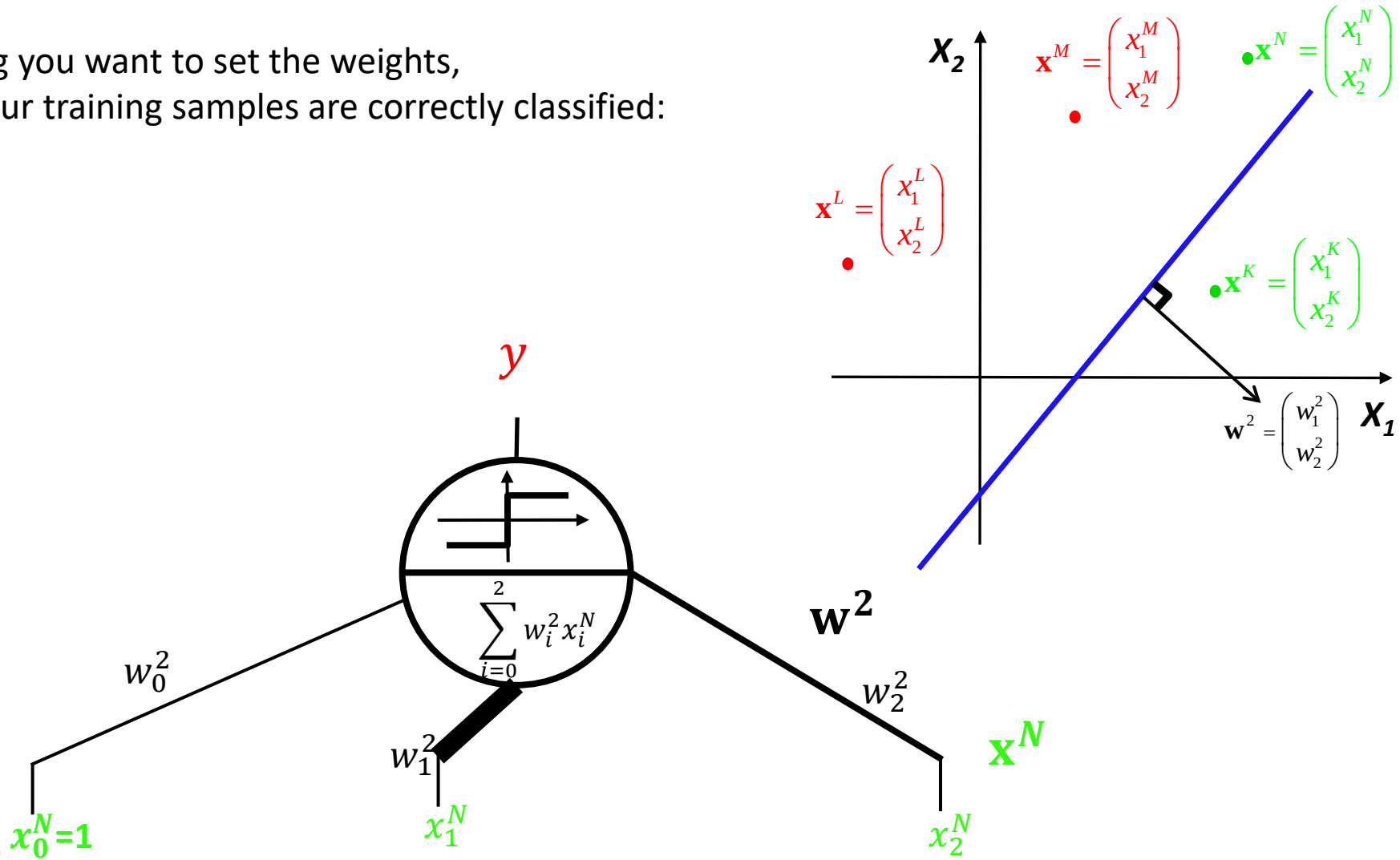

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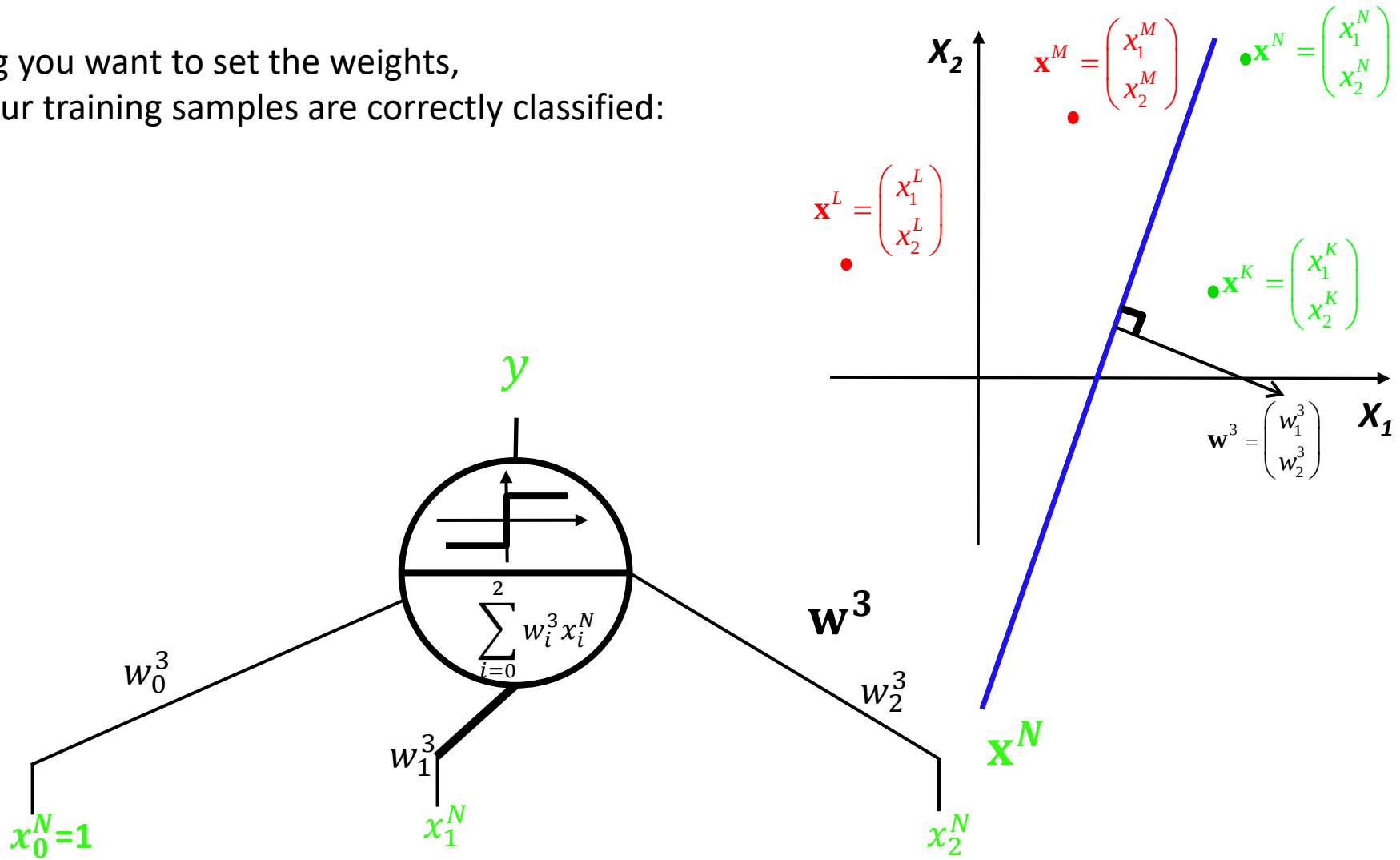

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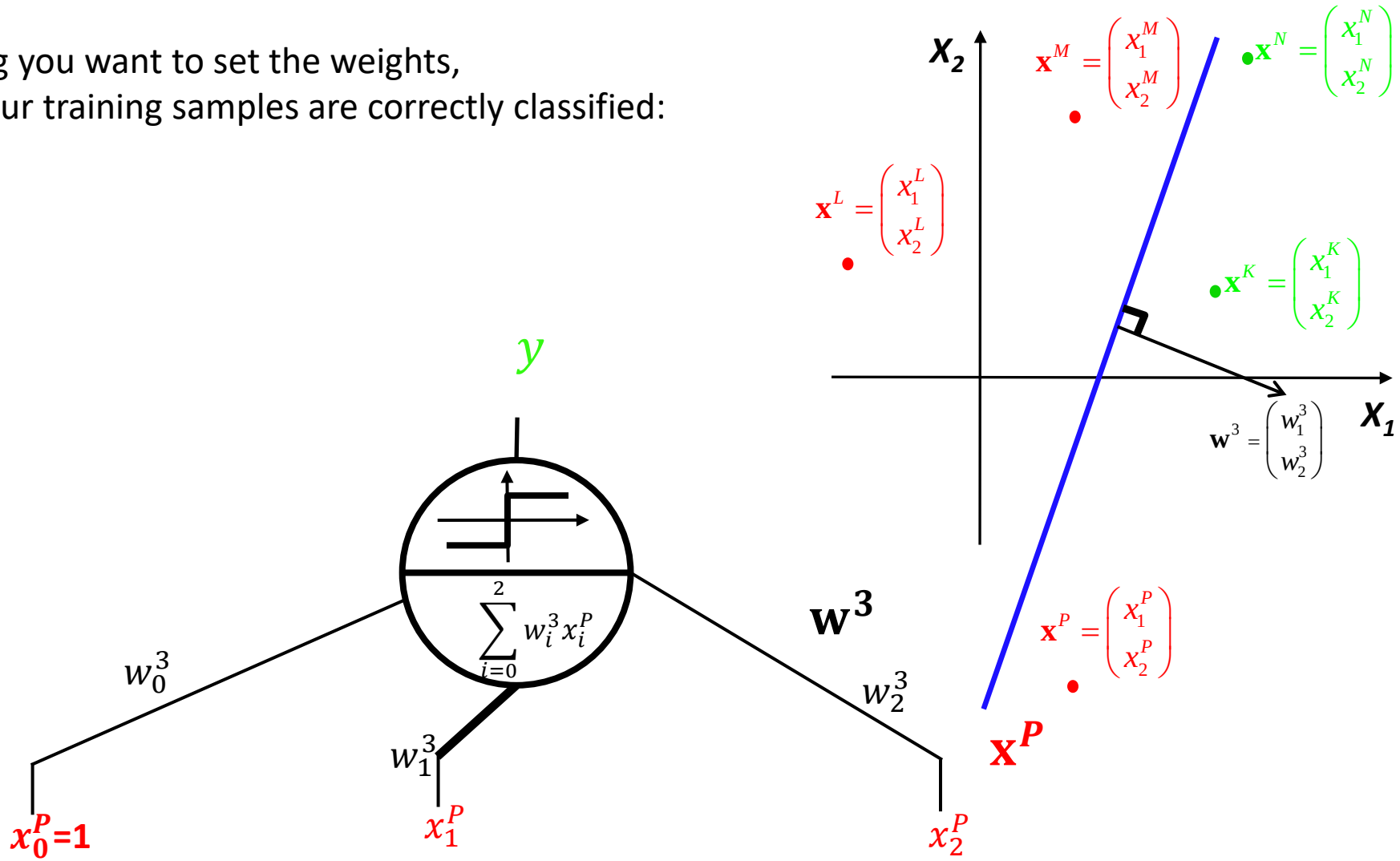

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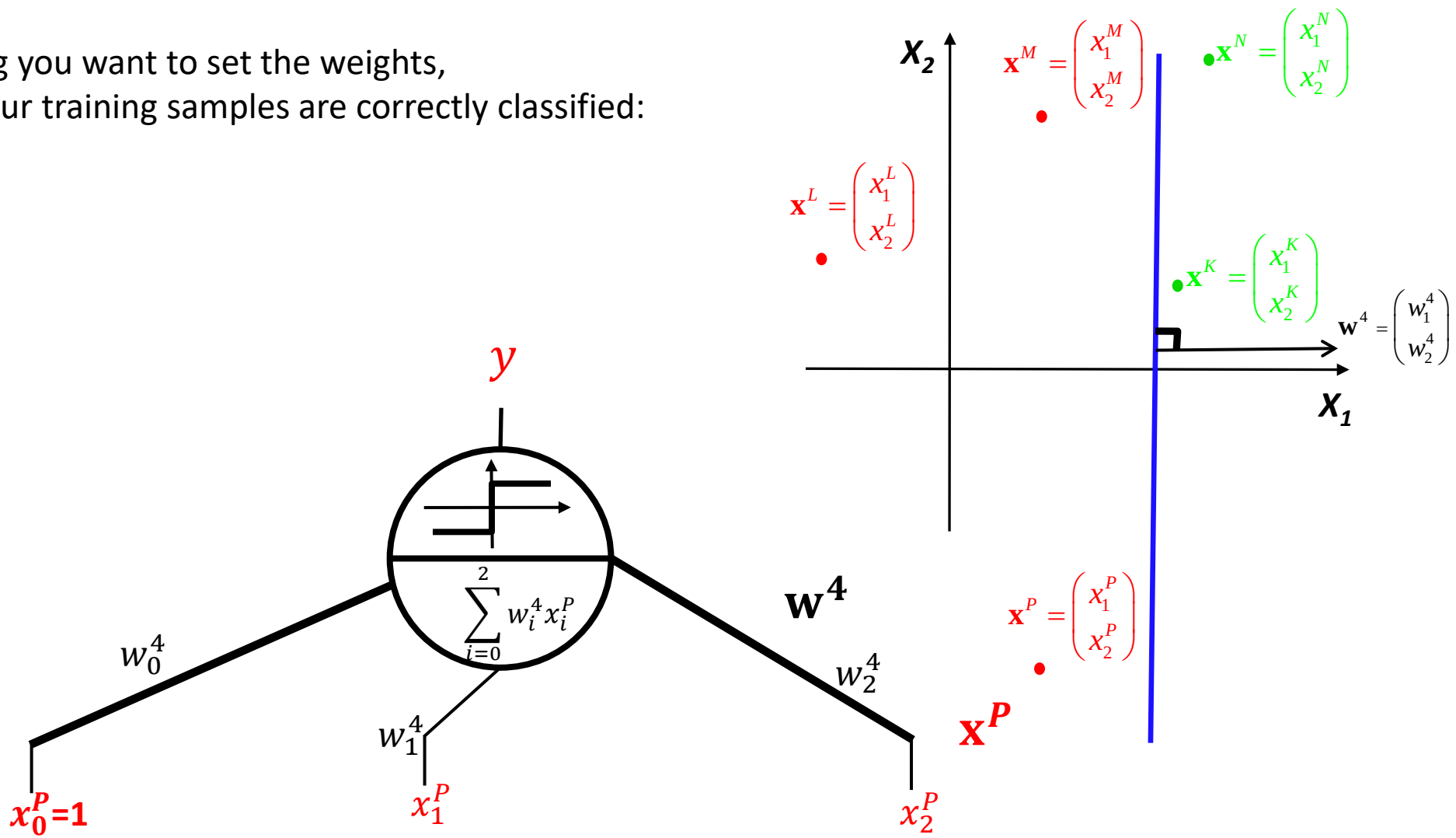

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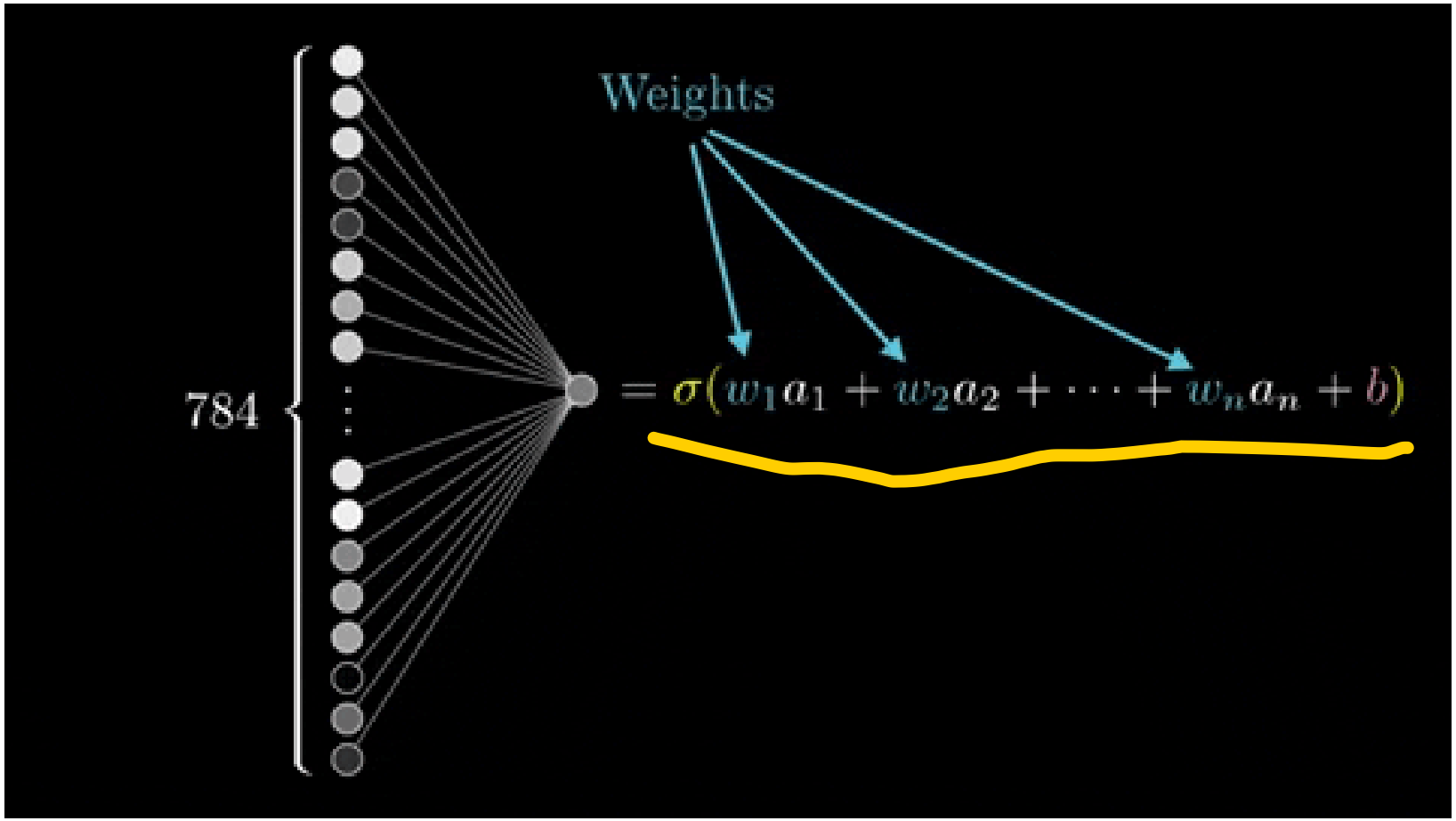
One neuron = simple linear decision



Source: https://www.3blue1brown.com/neural-networks

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Perceptron: Rosenblatt's Algorithm (1956-1958)

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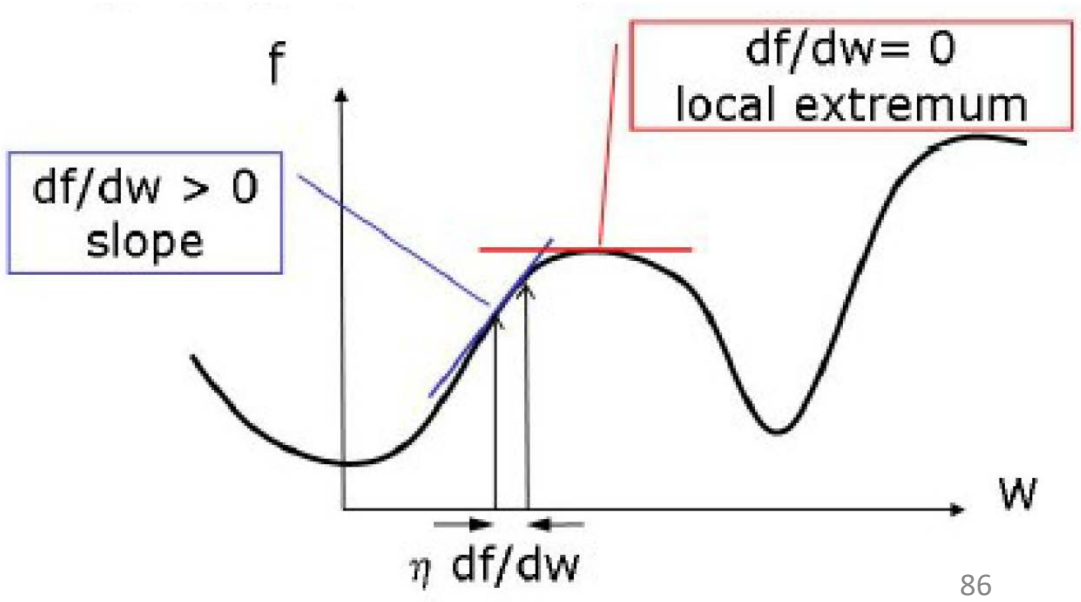
Perceptron Algorithm

- Pick initial weight vector (including w_0), e.g. (0, 0,…,0)
- Repeat until all points are correctly classified
  - *Repeat for each point*
    - Calculate $y^i\mathbf{w}\mathbf{x}^i$ for point i
    - If $y^i\mathbf{w}\mathbf{x}^i > 0$, the point is correctly classified
    - Else change the weights to increase the value of $y^i\mathbf{w}\mathbf{x}^i$; change in weight proportional to $y^i\mathbf{x}^i$

Rosenblatt, F. (1958). The perceptron: a probabilistic model for information storage and organization in the brain. Psychological review, 65(6):386.

Gradient Ascent

- Why pick $y^i\mathbf{x}^i$ as increment to weights?
- To maximize scalar function of one variable $f(\mathbf{w})$
  - Pick initial $\mathbf{w}$
  - Change $\mathbf{w}$ to $\mathbf{w} + \eta\, df/d\mathbf{w}$ ($\eta > 0$, small)
  - Until f stops changing ($df/d\mathbf{w} \approx 0$)



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Gradient Ascent

- To maximize a multivariate function $f(\mathbf{w})$
  - Pick initial $\mathbf{w}$
  - Change $\mathbf{w}$ to $\mathbf{w} + \eta \nabla f_{\mathbf{w}}$ ($\eta > 0$, small)
  - Until f stops changing ($\nabla f_{\mathbf{w}} \approx 0$)
- Find local maximum, unless function is globally convex

$$\nabla f_{\mathbf{w}} = \left[\frac{\partial f}{\partial \mathbf{w}_1}, \quad \dots \quad , \frac{\partial f}{\partial \mathbf{w}_n} \right]$$

Gradient Ascent

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  - Pick initial $\mathbf{w}$
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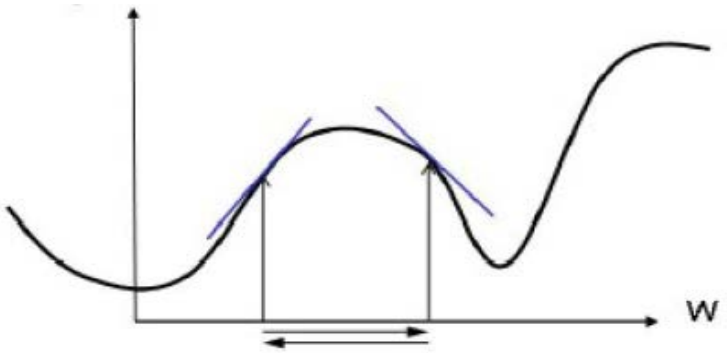
$$\nabla f_{\mathbf{w}} = \left[\frac{\partial f}{\partial \mathbf{w}_1}, \quad \ldots \quad , \frac{\partial f}{\partial \mathbf{w}_n} \right]$$

- Find local maximum, unless function is globally convex
- If f is non-linear, the learning rate η has to be chosen very carefully
  - Too small $\Rightarrow$ slow convergence
  - Too big $\Rightarrow$ osccilations



Gradient Ascent

- Maximize margin of misclassified points

$$f(\mathbf{w}) = \sum_{on\ \mathbf{i}\ misclassified\ points} y^i \mathbf{w}\mathbf{x}^{\mathrm{i}}$$

$$\nabla_{\mathbf{w}} f(\mathbf{w}) = \sum_{on\ \mathbf{i}\ misclassified\ points} y^i \mathbf{x}^{\mathrm{i}}$$

- Off-line training: Compute, at each iteration, the gradient as sum over all training points
- On-line training: Approximate gradient by one of the terms in the sum: $y^i \mathbf{x}^{\mathrm{i}}$ (principle of the *Stochastic Gradient Descent*, SGD)

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Perceptron Algorithm

- Each change of **w** decreases the error on a specific point. However, changes for several points are correlated, that is different points could change the weights in opposite directions. Thus, this iterative algorithm requires several loops to converge.

- Guarantee to find a separating hyperplane if one exists – if data is linearly separable.

- If data are not linearly separable, then this algorithm loops indefinitely.

Rosenblatt, F. (1958). The perceptron: a probabilistic model for information storage and organization in the brain. Psychological review, 65(6):386.

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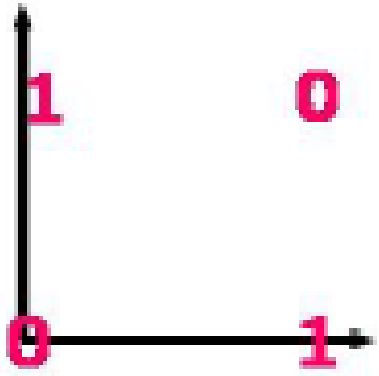
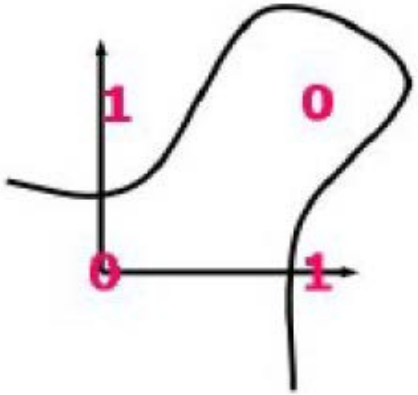
Beyond Linear Separability

- Values of the XOR boolean function cannot be separated by a single perceptron unit
  [Minsky and Papert, 1969].





Minsky, M. and Papert, S. (1969). Perceptrons: An Introduction to Computational Geometry. MIT Press.

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Overview

- Machine Learning vs Statistics
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FROM SIMPLE TO COMPLEX

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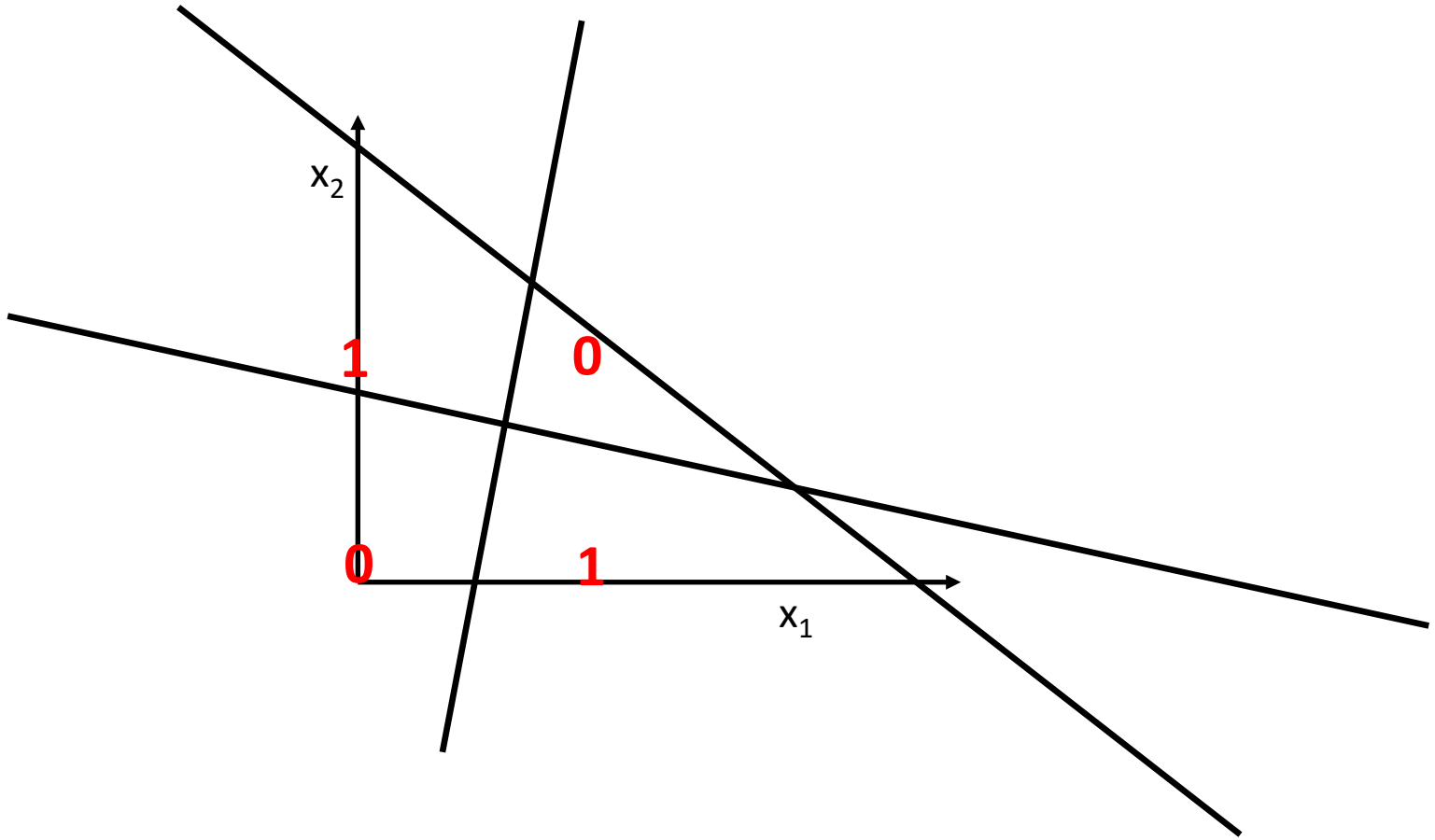
Problem which cannot be solved with a unique straight line



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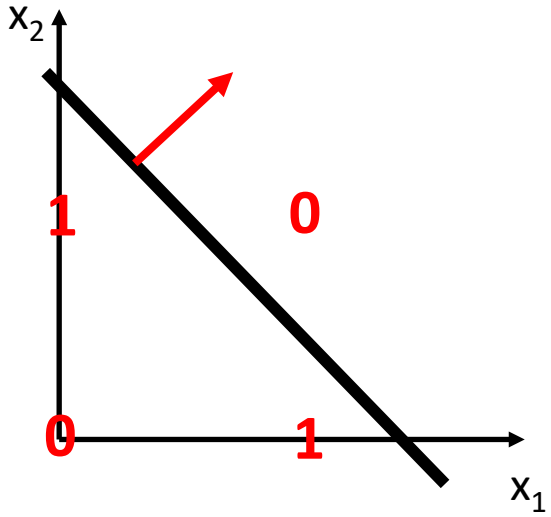
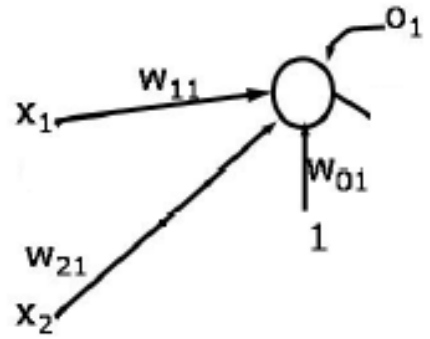
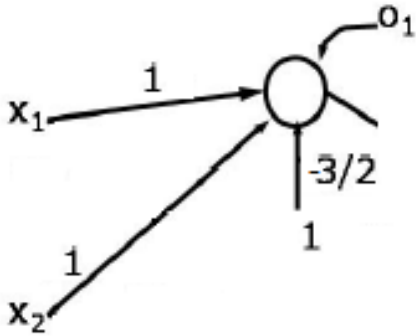
Problem which cannot be solved with a unique straight line





$w_{01} = -3/2 \quad w_{11} = w_{21} = 1$

x_1	x_2	o_1
0	0	0
0	1	0
1	0	0
1	1	1



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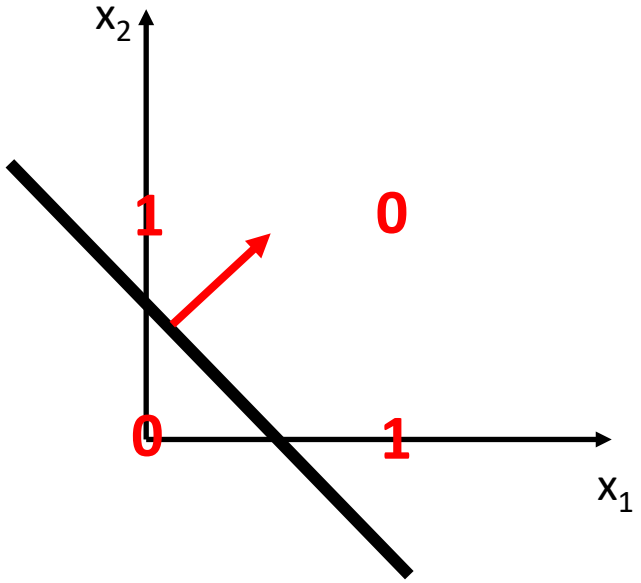
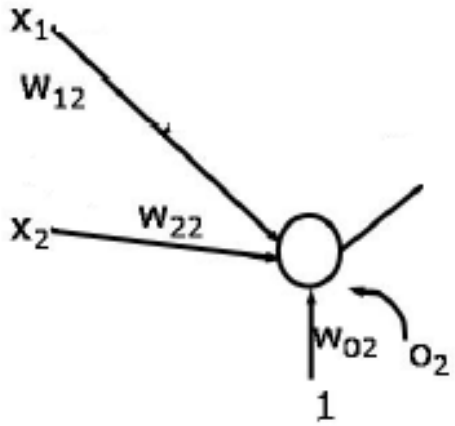
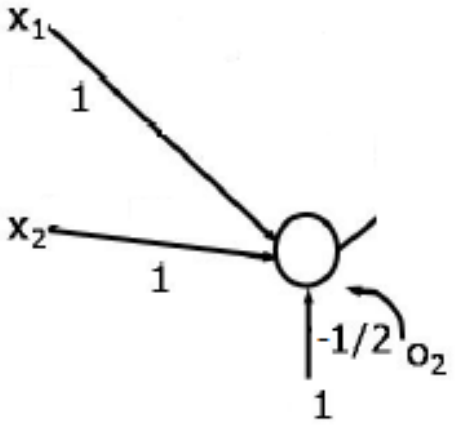
Problem which cannot be solved with a unique straight line



x_1	x_2	o_1	o_2
0	0	0	0
0	1	0	1
1	0	0	1
1	1	1	1



$w_{02} = -1/2 \quad w_{12} = w_{22} = 1$



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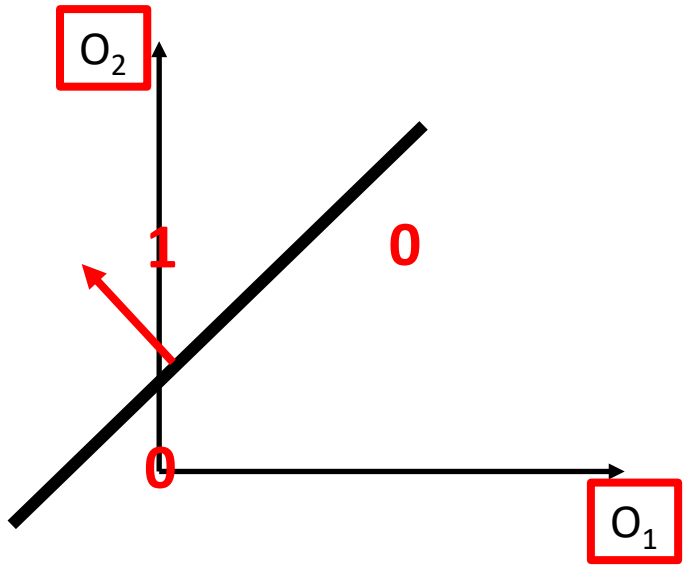
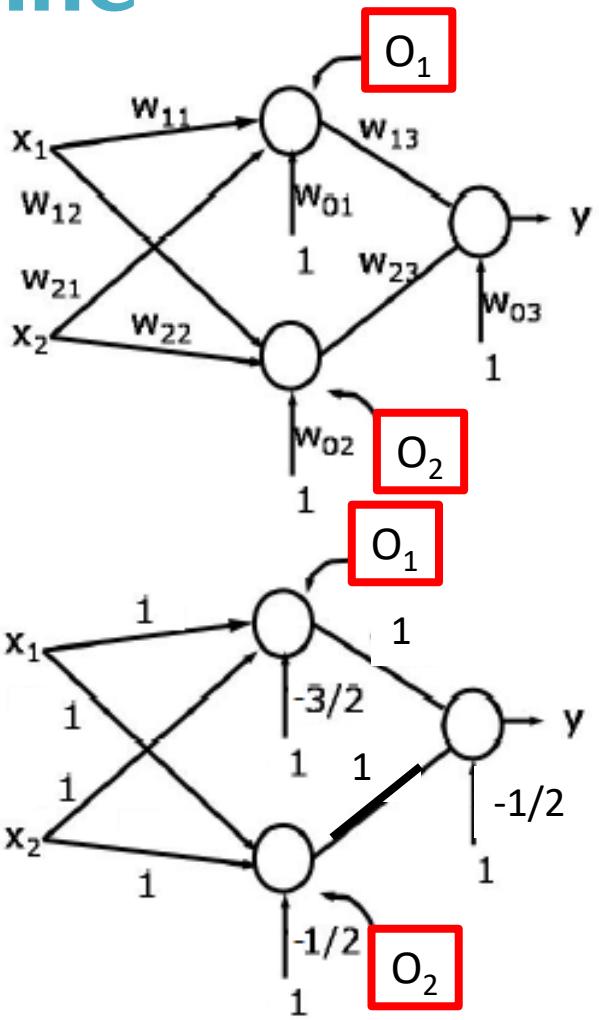
Problem which cannot be solved with a unique straight line



$O_2-O_1-1/2=0$

o_1	o_2	y
0	0	0
0	1	1
0	1	1
1	1	0



$w_{23}o_2+w_{13}o_1+w_{03}=0$

$w_{03}=-1/2$, $w_{13}=-1$, $w_{23}=1$

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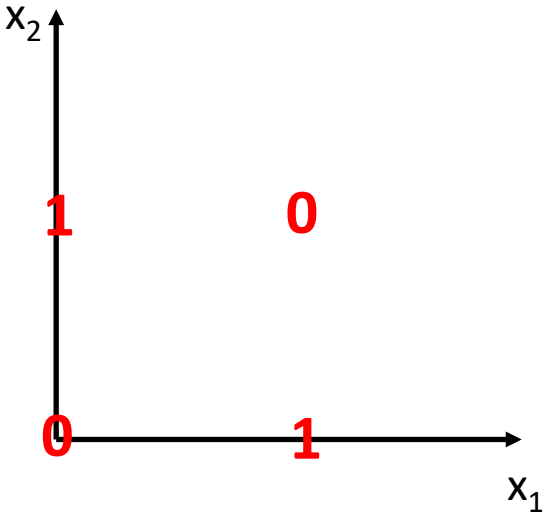
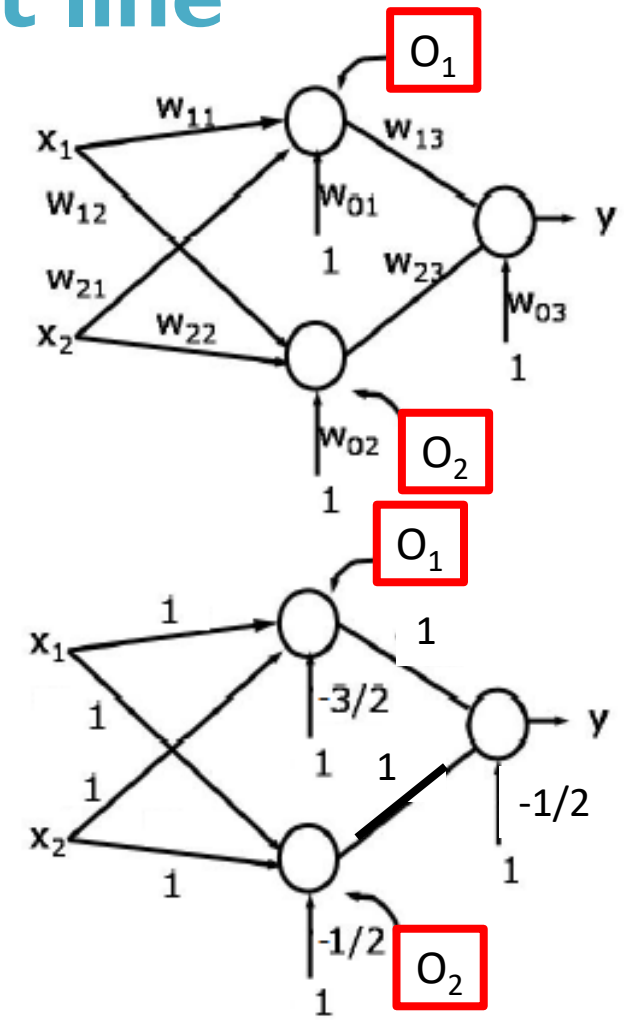
Problem which cannot be solved with a unique straight line



x_1	x_2	o_1	o_2	y
0	0	0	0	0
0	1	0	1	1
1	0	0	1	1
1	1	1	1	0



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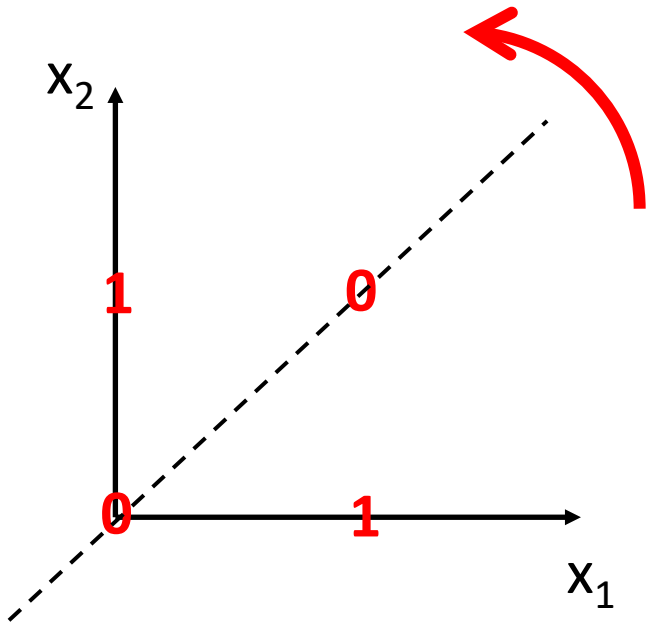

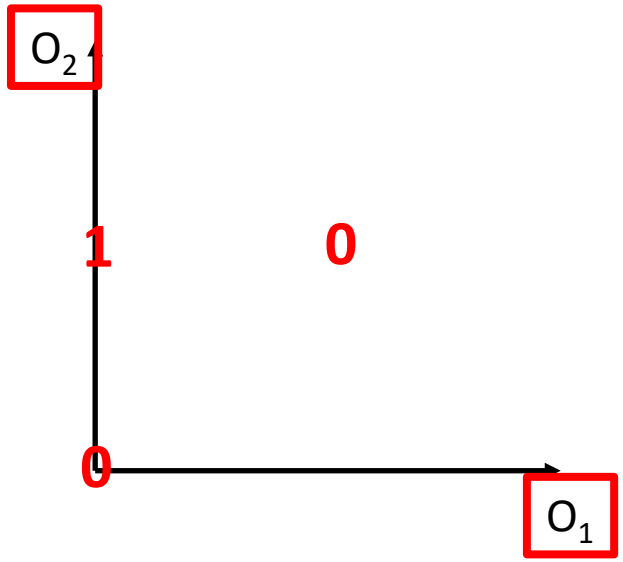

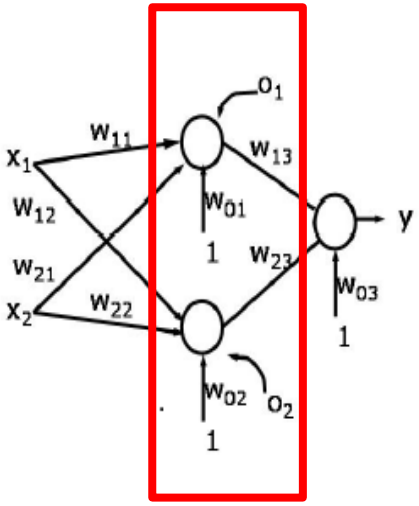

Adding a hidden layer of neurons has fold the input space

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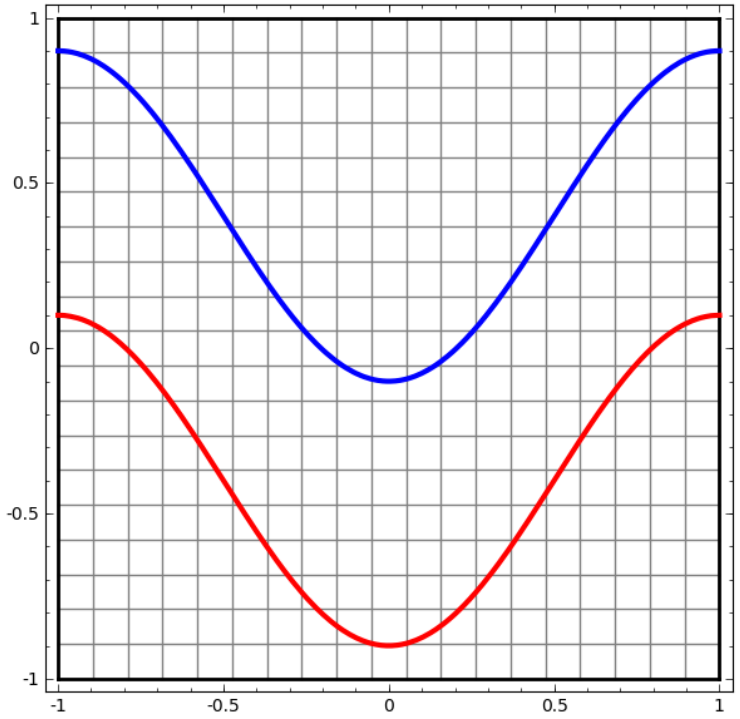
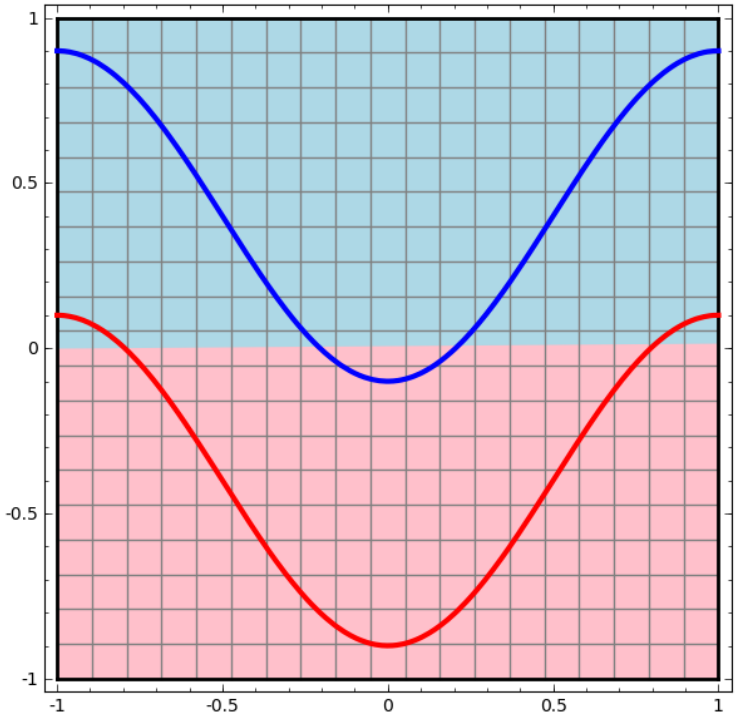
One perceptron





Illustrations from: http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

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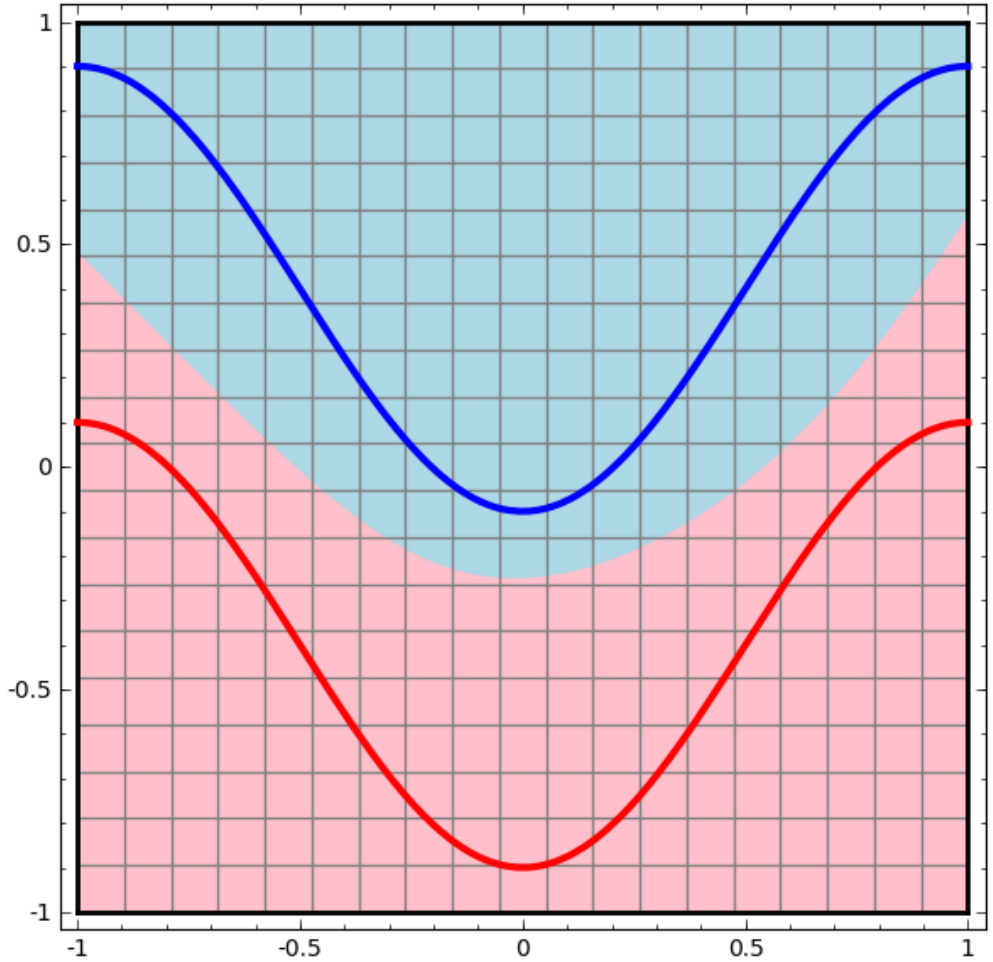
Multi-Layer Perceptron, manifold disentanglement



Illustrations from: http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

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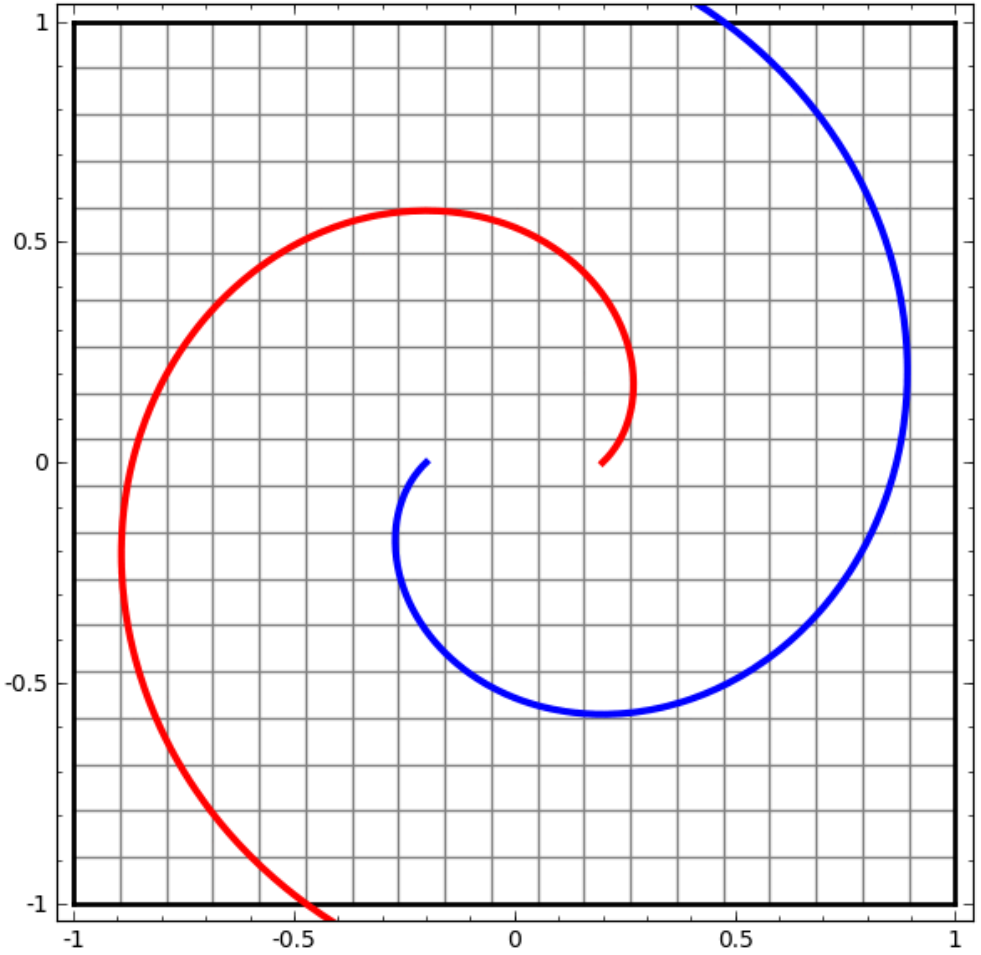
Multi-Layer Perceptron, manifold disentanglement



Illustrations from: http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

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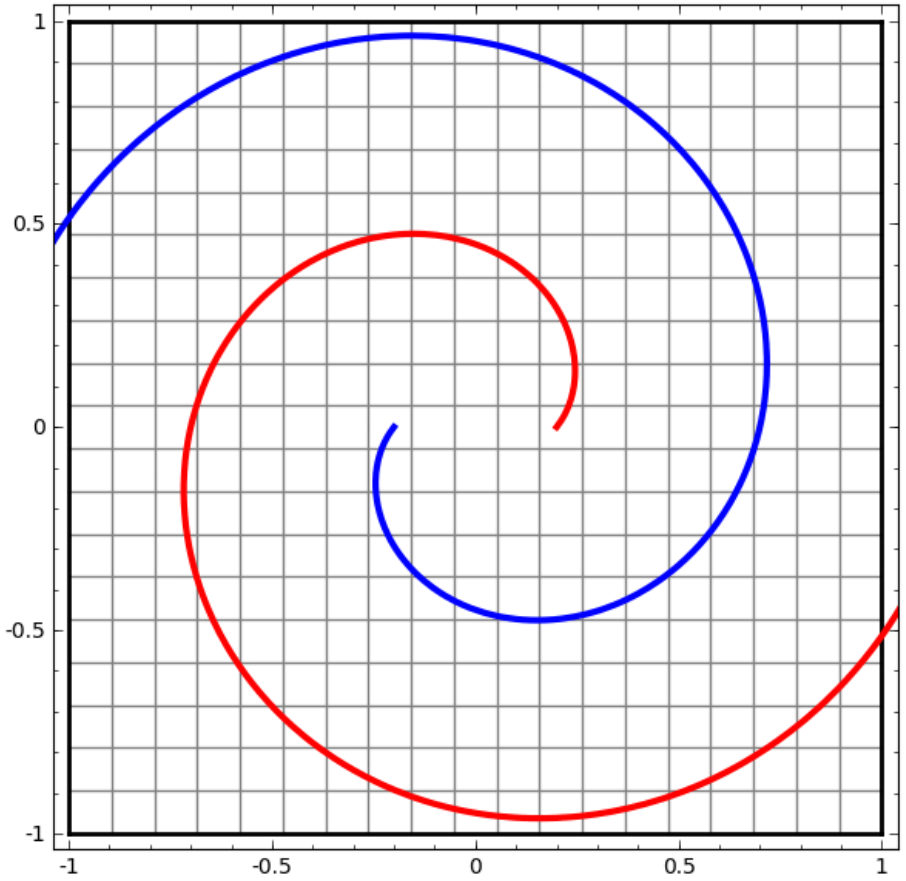
Multi-Layer Perceptron, manifold disentanglement



Illustrations from: http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

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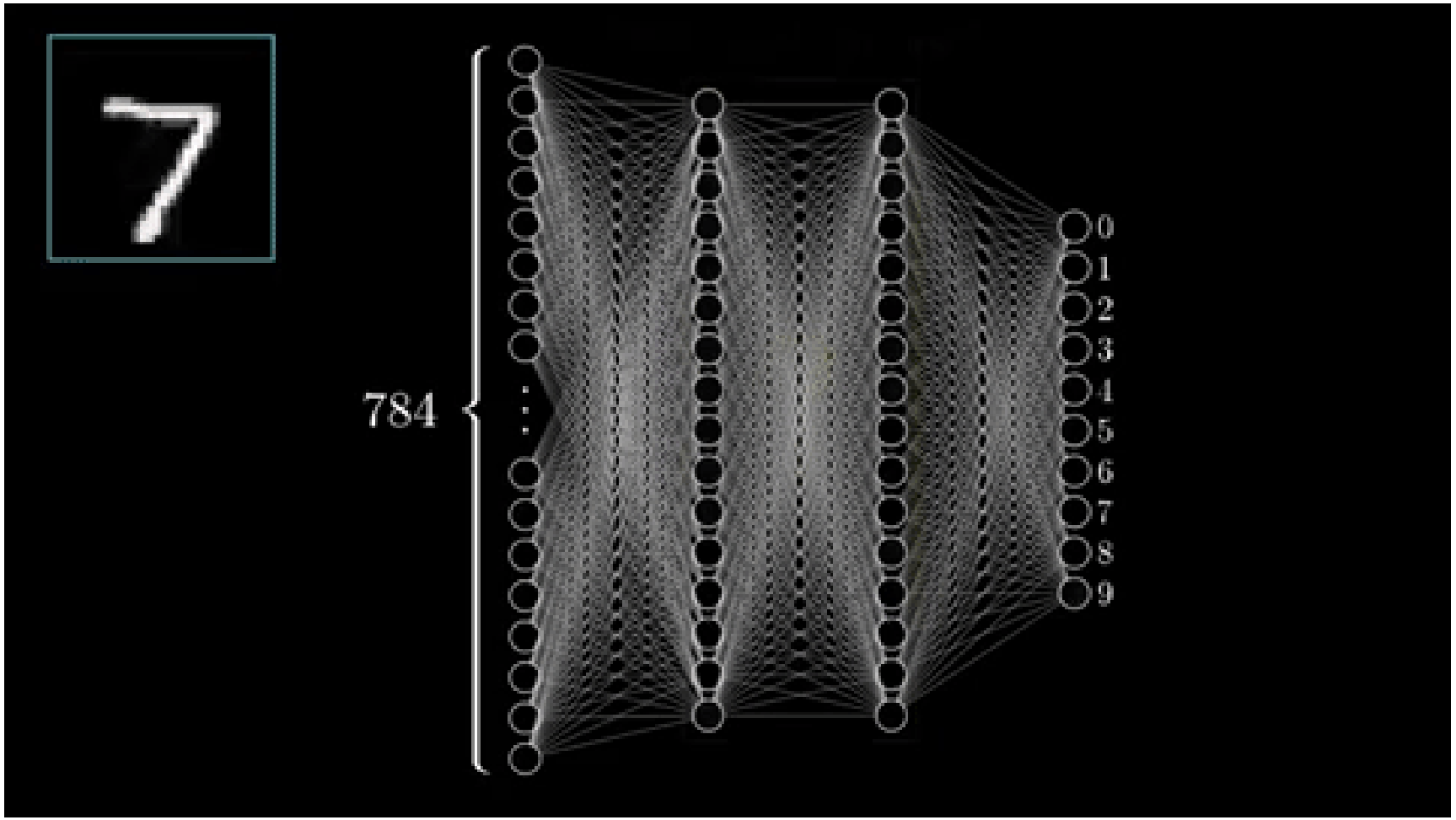
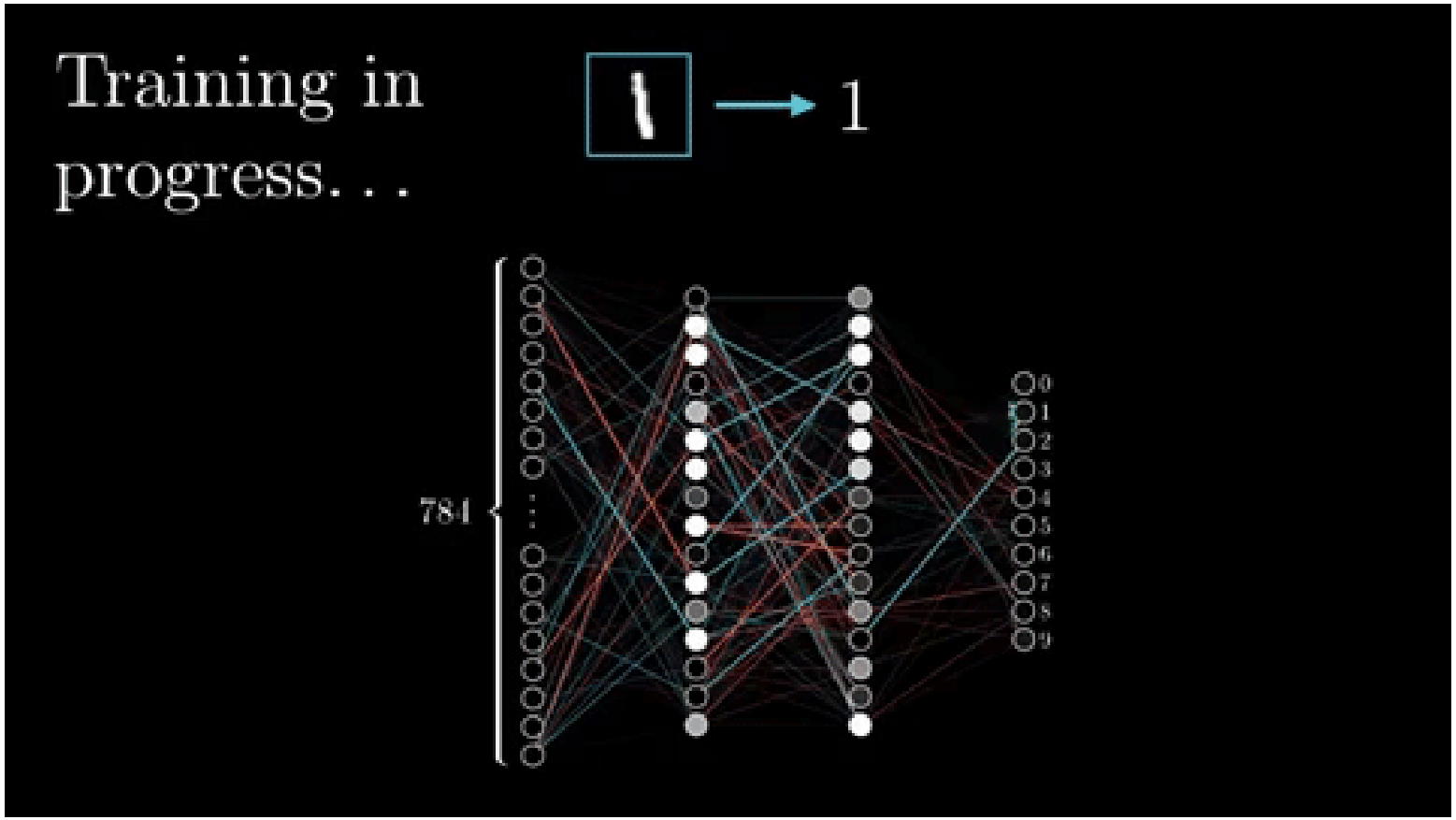
Solution: Neural Network



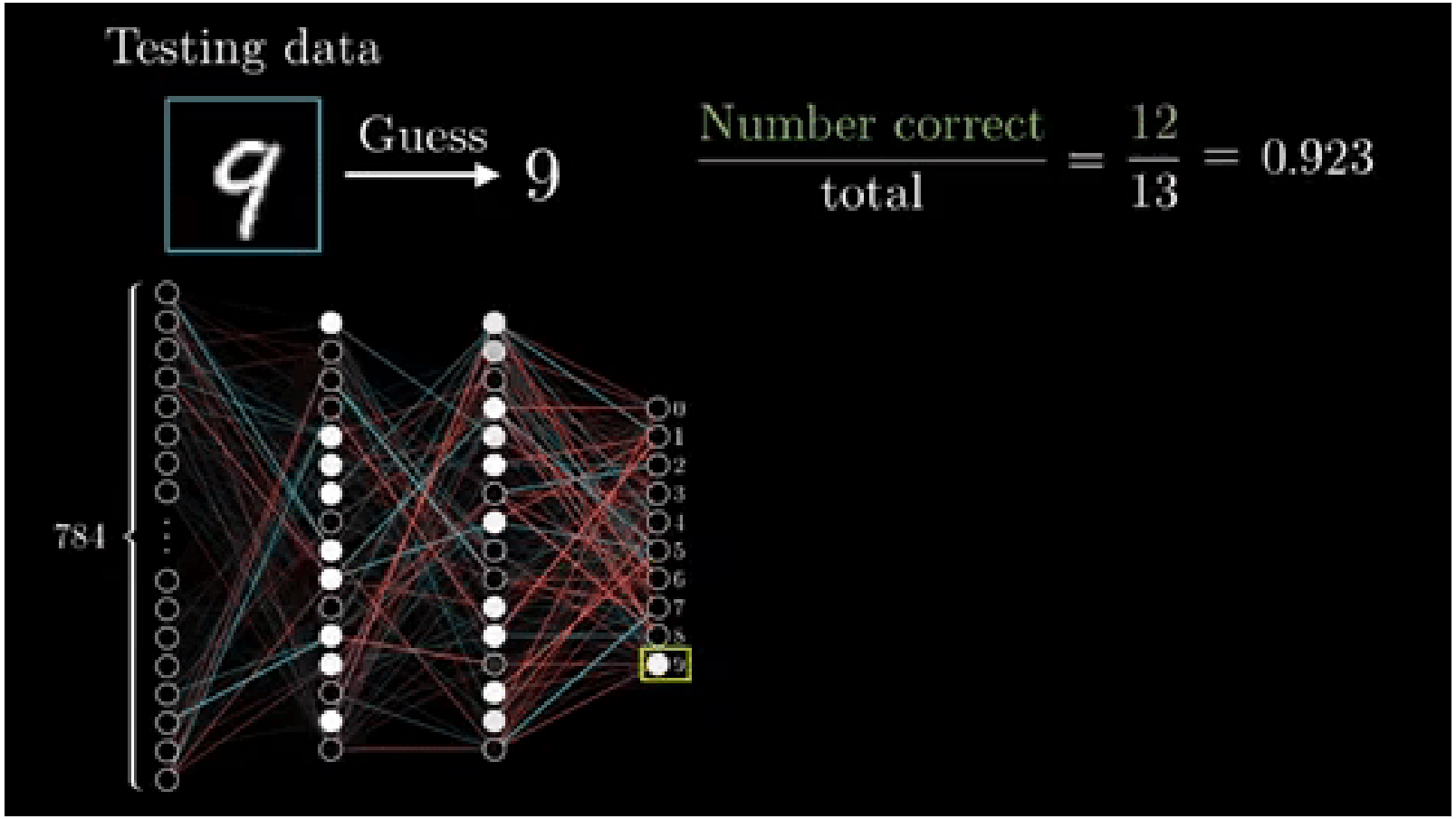
Source: https://www.3blue1brown.com/neural-networks

Training



Source: https://www.3blue1brown.com/neural-networks

Inference/Test



Source: https://www.3blue1brown.com/neural-networks

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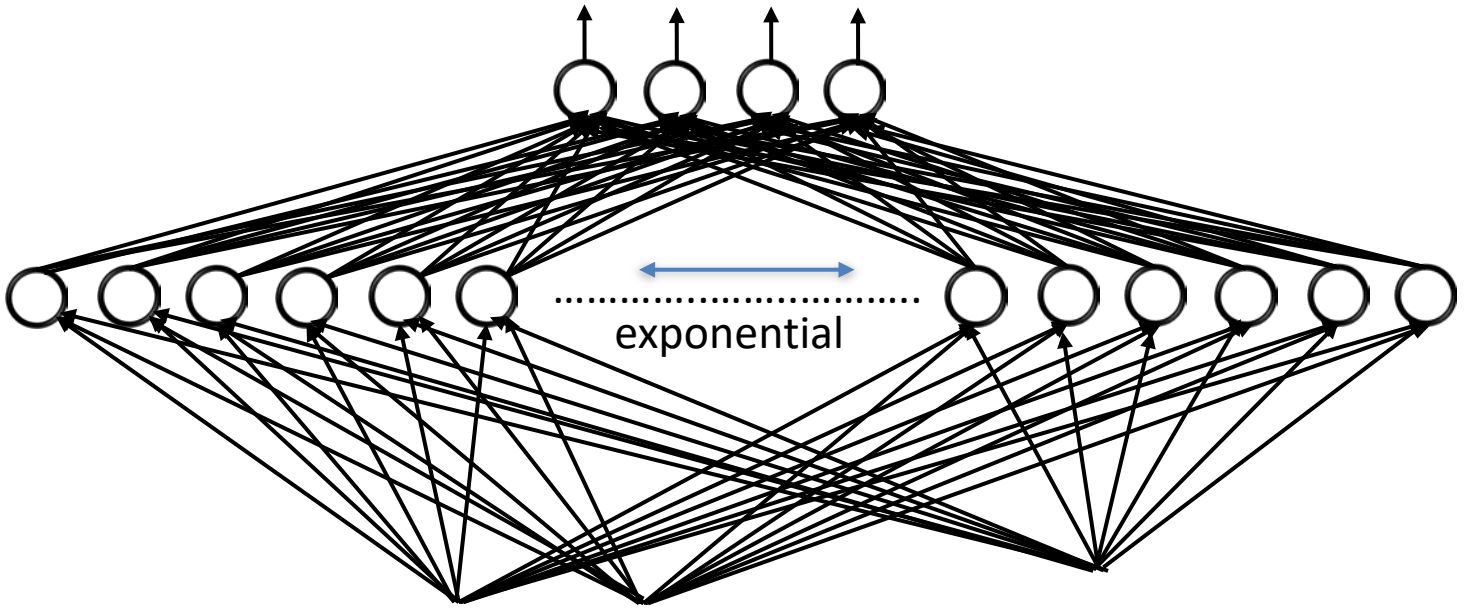
DEEP LEARNING PRINCIPLES

Deep representation origins

- **Theorems (Cybenko (1989), Hornik & Stinchcombe & White (1989)), Allan Pinkus (1999)):** *A neural network with one single hidden layer is a **universal approximator**, i.e. it can represent any continuous function on compact subsets of $\mathbf{R}^n$ with error 0!!*

  *$\Rightarrow$ 1 layers is enough…but hidden layer size may be **exponential** to get error prediction lower than ε, or even **infinite** for a prediction error 0*



Cybenko, G. (1989). Approximation by superpositions of a sigmoidal function. Mathematics of control, signals and systems, 2(4), 303-314.
Hornik, K., Stinchcombe, M., & White, H. (1989). Multilayer feedforward networks are universal approximators. Neural networks, 2(5), 359-366.
Pinkus, Allan (1999). "Approximation theory of the MLP model in neural networks". Acta Numerica. 8: 143–195.

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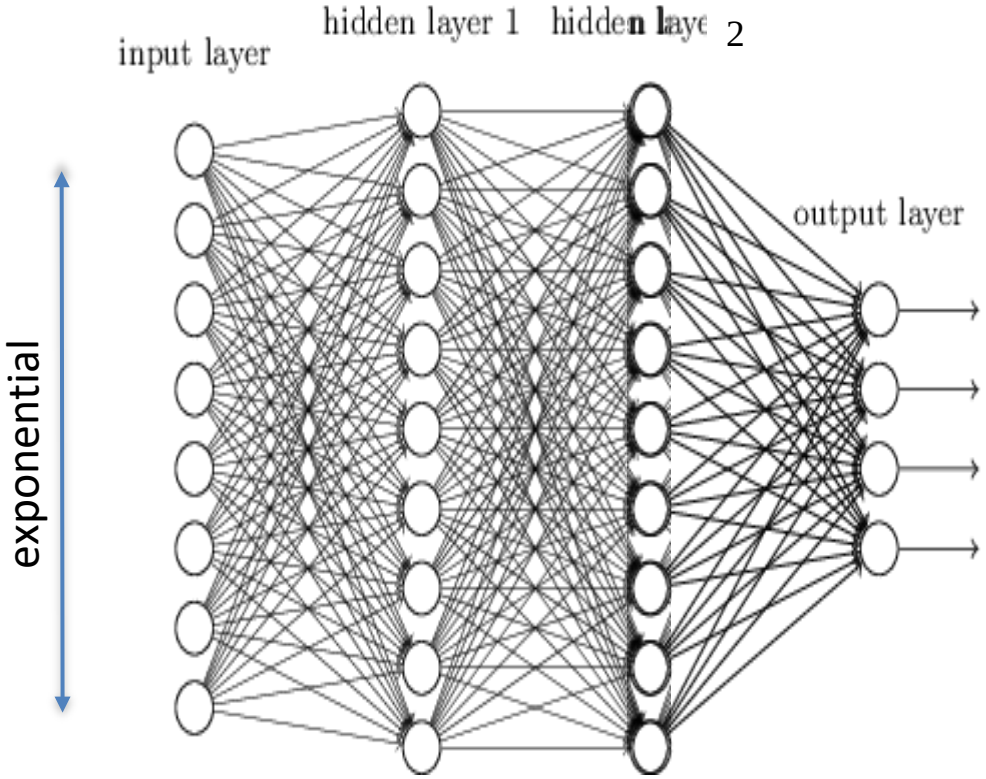
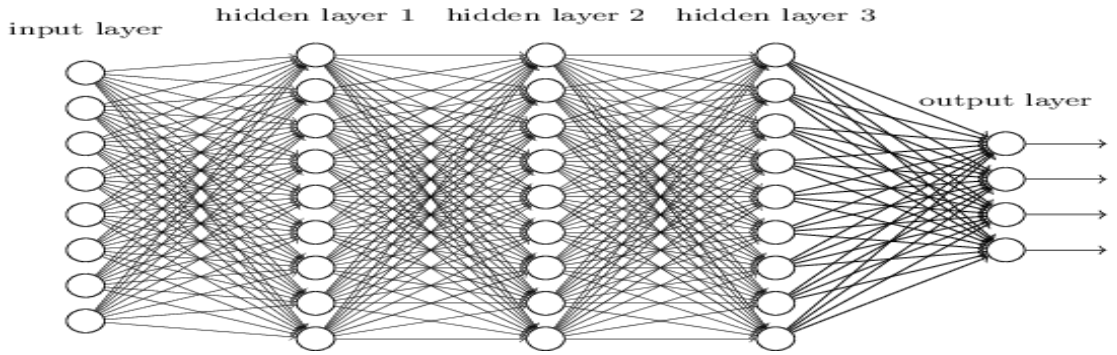
Deep representation origins

- **Theorem Hastad** (1986), **Bengio** et al. (2007) Functions representable compactly with *k* layers would require *k-1* layers with exponential size



Go Deep!



Hastad, J. (1986). Almost optimal lower bounds for small depth circuits. In Proceedings of the 18th annual ACM Symposium on Theory of Computing, pp. 6–20 Berkeley, California. ACM Press.
Johan T. Hastad. Computational Limitations for Small Depth Circuits. MIT Press,Cambridge, MA, 1987.
Yoshua Bengio and Yann LeCun. Scaling learning algorithms towards AI. In L. Bottou,O. Chapelle, D. DeCoste, and J. Weston, editors, Large Scale Kernel Machines. MIT Press, 2007.

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The Blessing of dimensionality: Thomas Cover's Theorem (1965)

Cover's theorem states: A complex pattern-classification problem cast in a high-dimensional space nonlinearly is more likely to be linearly separable than in a low-dimensional space.

Through repeated sequence of Bernoulli trials:

The number of groupings that can be formed by (l-1)-dimensional hyperplanes to separate N points in two classes is: $$O(N,l) = 2\sum_{i=0}^{l} \frac{(N-1)!}{(N-1-i)!i!}$$

Notice: The total number of possible groupings is 2^N

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Deep Neural Network Approximation Theory (2021)

"…deep networks provide exponential approximation accuracy—i.e., the approximation error decays exponentially in the number of nonzero weights in the network—of the multiplication operation, polynomials, sinusoidal functions, and certain smooth functions.

Moreover, this holds true even for one-dimensional oscillatory textures and the Weierstrass function—a fractal function, neither of which has previously known methods achieving exponential approximation accuracy.

We also show that in the approximation of sufficiently smooth functions finite-width deep networks require strictly smaller connectivity than finite-depth wide networks."

Elbrächter, D., Perekrestenko, D., Grohs, P., & Bölcskei, H. (2021). Deep neural network approximation theory. IEEE Transactions on Information Theory, 67(5), 2581-2623.

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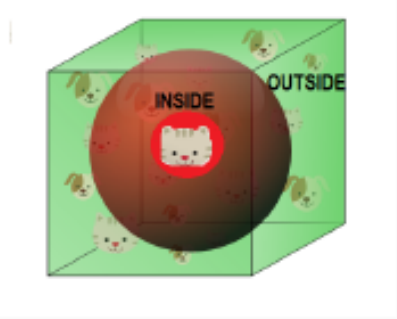
The curse of dimensionality [Bellman, 1956]

- Euclidian distance is not relevant in high dimension: d $\geq$10
  1. look at the examples at distance at most r
  2. the hypersphere volume is too small: practically empty of examples

$$\frac{volume\ of\ the\ sphere\ of\ radial\ r}{hypersphere\ of\ 2r\ width} \rightarrow_{d\rightarrow\infty} 0$$



  3. need a number of examples exponential in d

Remark

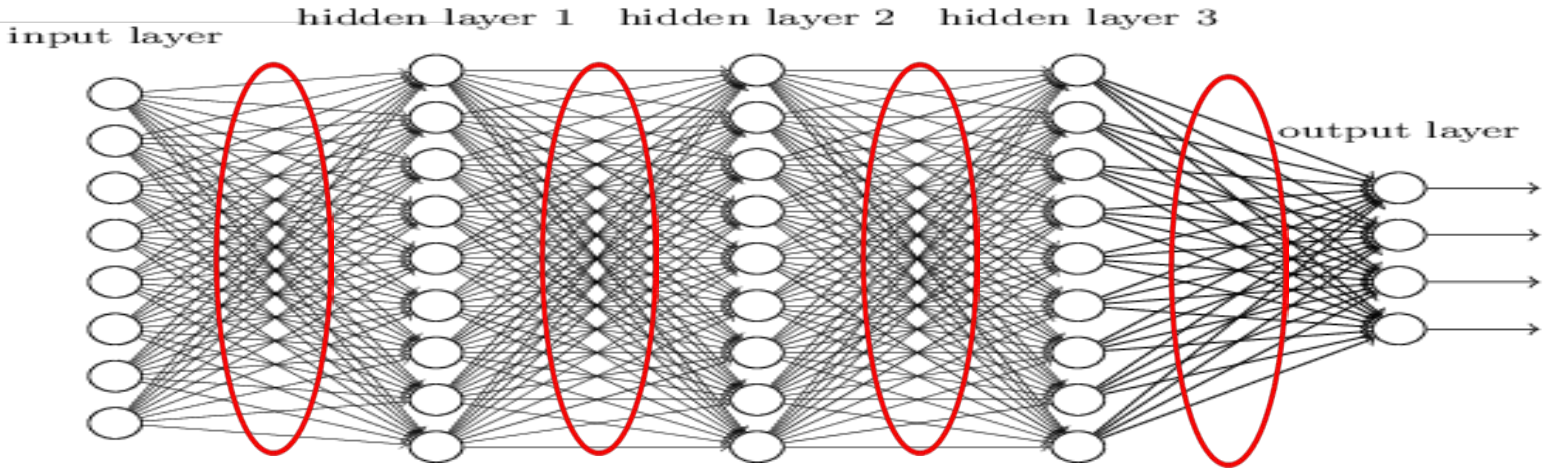
Specific care for data representation

Structure the network?

- Can we put any structure reducing the space of exploration and providing useful properties (invariance, robustness, sequentiality…)?

$$y = s(w_{13}\, s(w_{11}x_1 + w_{21}x_2 - w_{01}) + w_{23}\, s(w_{12}x_1 + w_{22}x_2 - w_{02}) - w_{03})$$

(z_1 over $w_{11}x_1 + w_{21}x_2 - w_{01}$, z_2 over $w_{12}x_1 + w_{22}x_2 - w_{02}$, z_3 over the whole expression)



Enabling factors

- Why do it now ? Before 2006, training deep networks was unsuccessful because of practical aspects
  - faster CPU's
  - parallel CPU architectures
  - advent of GPU computing
  - Advances in ML/Optim (1995 -> 2005)

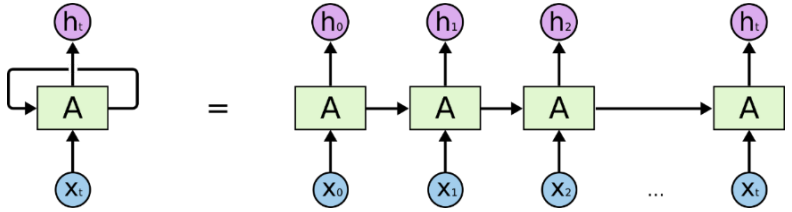
- Hinton, Osindero & Teh « A Fast Learning Algorithm for Deep Belief Nets », *Neural Computation*, 2006
- Bengio, Lamblin, Popovici, Larochelle « Greedy Layer-Wise Training of Deep Networks », *NIPS'2006*
- Ranzato, Poultney, Chopra, LeCun « Efficient Learning of Sparse Representations with an Energy-Based Model », *NIPS'2006*

- Results…
  - 2009, sound, interspeech +~24%
  - 2011, text, +~15% without linguistic at all
  - 2012, images, ImageNet +~20%
  - 2020, molecules/graphs, AlphaFold, +~24%
    (sorry in French, https://www.youtube.com/watch?v=OGewxRMME8o)

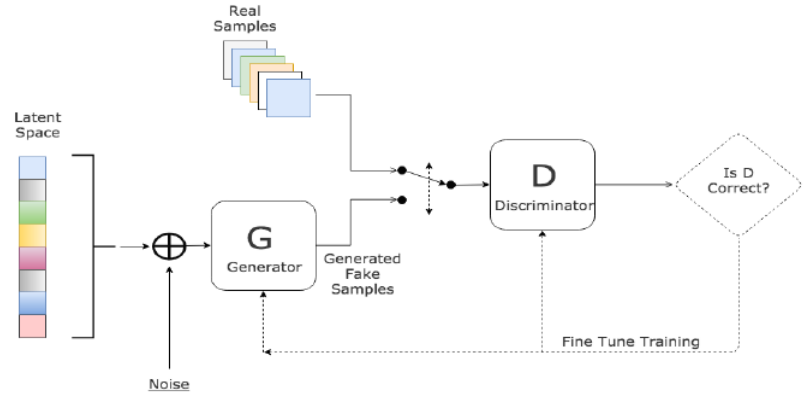
Slide from Yoshua Bengio

Network architectures

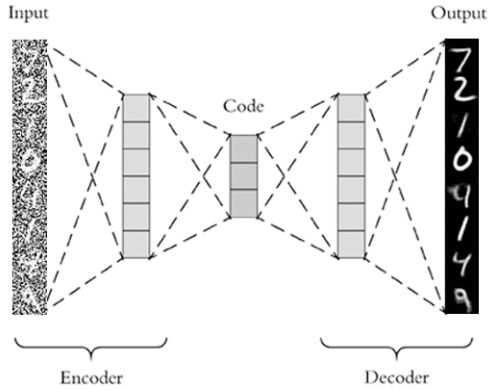
Spatial Correlation
(images, sounds...)



Sequential Correlation
(machine translation, speech 2 text, time series...)



Generative Adversarial Network
(Data Generator)



Dimension reduction, compression, denoising/data cleansing, data generator

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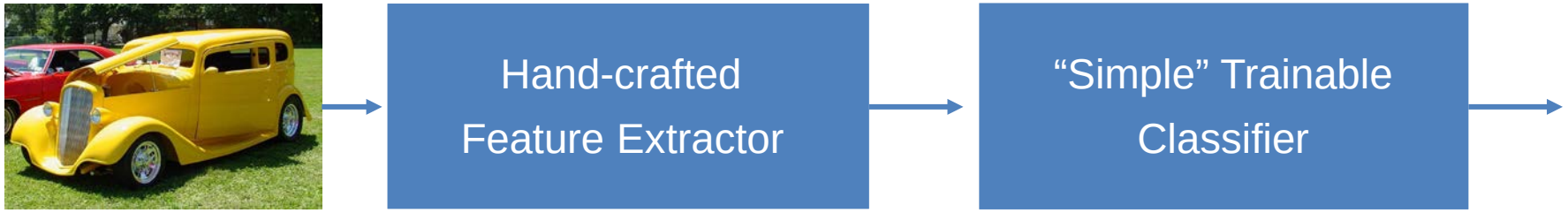
Deep learning = Learning representations/features

- The traditional model of pattern recognition (since the late 50's)
  - Fixed/engineered features (or fixed kernel) + trainable classifier



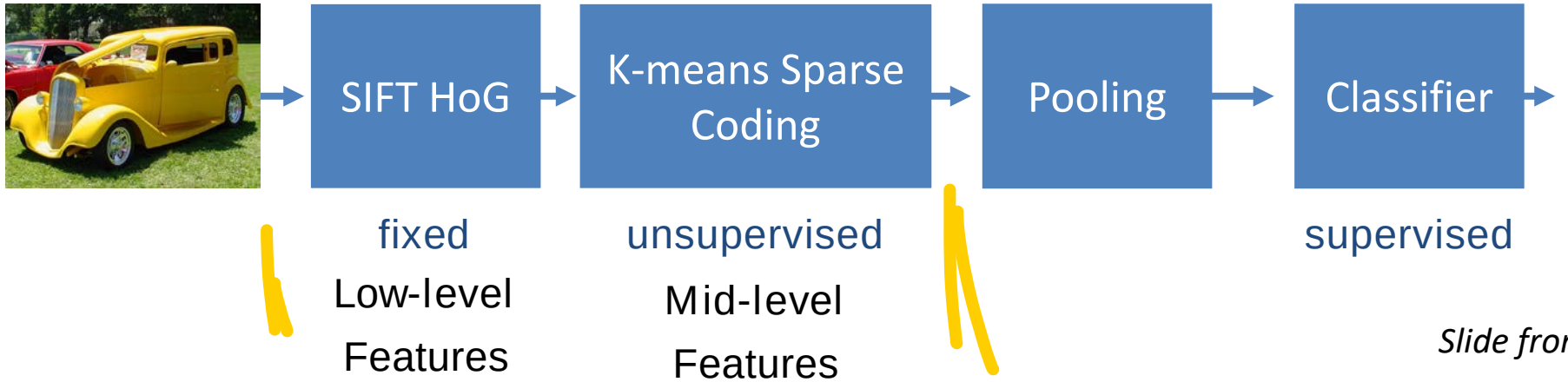
- End-to-end learning / Feature learning / Deep learning
  - Trainable features (or kernel) + trainable classifier

Slide from Yann LeCun

Architecture of "mainstream" pattern recognition systems

- Modern architecture for pattern recognition
  - Speech recognition: early 90's – 2011

  - Object Recognition: 2006 - 2012



Slide from Yann LeCun

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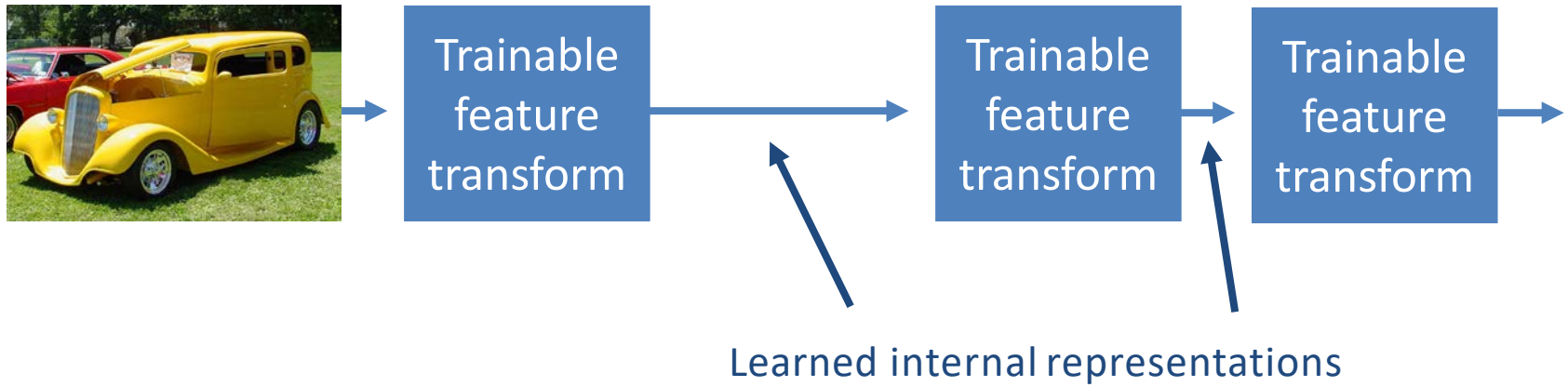
Trainable feature hierarchies: end-to-end learning

- A hierarchy of trainable feature transforms
  - Each module transforms its input representation into a higher-level one.
  - High-level features are more global and more invariant
  - Low-level features are shared among categories



- How can we make all the modules trainable and get them to learn appropriate representations?

Slide from Yann LeCun

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Spatial correlations

Convolutional Neural Networks (aka CNN, ConvNet)

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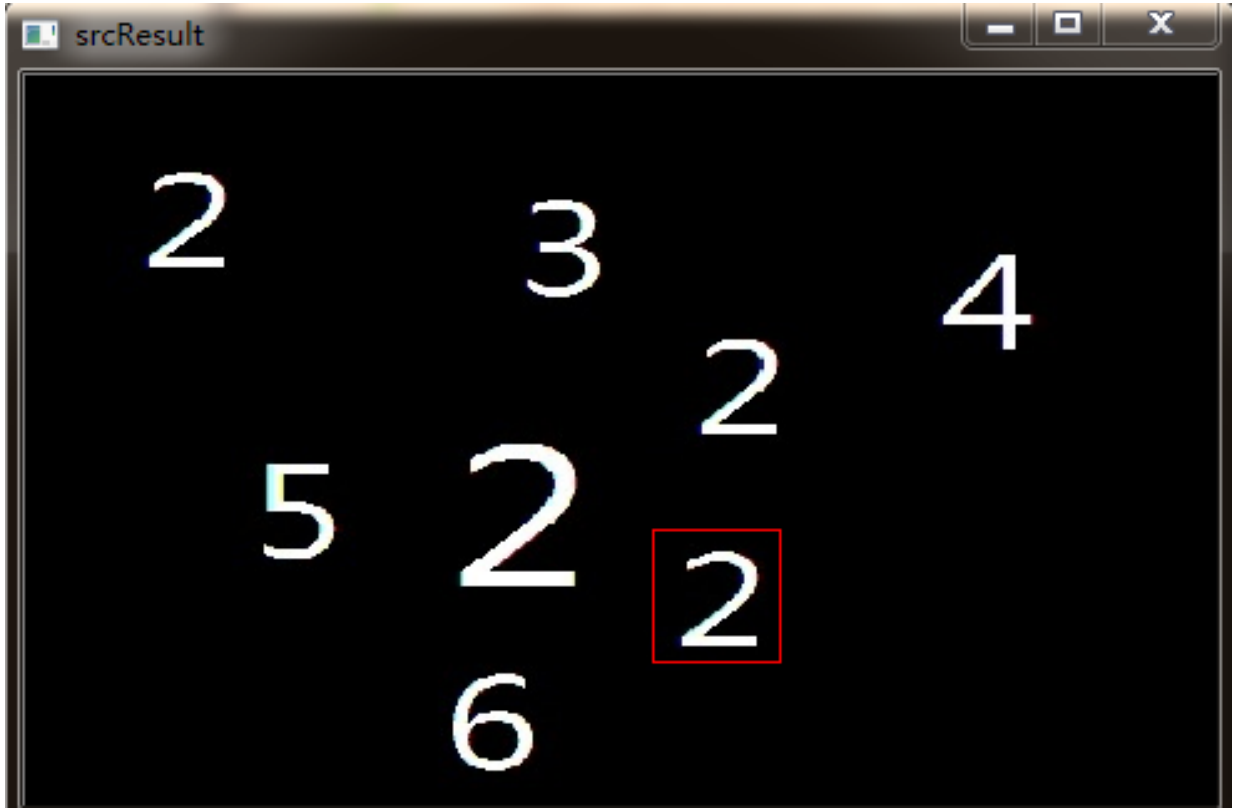
Do you know template matching?

Single target matching results:



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(picture from https://programmer.group/5ca5086fed10b.html)

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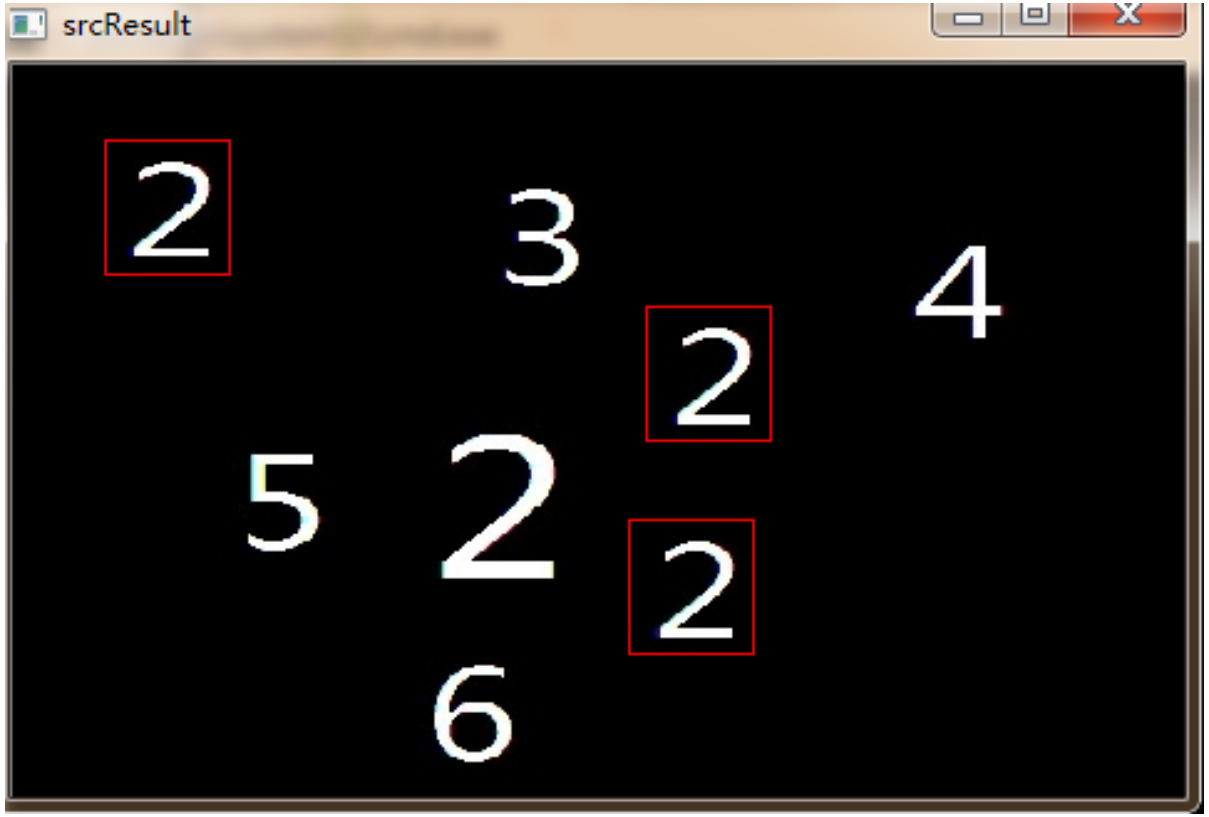
Do you know template matching?

Multi-objective matching result:



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(picture from https://programmer.group/5ca5086fed10b.html)

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Do you know template matching?

How to compute Template matching? Cross-correlation!

$$F \circ I(x,y) = \sum_{j=-N}^{N} \sum_{i=-N}^{N} F(i,j) I(x+i, y+j)$$

When this is maximal, the Filter is perfectly positioned with respect to the pattern to detect.

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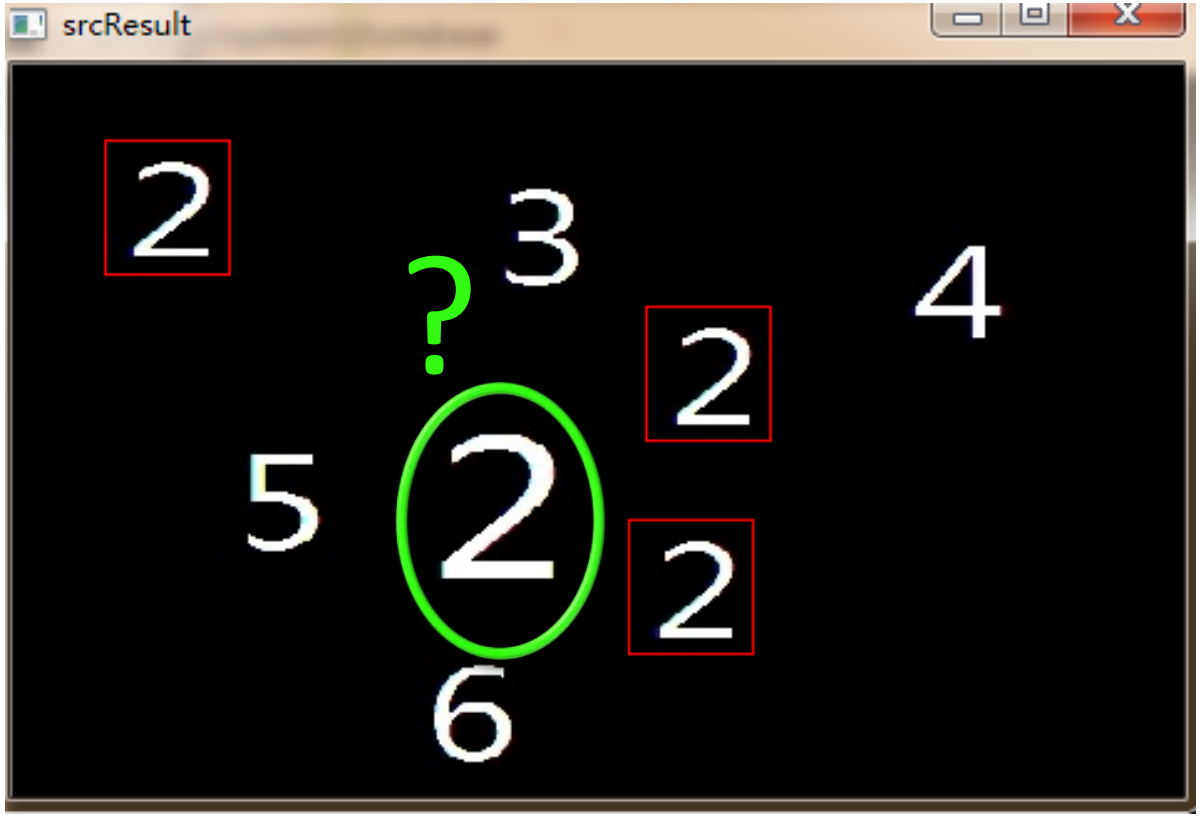
Do you know template matching?

Multi-objective matching result:



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(picture from https://programmer.group/5ca5086fed10b.html)

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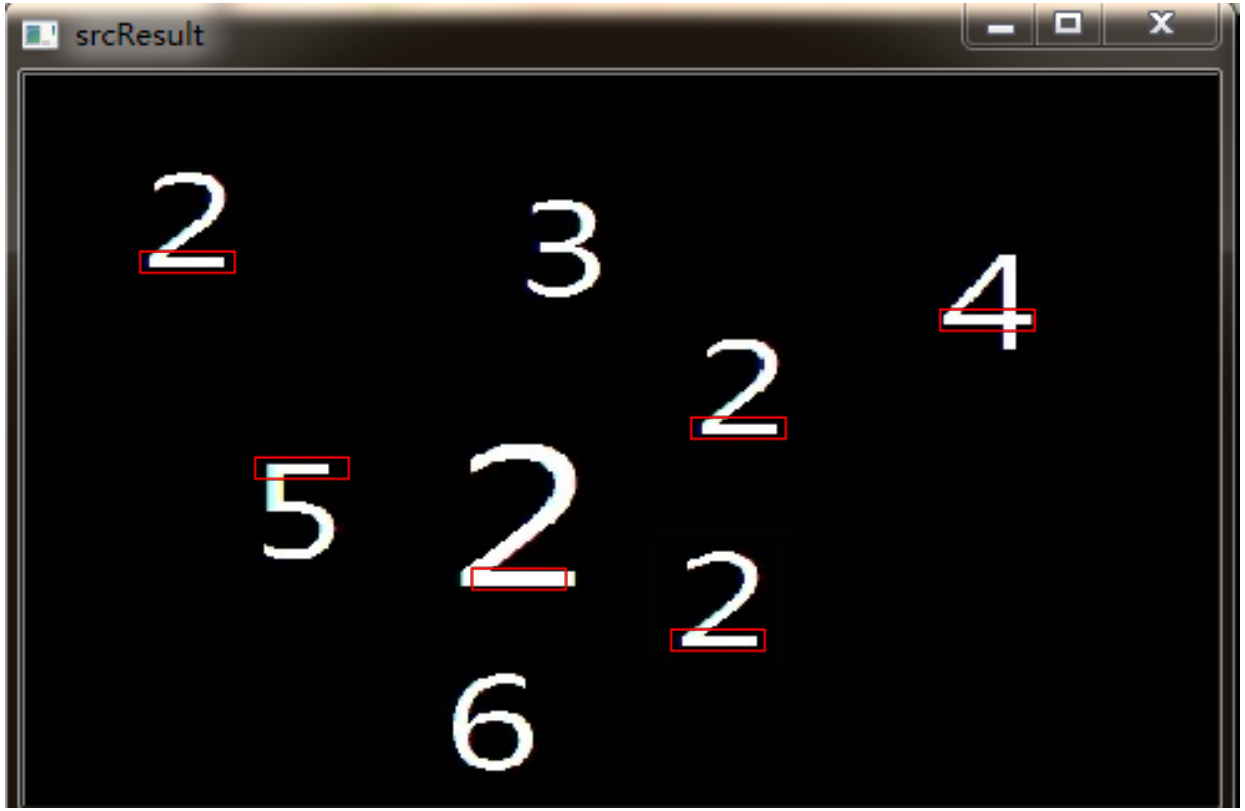
Are there more universal templates?

Multi-objective matching result:



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(picture from https://programmer.group/5ca5086fed10b.html)

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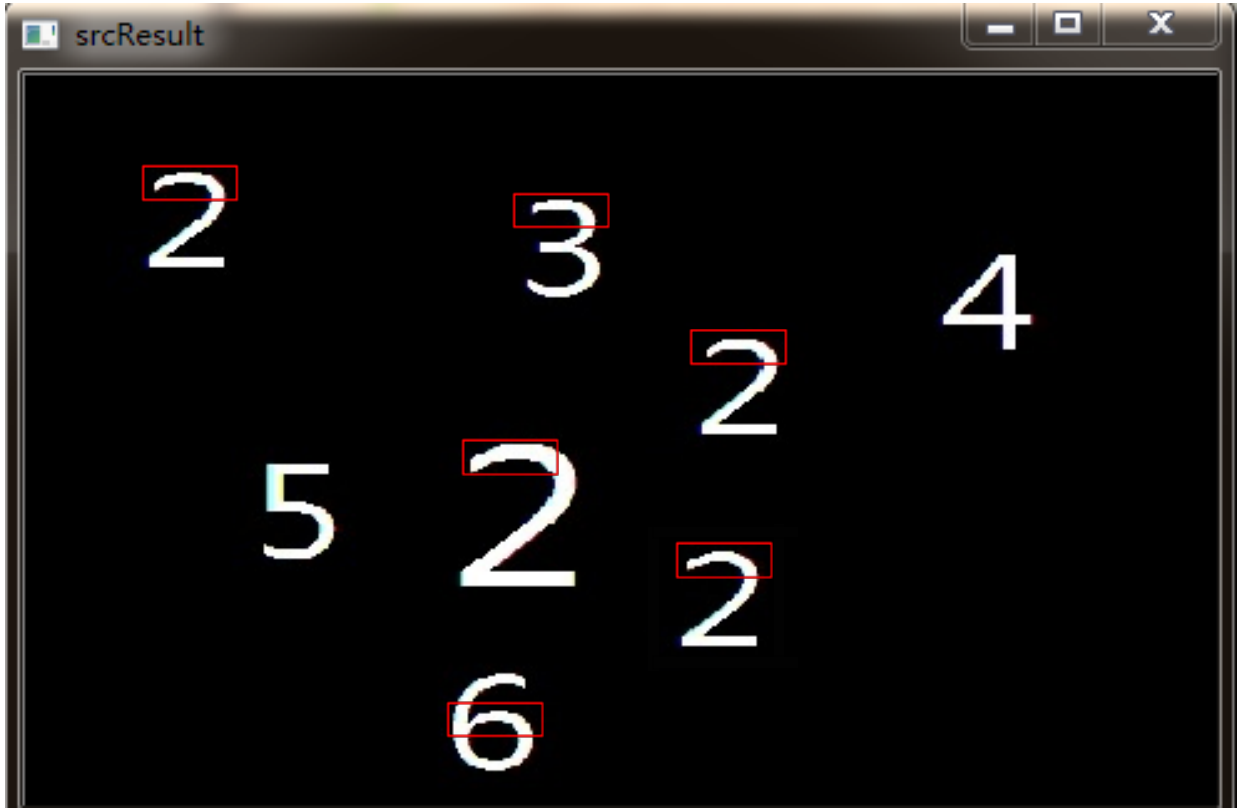
Are there more universal templates?

Multi-objective matching result:



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(picture from https://programmer.group/5ca5086fed10b.html)

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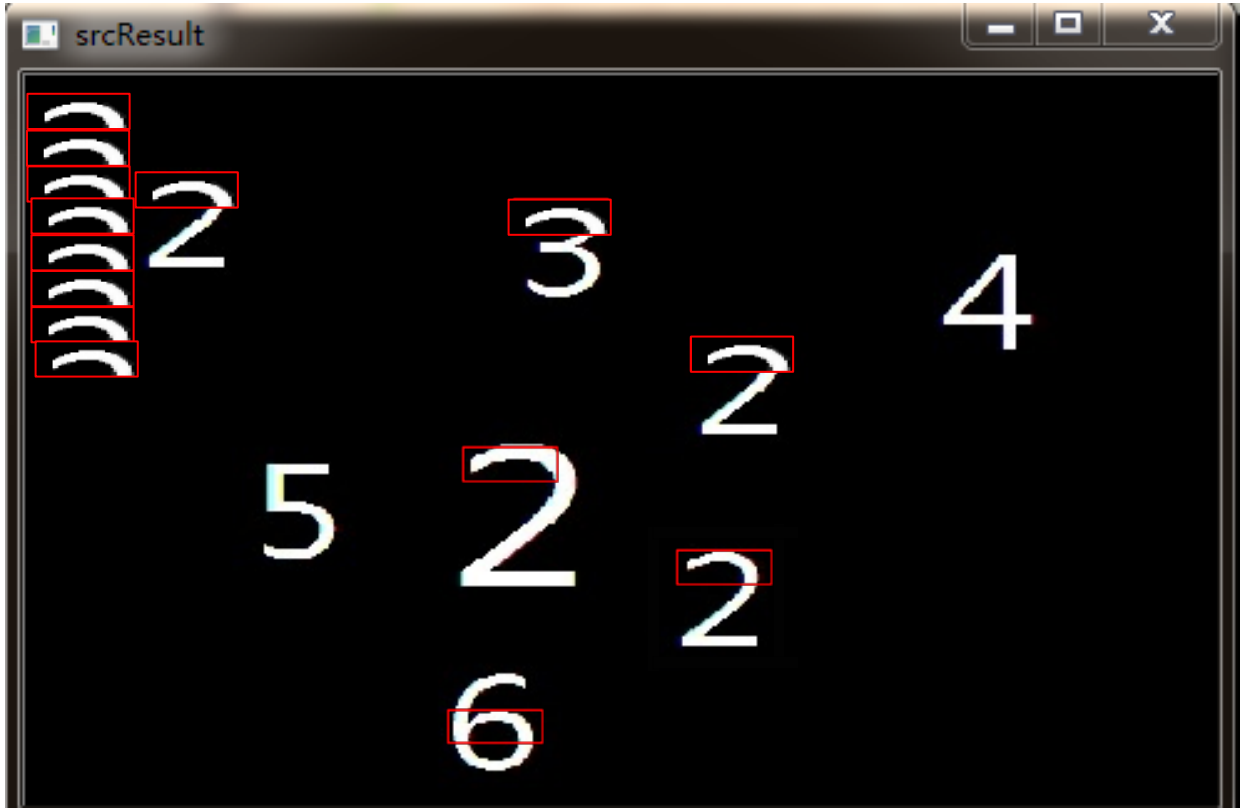
How to locate these templates?

By scanning I, we acquire **translation invariance**



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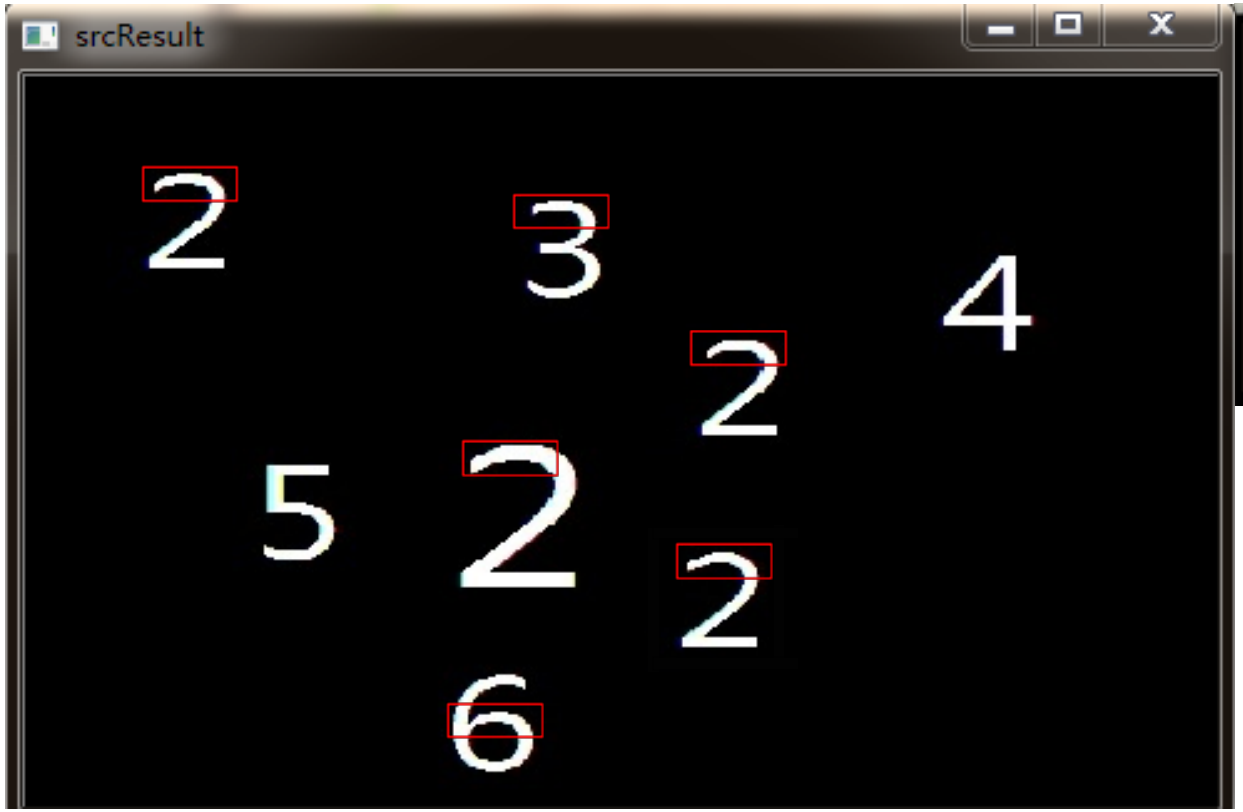
How to define these templates?

By learning what filter maximizes **local cross-correlations**



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Cross-correlation or Convolution?

- How to define these templates?

By learning what filter maximizes **local cross-correlations**

$$F \circ I(x,y) = \sum_{j=-N}^{N} \sum_{i=-N}^{N} F(i,j) I(x+i, y+j)$$

Or **local convolutions**

$$F * I(x,y) = \sum_{j=-N}^{N} \sum_{i=-N}^{N} F(i,j) I(x-i, y-j)$$

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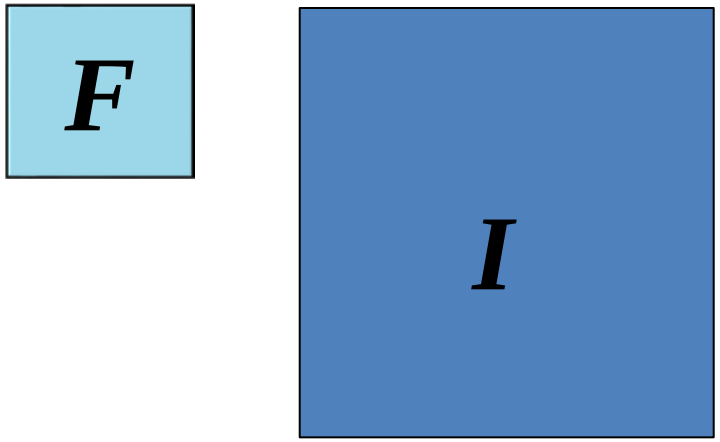
Cross-correlation or Convolution?

- Convolution:
  - Flip the filter in both dimensions (bottom to top, right to left)
  - Then apply cross-correlation



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Cross-correlation or Convolution?

- Convolution:
  - Flip the filter in both dimensions (bottom to top, right to left)
  - Then apply cross-correlation

- Actually, The Convolutional operation widely used in Convolution Neural Network (CNN) is commonly and largely considered as a **misnomer**
  - The operation that is used is strictly speaking a correlation.
  - Both the operators have **translational invariance** and **locality**.

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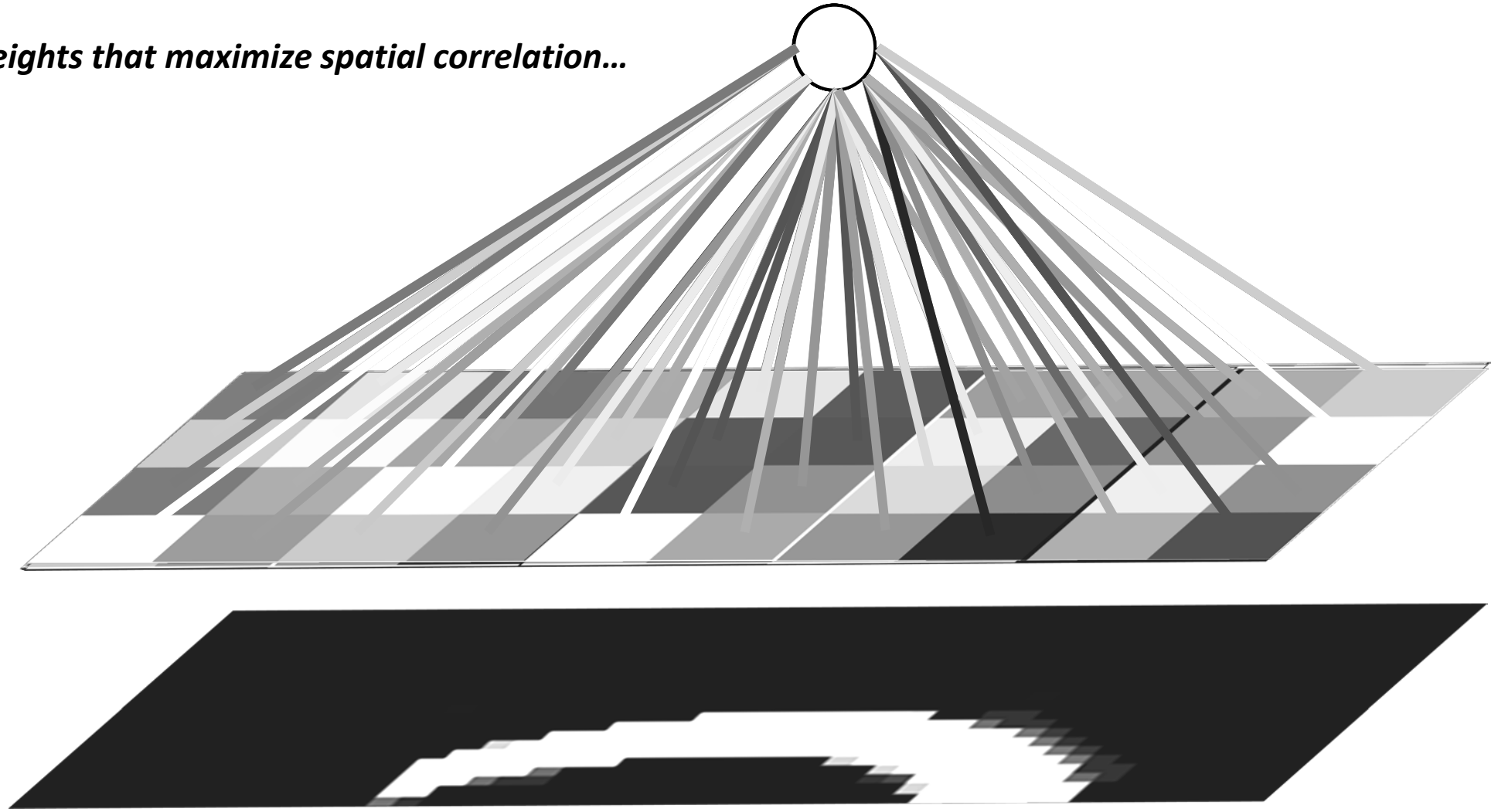
One single neuron is a correlator

Set the weights that maximize spatial correlation…



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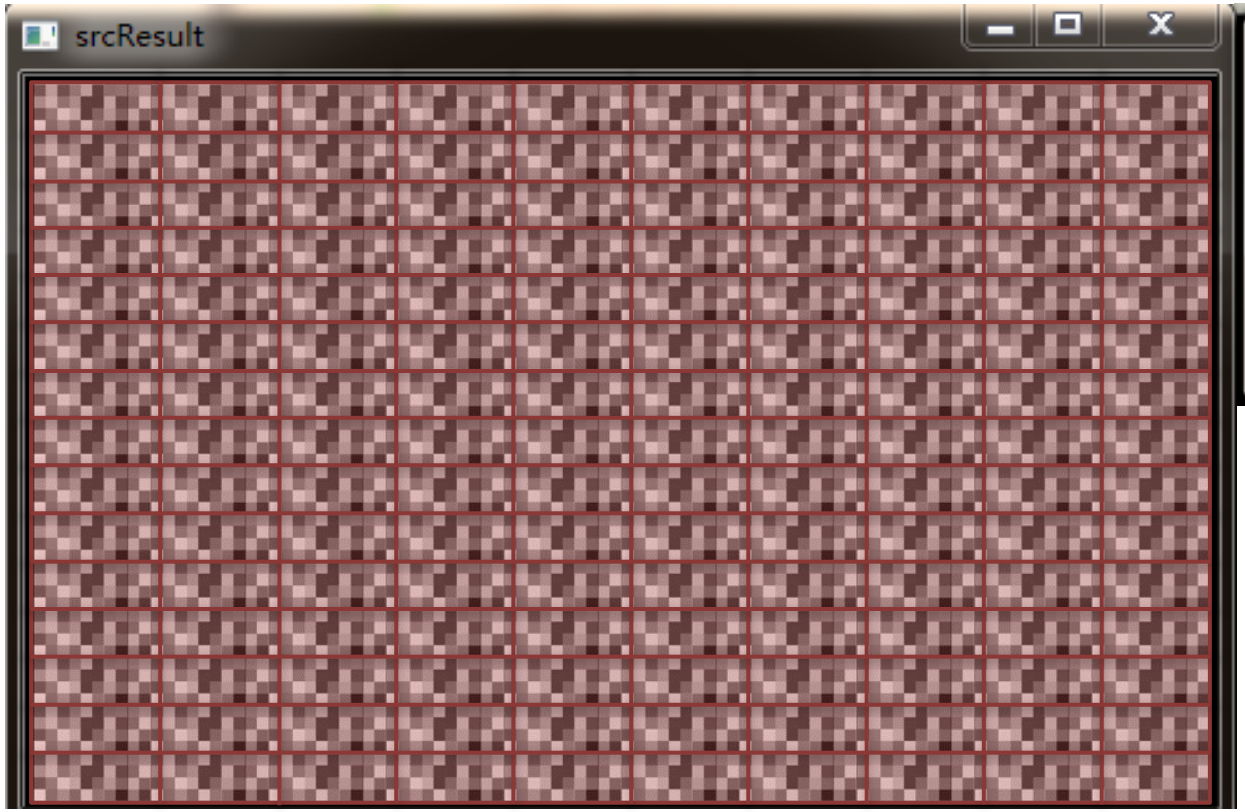
How to define these templates?

And instead of scanning I, let us just **duplicate** the template **into a grid**.



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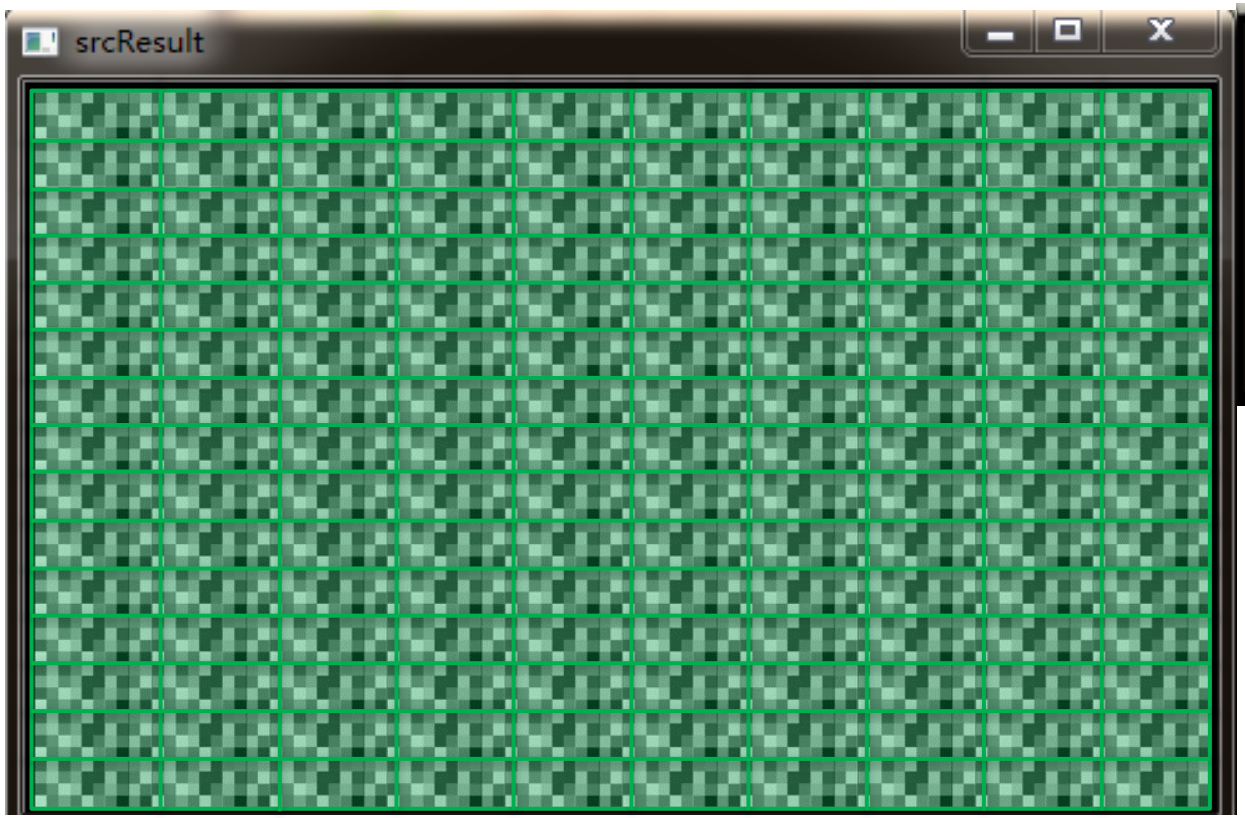

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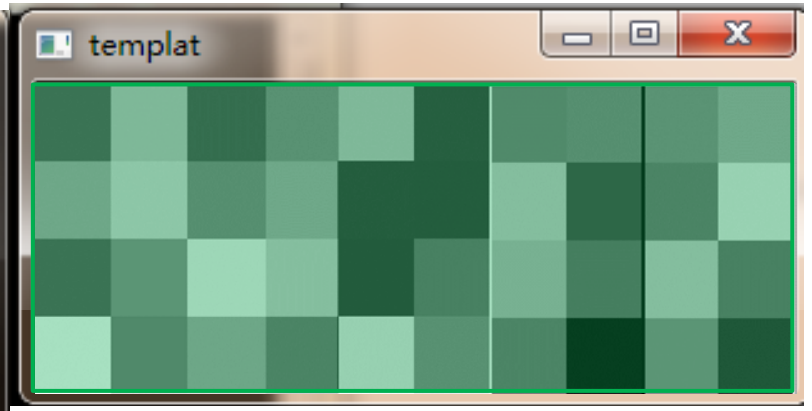

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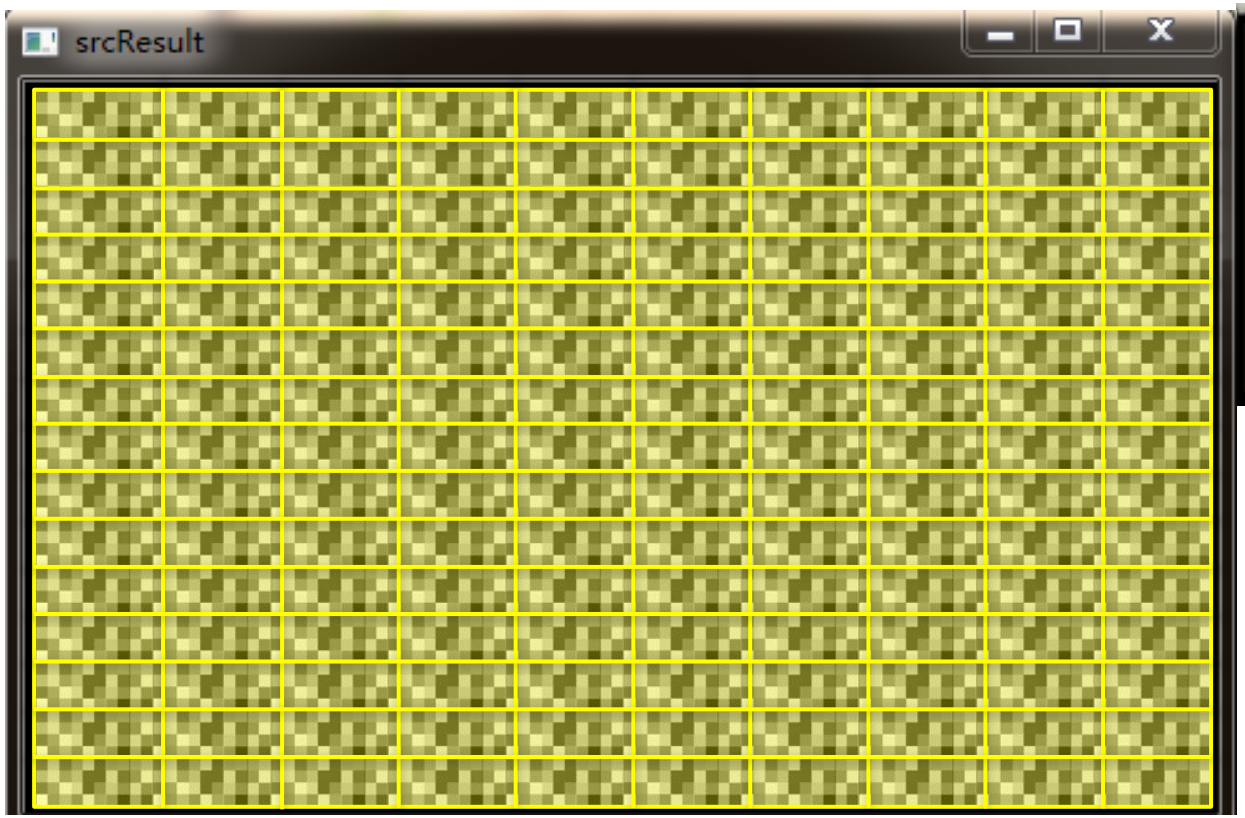

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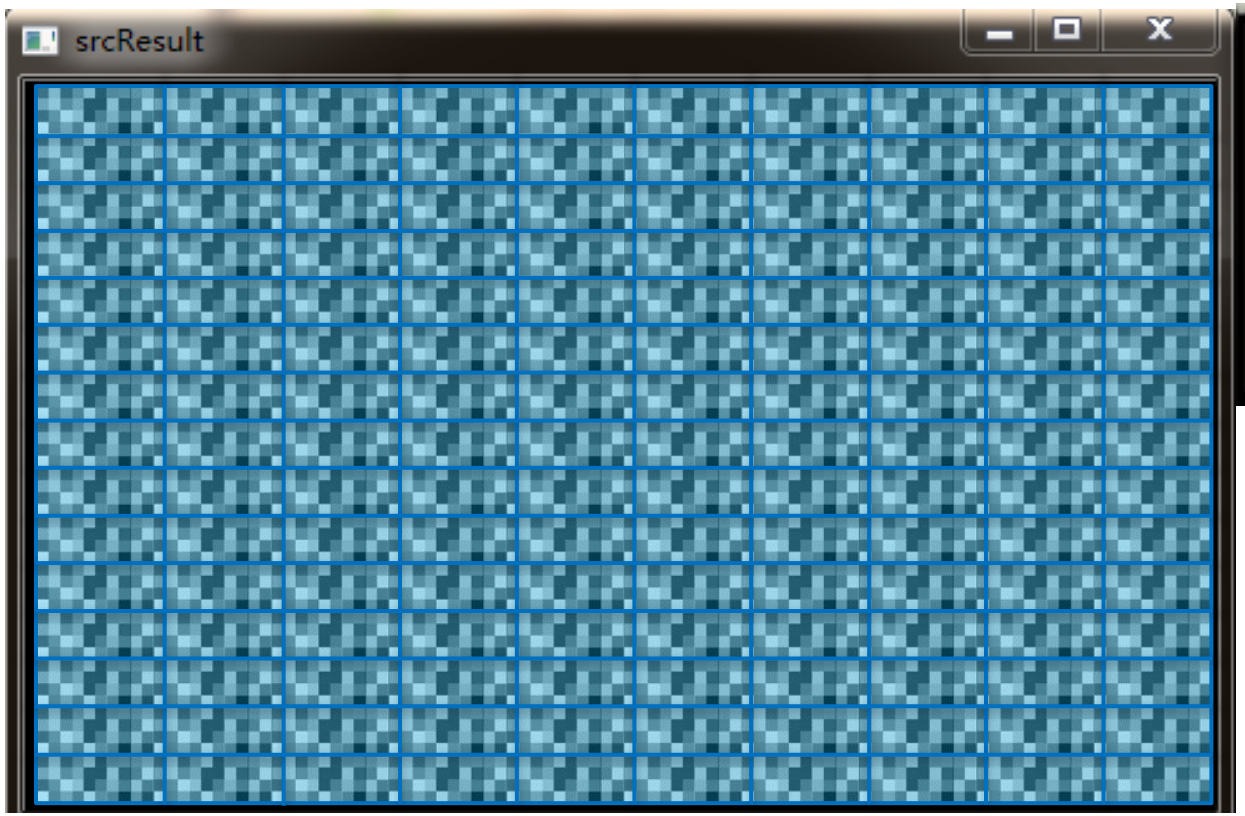

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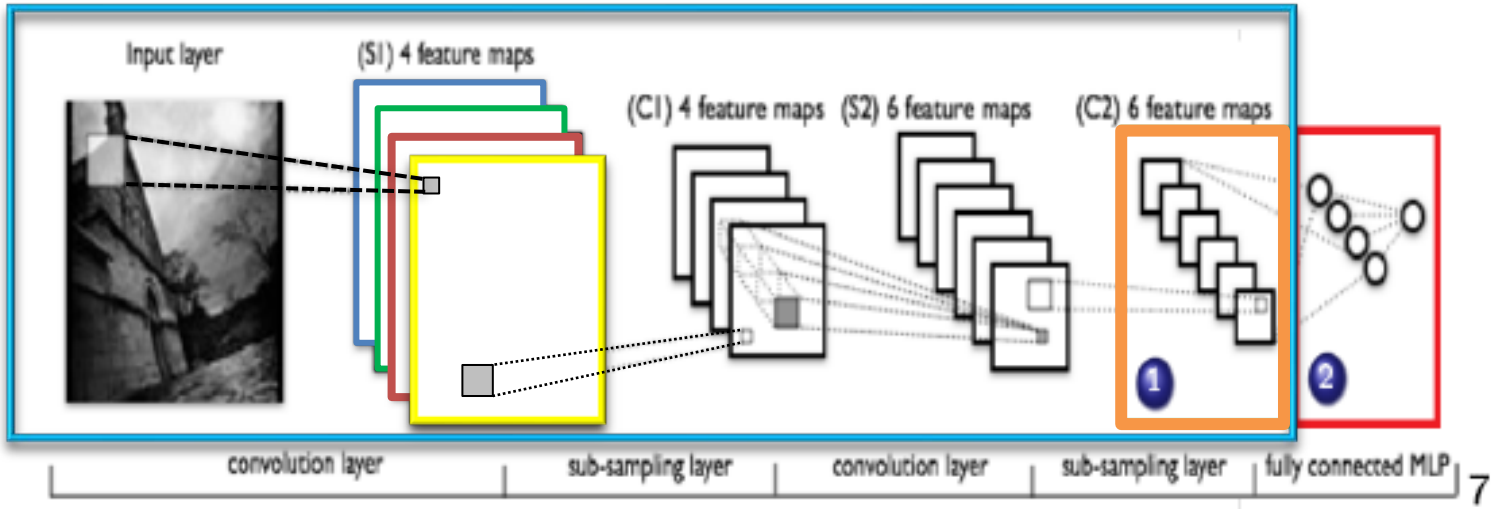
Deep representation by CNN

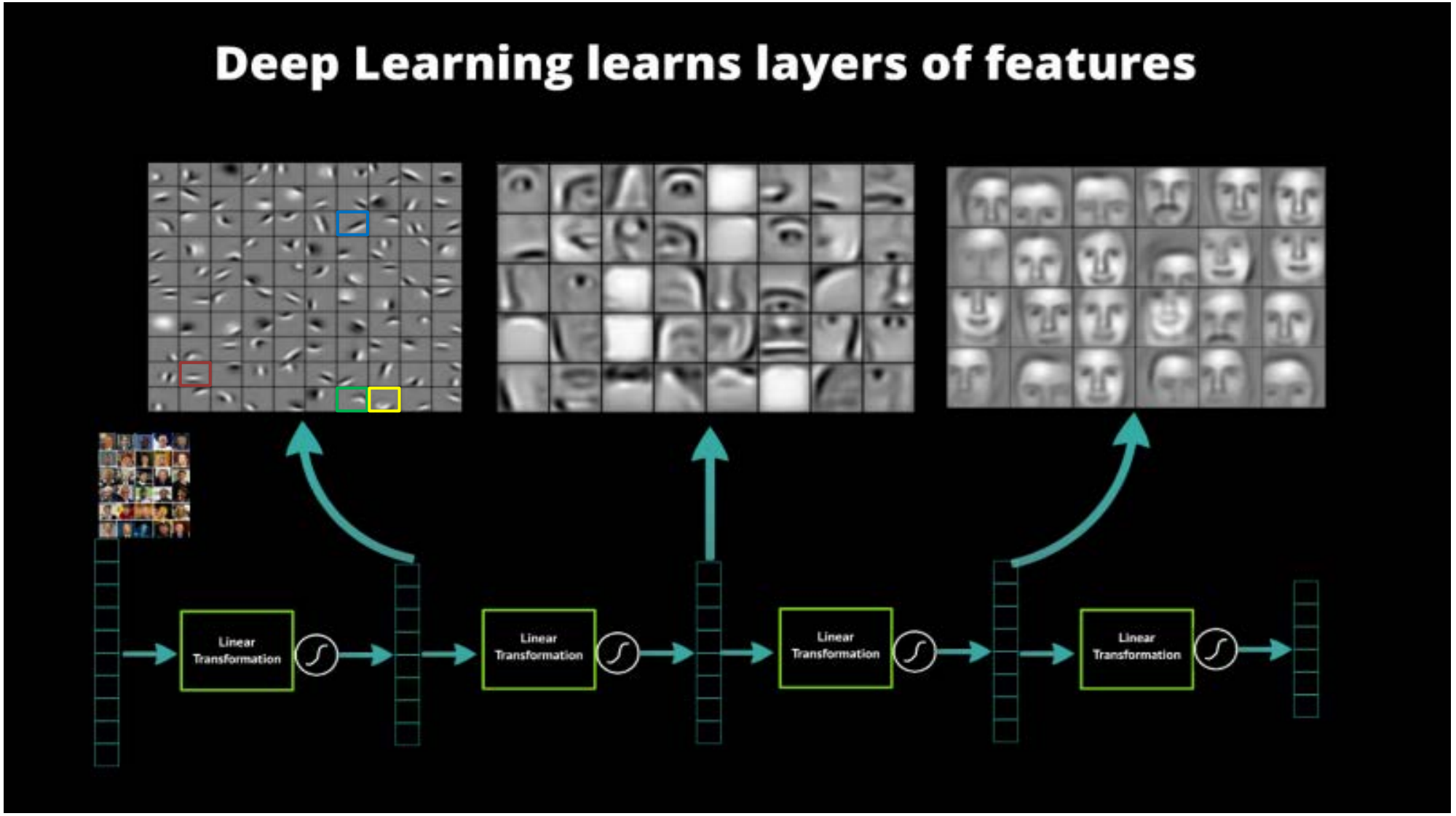
- feature map = result of the convolution
- convolution with a filter extract characteristics (*edge detectors*)
- extract parallelised characteristics at each layer



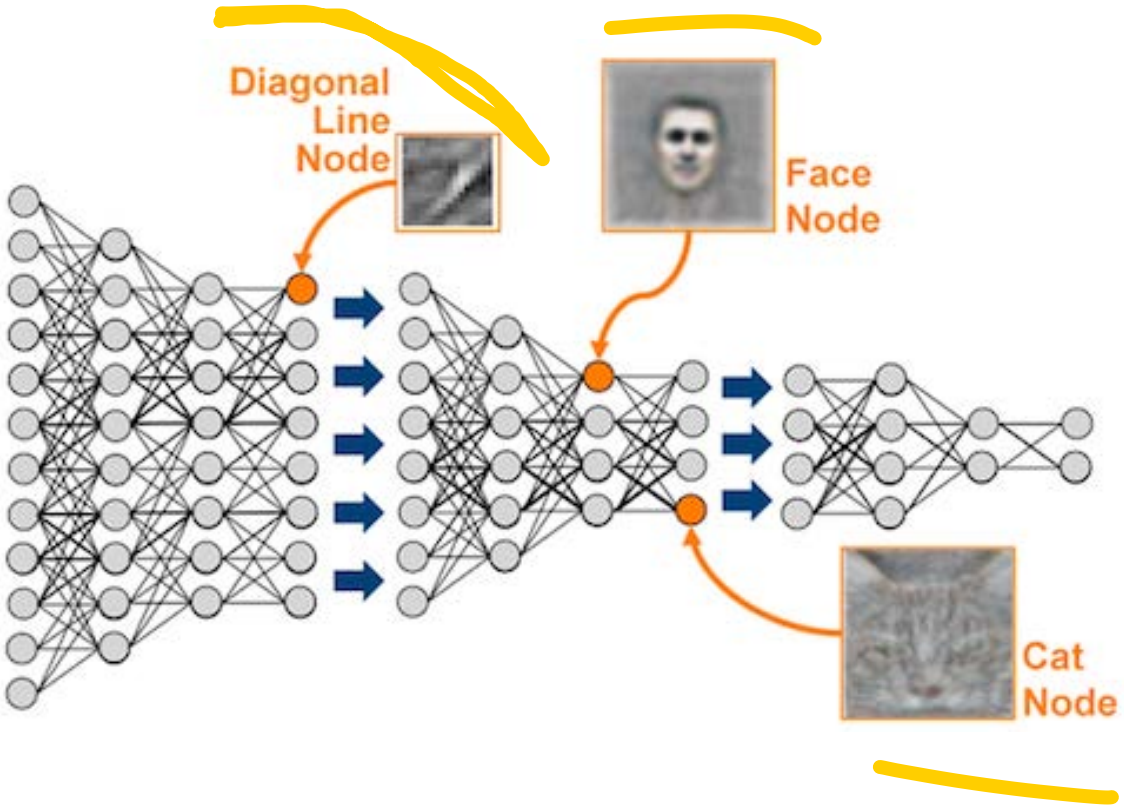
7

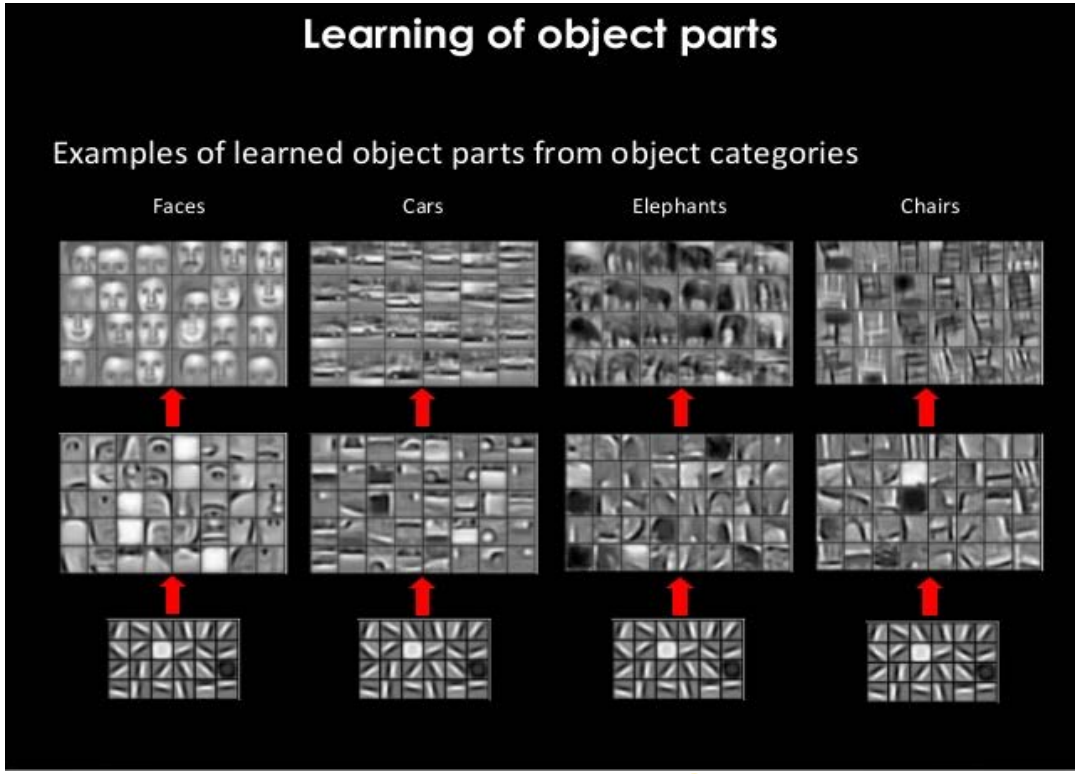
1. final representation of our data
2. classifier (MLP)

Deep representation by CNN



Deep representation by CNN





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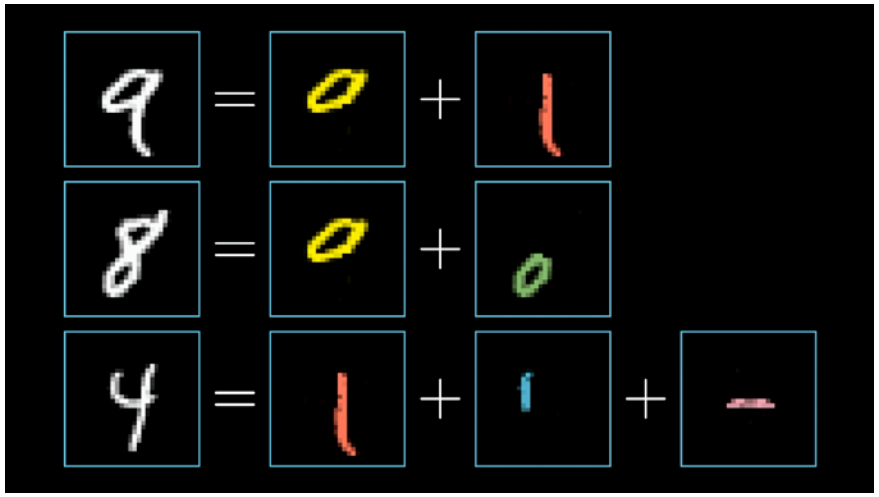
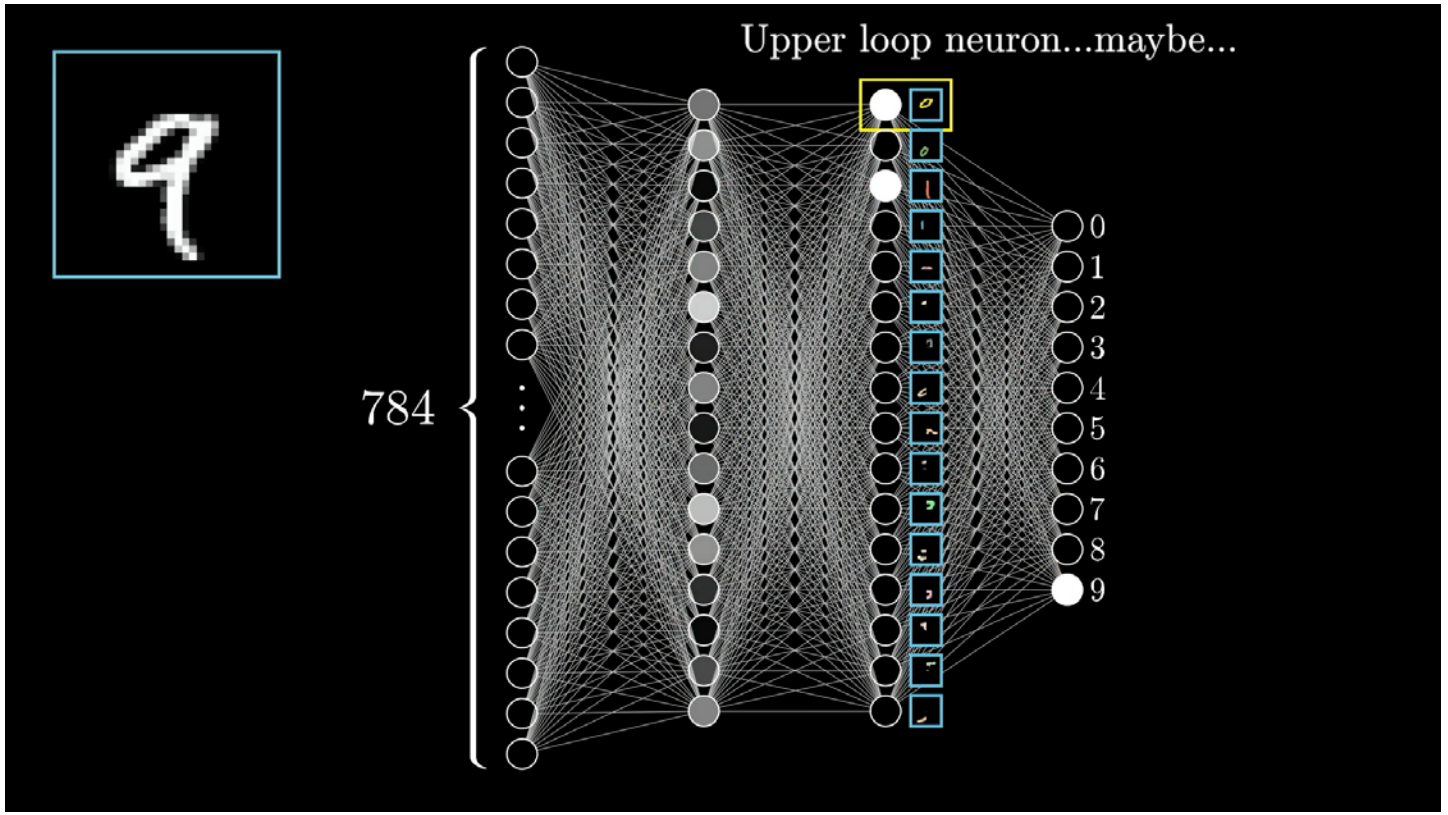
Deep representation by CNN

- We hope that the inner layers will detect basic patterns, "as we" break down our visual reasoning:





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Extracted from 3Blue1Brown tutoriel : https://www.youtube.com/watch?v=aircAruvnKk

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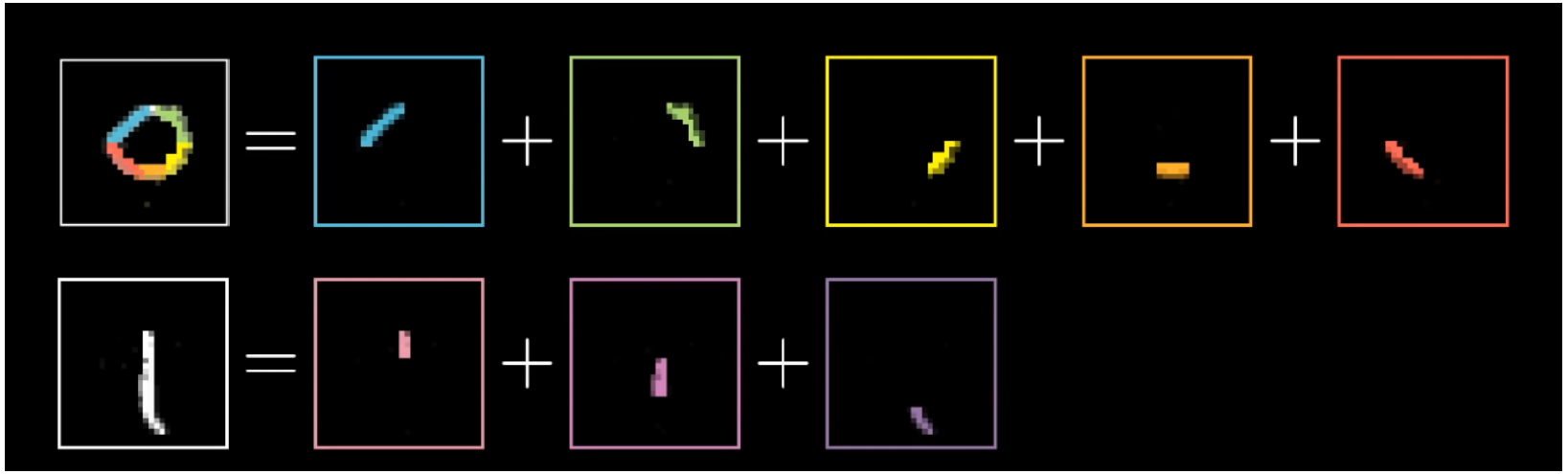
Deep representation by CNN

- These patterns (loops, bars, etc.) are in turn broken down into sub-patterns:



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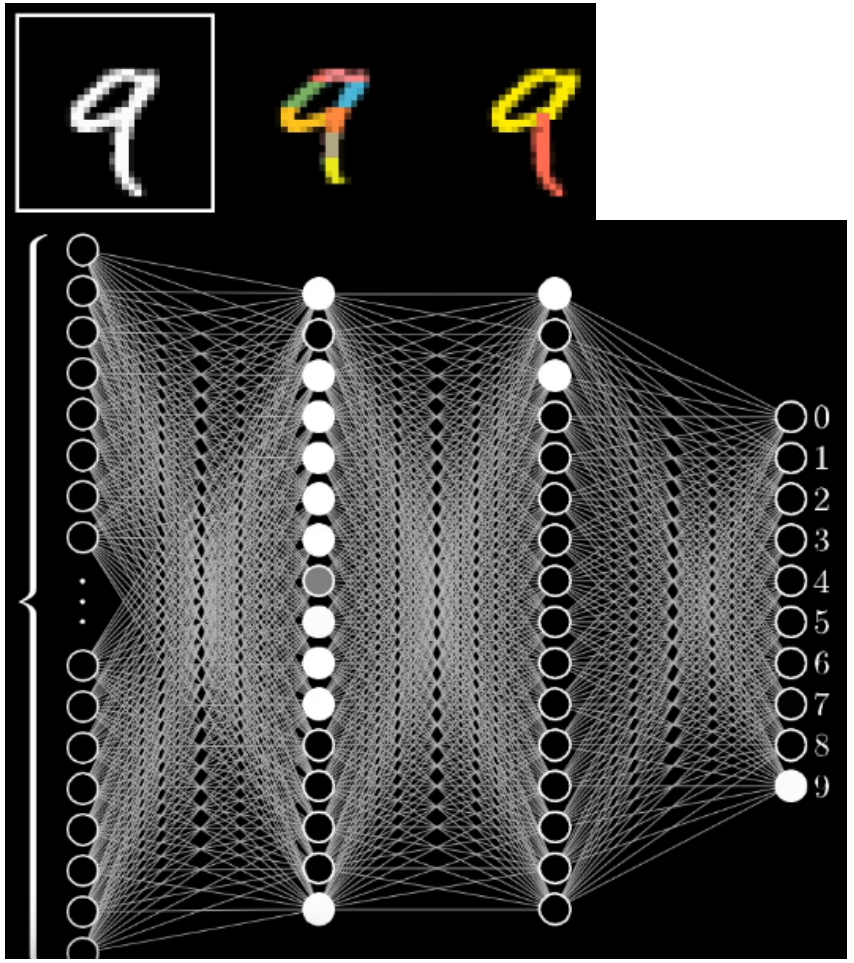
Deep representation by CNN



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Transfer Learning

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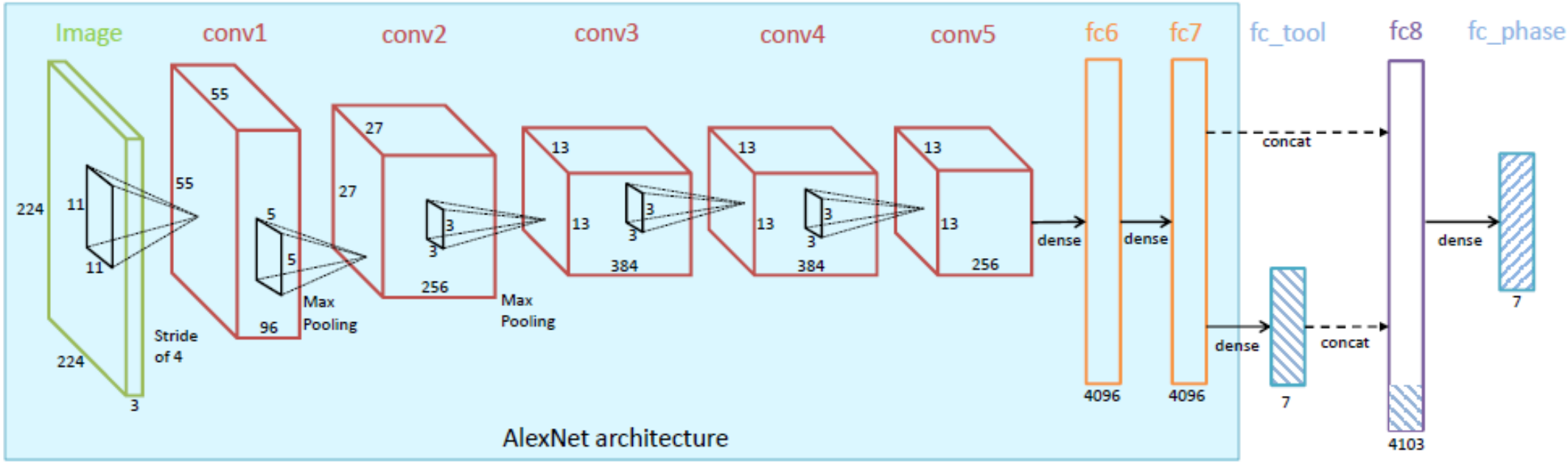
Transfer Learning



Grasper | Bipolar | Hook | Clipper

Scissors | Irrigator | Specimen bag

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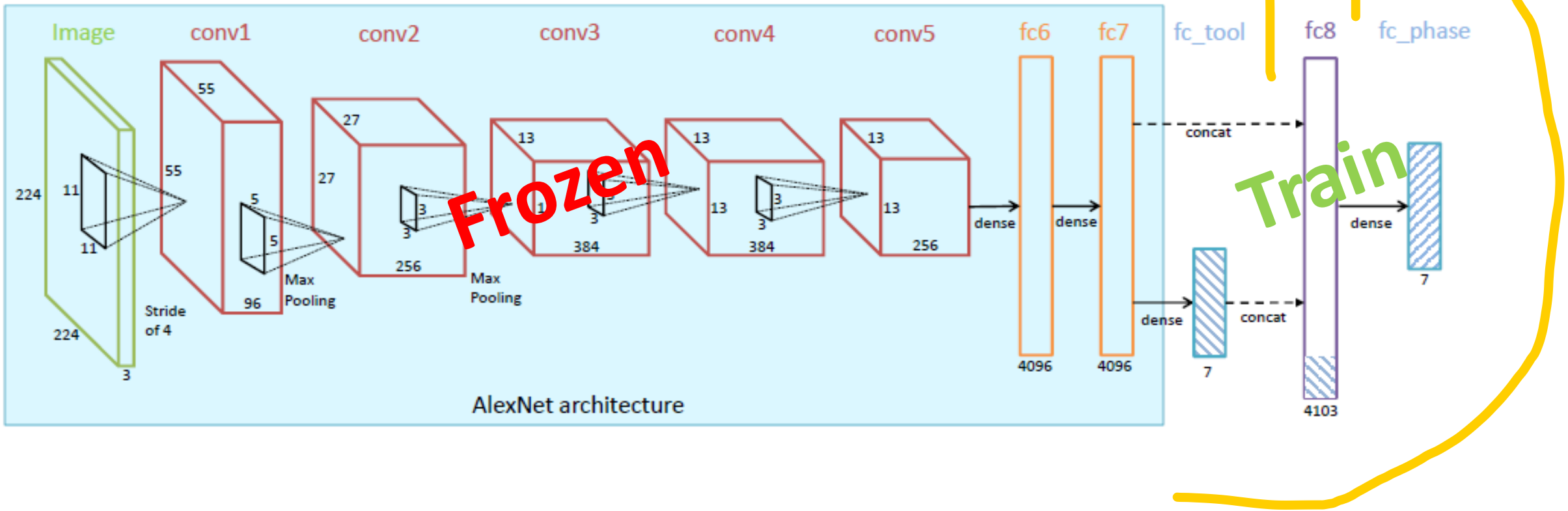
Transfer Learning!!

Very small training set



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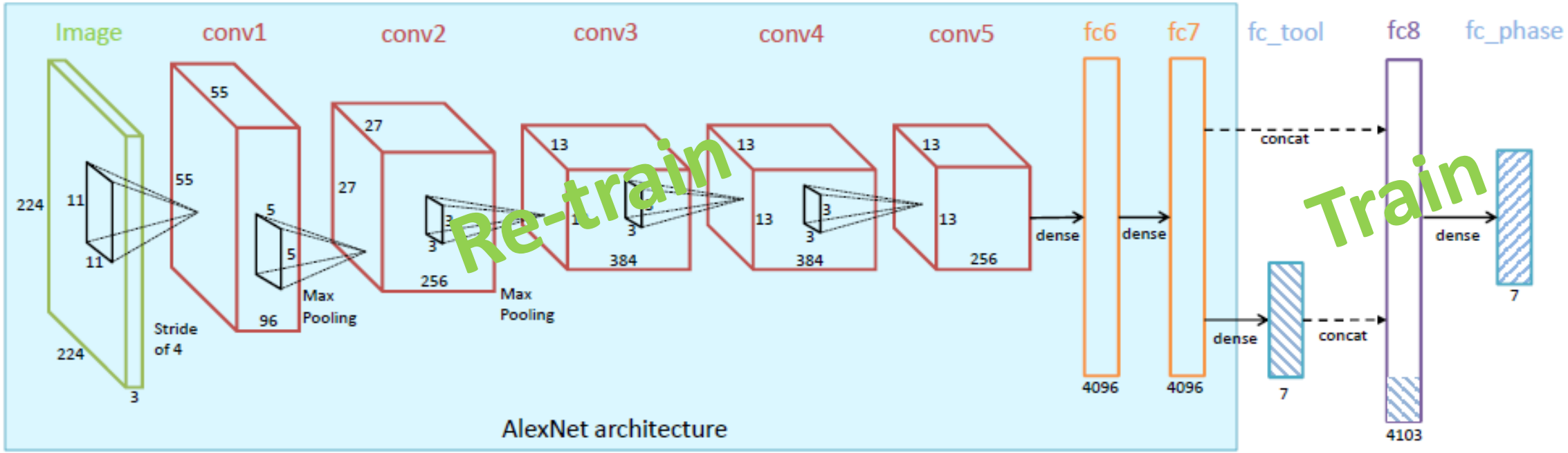
Transfer Learning!!

Small learning kit



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CNN for temporal data?

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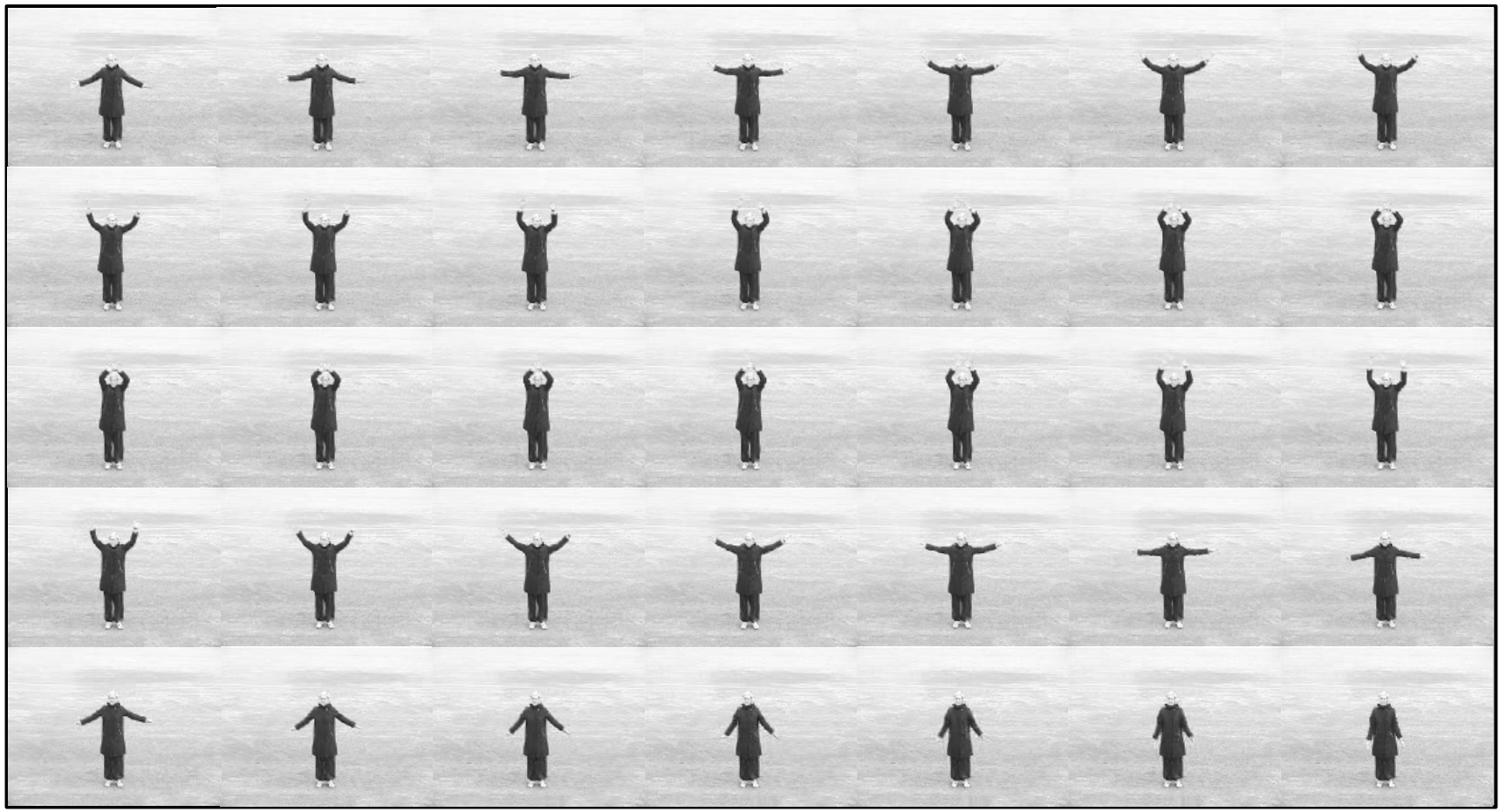
CNN for temporal data?



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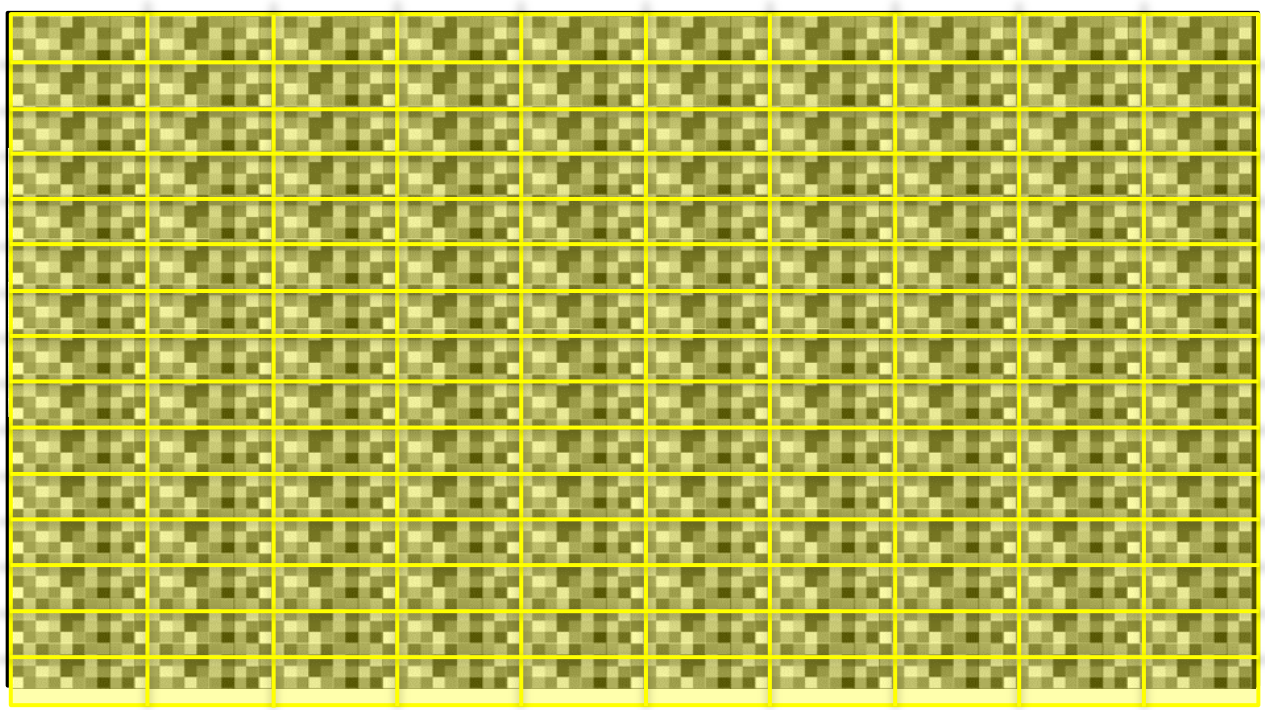
CNN for temporal data?



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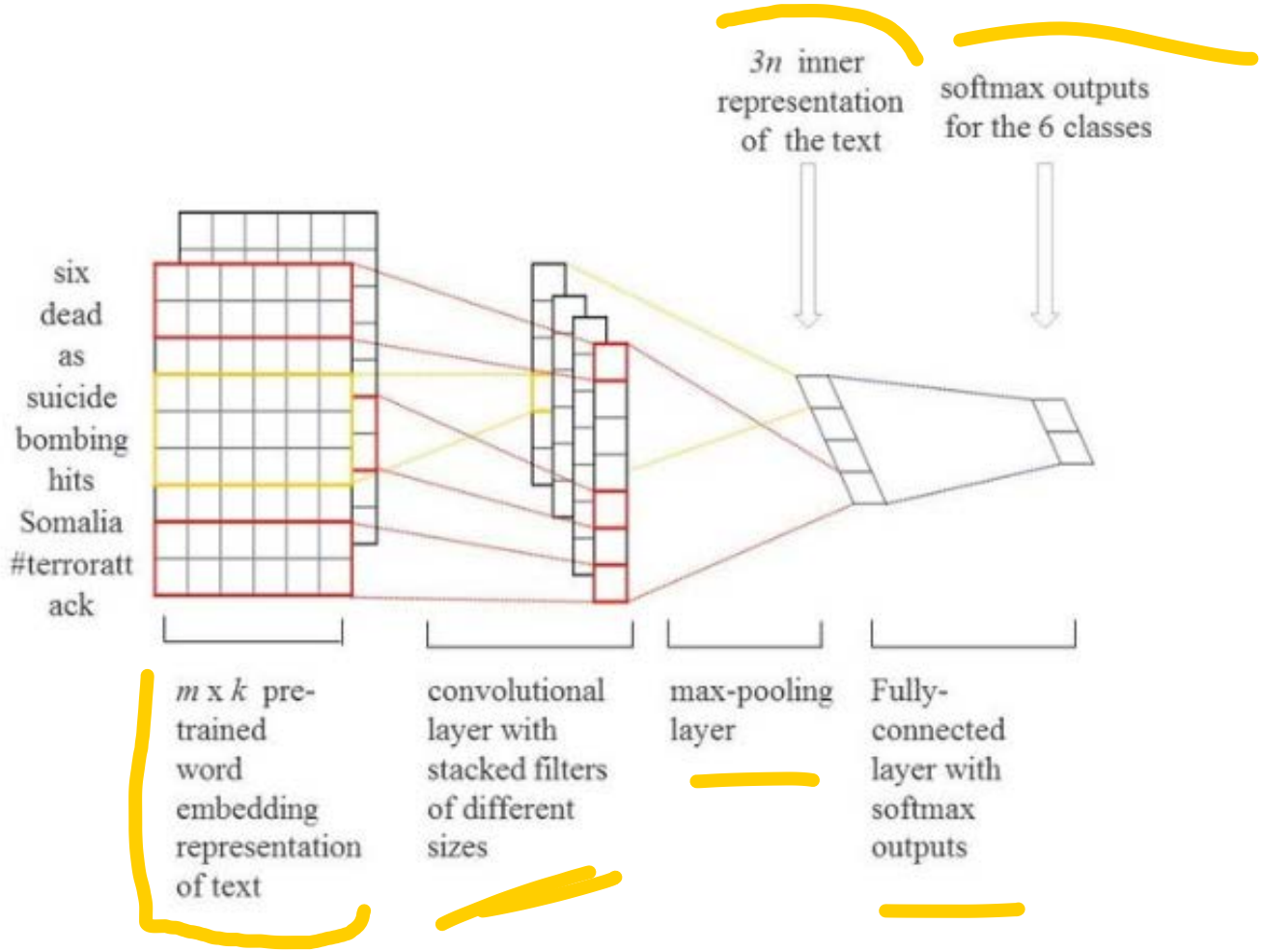
CNNs for Text



Yoon Kim. Convolutional neural networks for sentence classification. In Conference on Empirical Methods in Natural Language Processing (EMNLP), 2014.

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Sequential correlations

Recurrent Neural Networks (aka RNN, LSTM / GRU)

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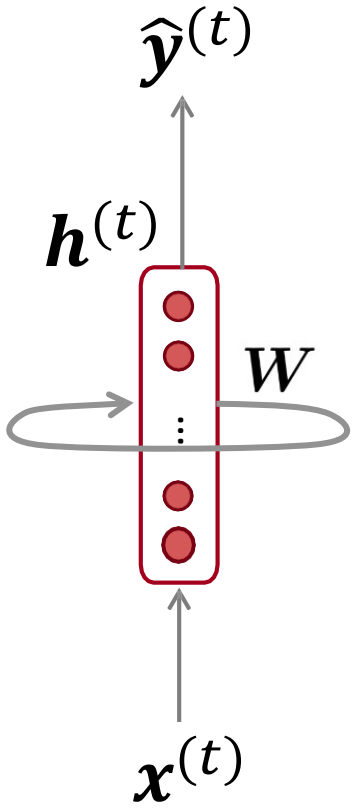
Recurrent Neural Networks (RNN)

A family of neural architectures

Core idea: Apply the same weights W *repeatedly*



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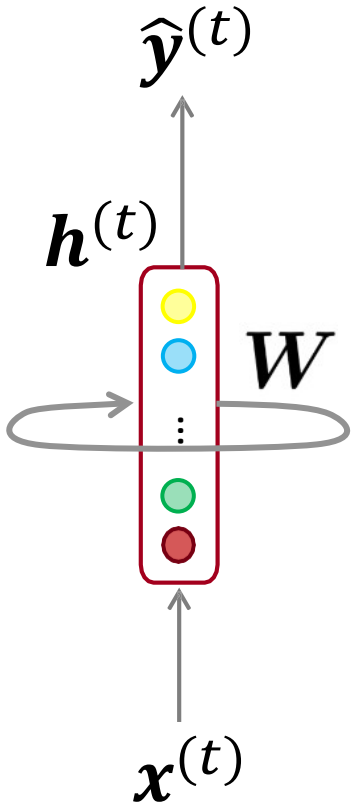

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Recurrent Neural Networks (RNN)

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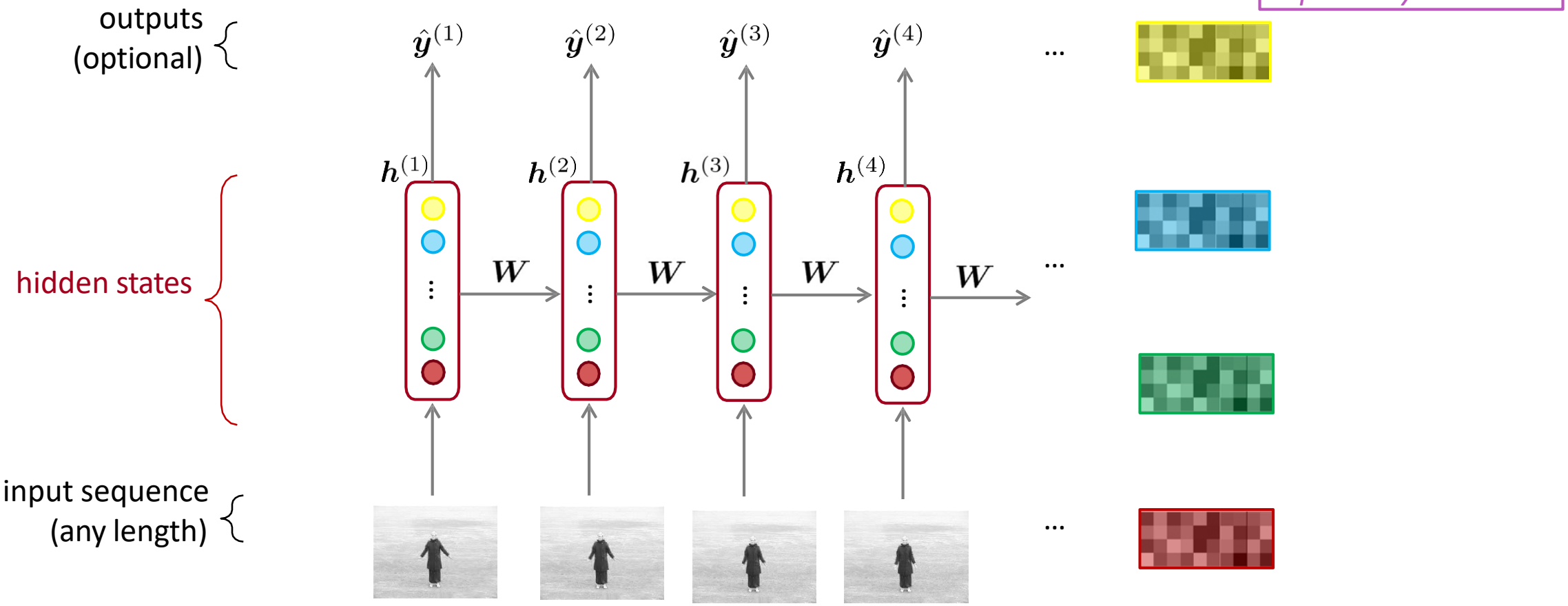

Abigail See

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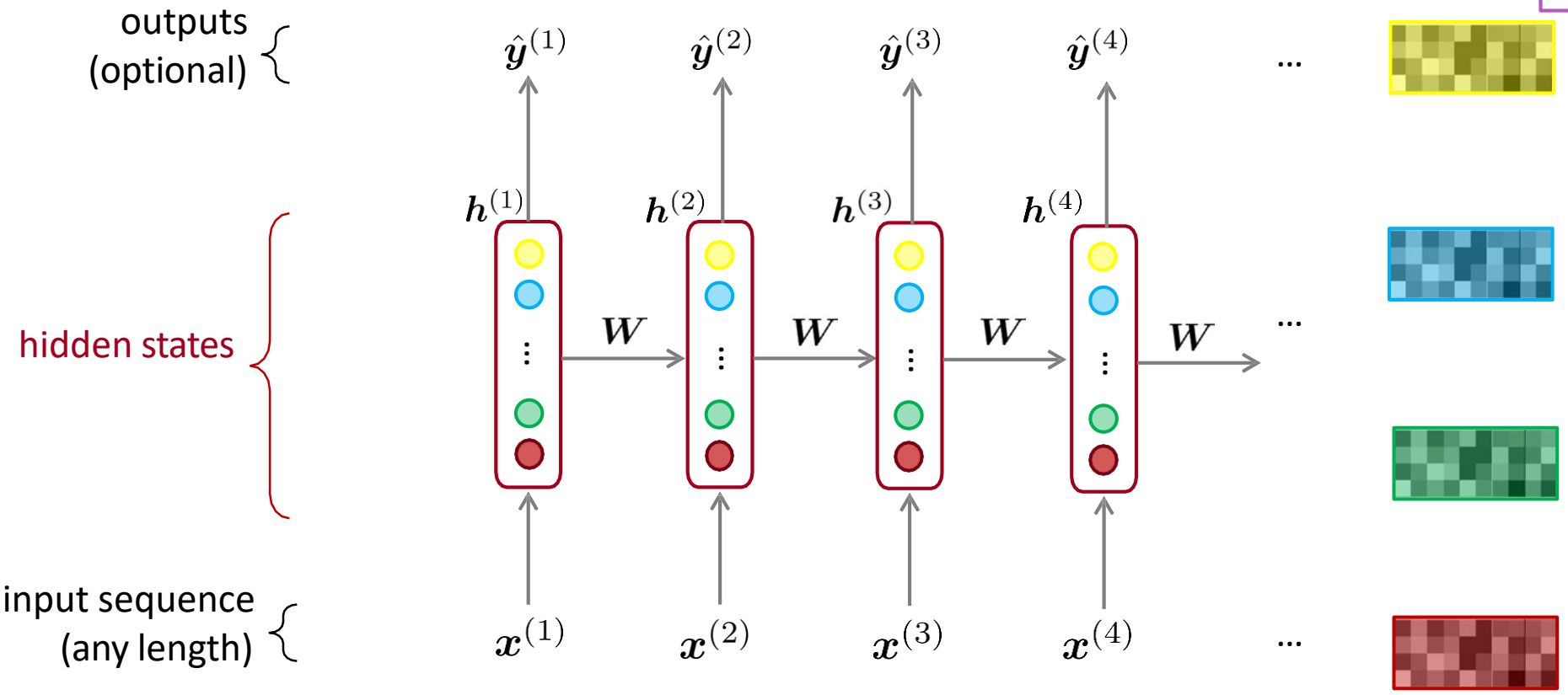

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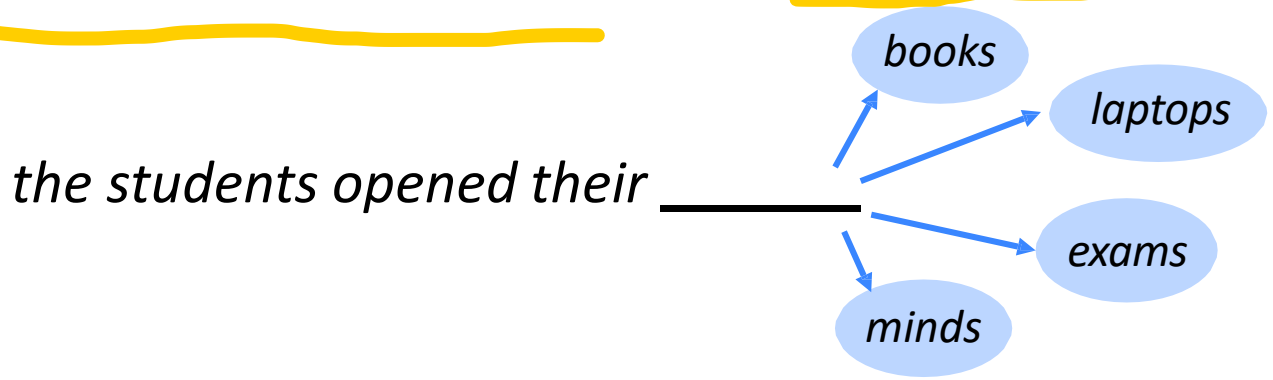
Language Modeling

- **Language Modeling** is the task of predicting what word comes next.



- More formally: given a sequence of words $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(t)}$, compute the probability distribution of the next word $\boldsymbol{x}^{(t+1)}$:

$$P(\boldsymbol{x}^{(t+1)} | \boldsymbol{x}^{(t)}, \ldots, \boldsymbol{x}^{(1)})$$

where $\boldsymbol{x}^{(t+1)}$ can be any word in the vocabulary $V = \{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_{|V|}\}$

- A system that does this is called a **Language Model**.

Abigail See

n-gram Language Models

- First we make a simplifying assumption: $\boldsymbol{x}^{(t+1)}$ depends only on the preceding *n-1* words.

n-1 words

$$P(\boldsymbol{x}^{(t+1)}|\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(1)}) = P(\boldsymbol{x}^{(t+1)}|\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)}) \quad \text{(assumption)}$$

prob of a n-gram

prob of a (n-1)-gram

$$= \frac{P(\boldsymbol{x}^{(t+1)},\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})}{P(\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})} \quad \text{(definition of conditional prob)}$$

- **Question:** How do we get these *n*-gram and (*n*-1)-gram probabilities?
- **Answer:** By counting them in some large corpus of text!

$$\approx \frac{\text{count}(\boldsymbol{x}^{(t+1)},\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})}{\text{count}(\boldsymbol{x}^{(t)},\ldots,\boldsymbol{x}^{(t-n+2)})} \quad \text{(statistical approximation)}$$

Sparsity Problems with n-gram Language Models

Sparsity Problem 1

Problem: What if *"students opened their* $\boldsymbol{w}$*"* never occurred in data? Then $\boldsymbol{w}$ has probability 0!

(Partial) Solution: Add small δ to the count for every $\boldsymbol{w} \in V$. This is called *smoothing*.

$$P(\boldsymbol{w}|\text{students opened their}) = \frac{\text{count}(\text{students opened their } \boldsymbol{w})}{\text{count}(\text{students opened their})}$$

Sparsity Problem 2

Problem: What if *"students opened their"* never occurred in data? Then we can't calculate probability for *any* $\boldsymbol{w}$!

(Partial) Solution: Just condition on *"opened their"* instead. This is called *backoff*.

Note: Increasing *n* makes sparsity problems *worse.* Typically we can't have *n* bigger than 5.

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A fixed-window neural Language Model

output distribution

$$\hat{\boldsymbol{y}} = \text{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

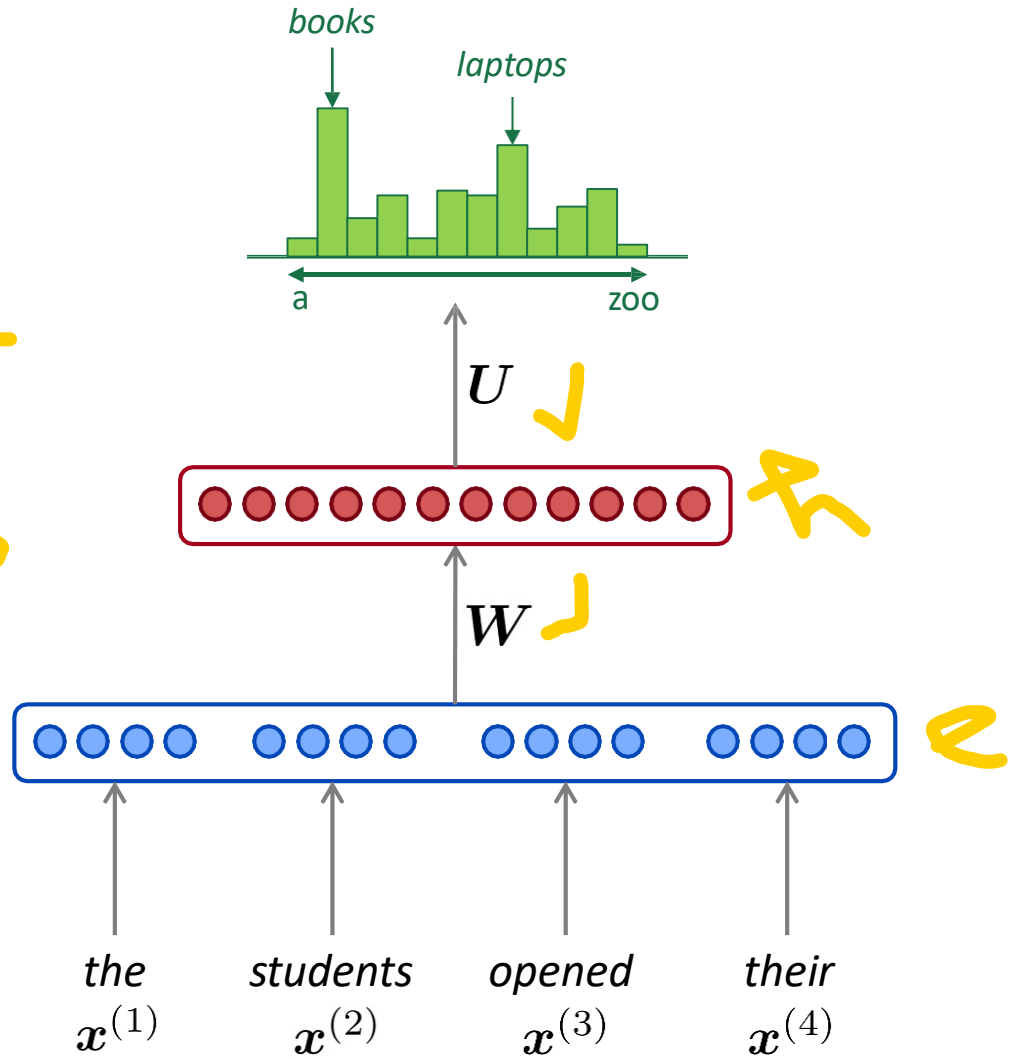
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

words / one-hot vectors

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$



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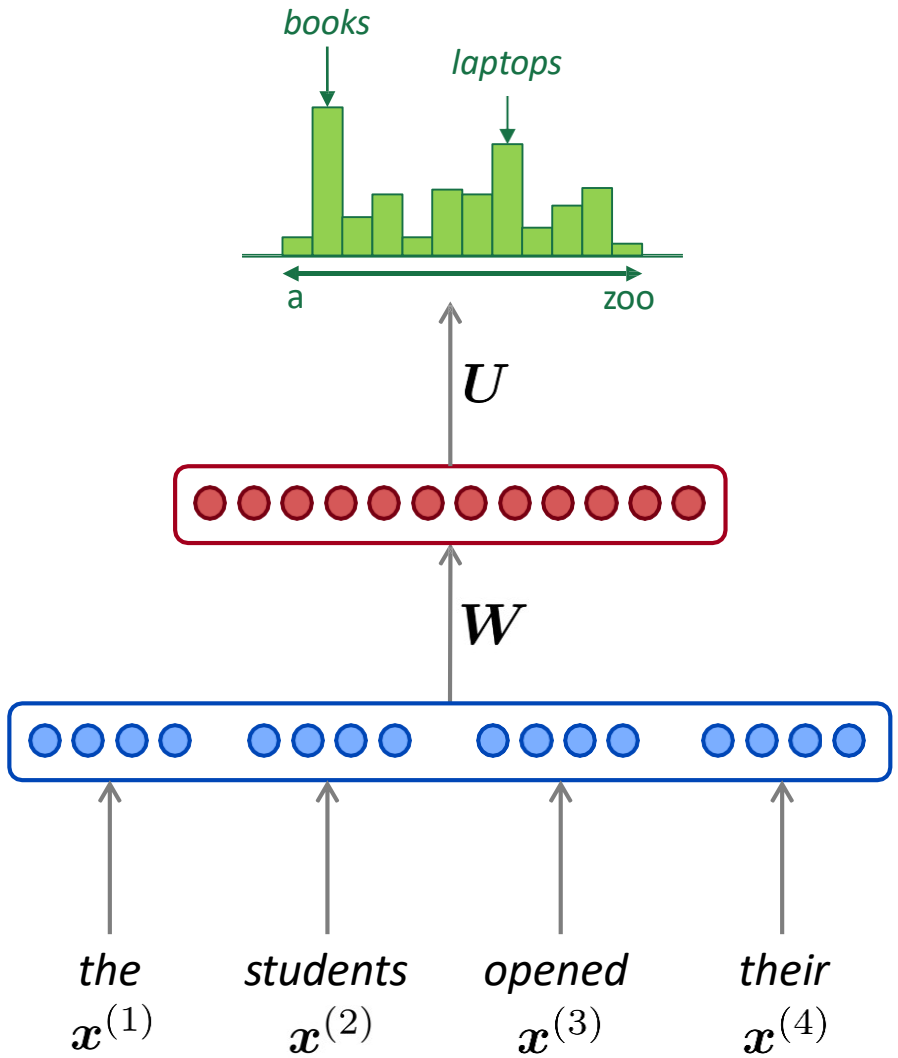
A fixed-window neural Language Model (as CNN)

Remaining **problems**:

- Fixed window is too small
- Enlarging window enlarges $\boldsymbol{W}$
- Window can never be large enough!

- $\boldsymbol{x}^{(1)}$ and $\boldsymbol{x}^{(2)}$ are multiplied by completely different weights in $\boldsymbol{W}$. No symmetry in how the inputs are processed.

We need a neural architecture that can process *any length input*



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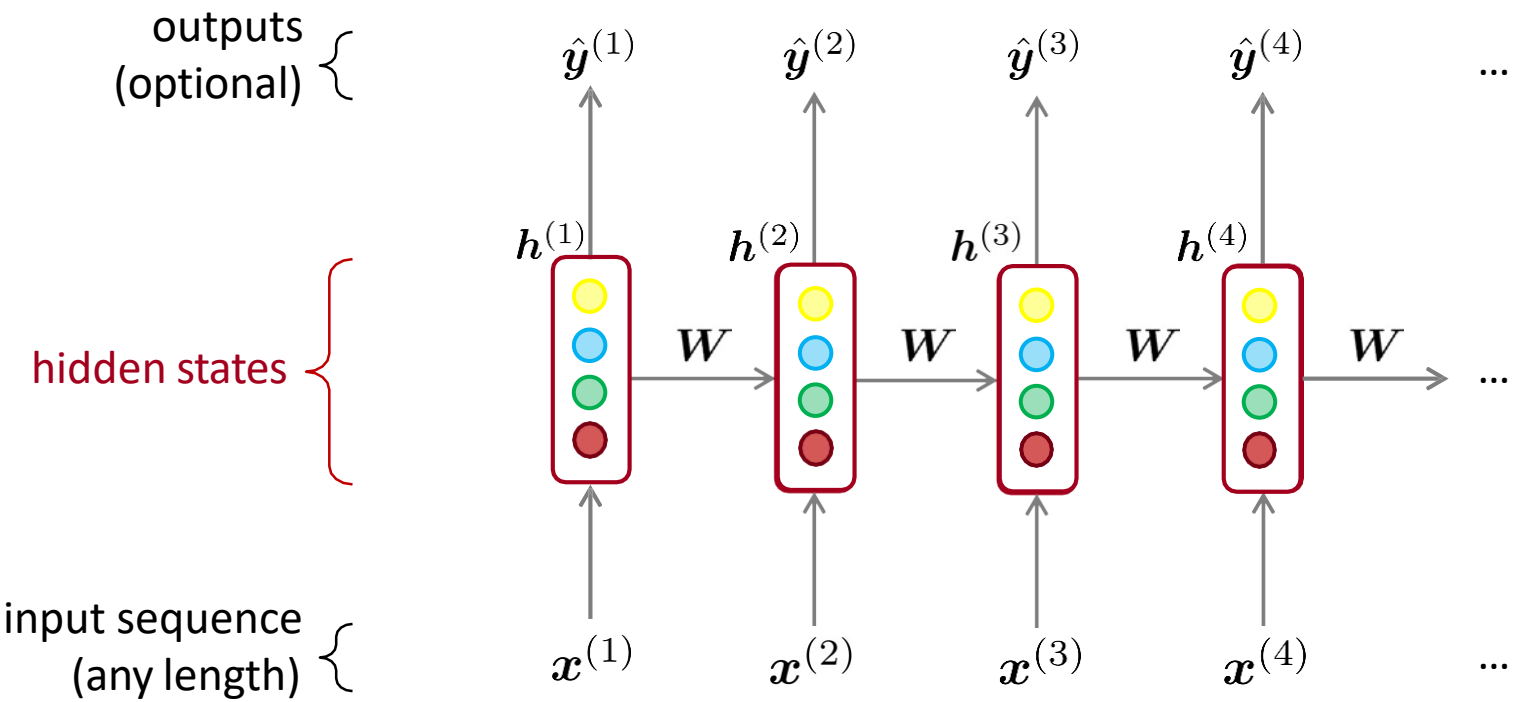
Recurrent Neural Networks (RNN)

A family of neural architectures

Core idea: Apply the same weights $\boldsymbol{W}$ *repeatedly*



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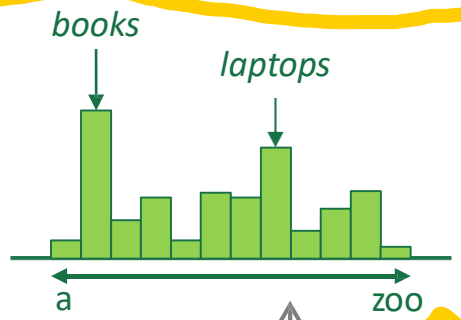
A RNN Language Model

$\hat{\boldsymbol{y}}^{(4)} = P(\boldsymbol{x}^{(5)}|\text{the students opened their})$



output distribution

$$\hat{\boldsymbol{y}}^{(t)} = \text{softmax}\left(\boldsymbol{U}\boldsymbol{h}^{(t)} + \boldsymbol{b}_2\right) \in \mathbb{R}^{|V|}$$

hidden states

$$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_e\boldsymbol{e}^{(t)} + \boldsymbol{b}_1\right)$$

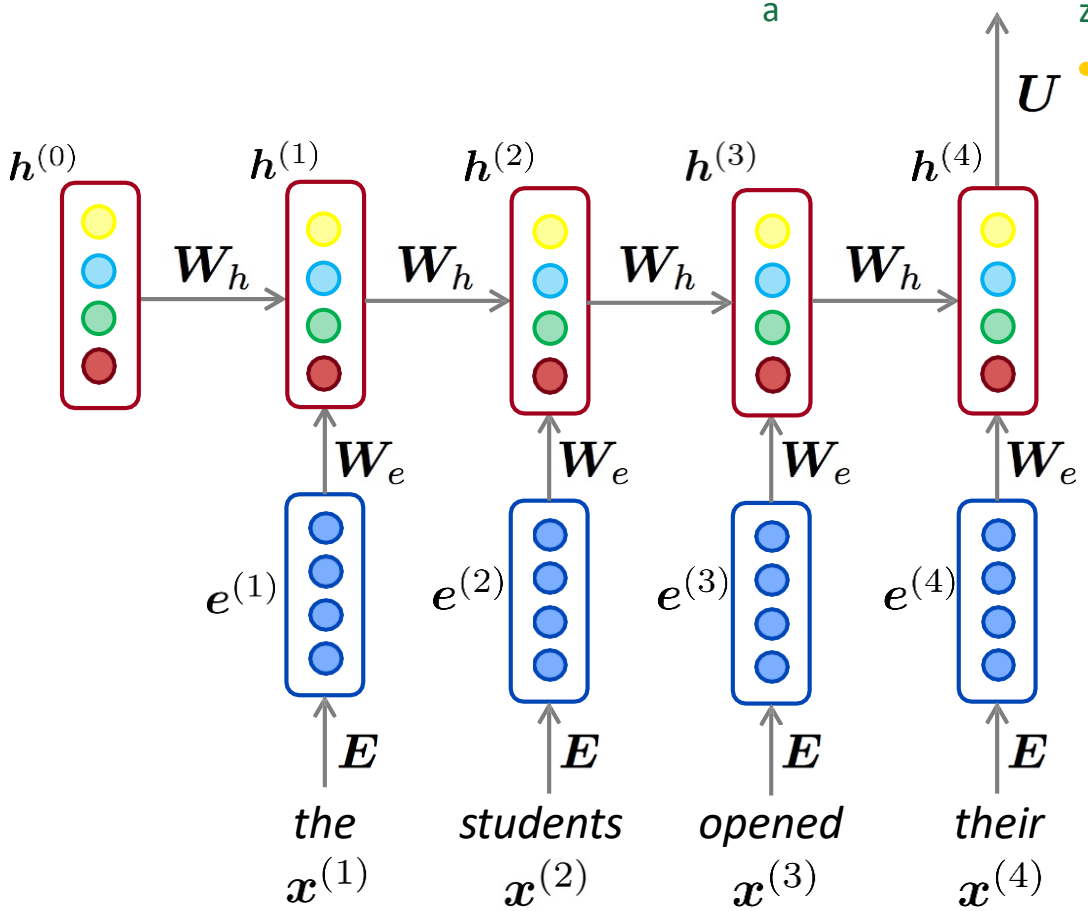
$\boldsymbol{h}^{(0)}$ is the initial hidden state

word embeddings

$$\boldsymbol{e}^{(t)} = \boldsymbol{E}\boldsymbol{x}^{(t)}$$

words / one-hot vectors

$$\boldsymbol{x}^{(t)} \in \mathbb{R}^{|V|}$$



***Note**: this input sequence could be much longer, but this slide doesn't have space!*

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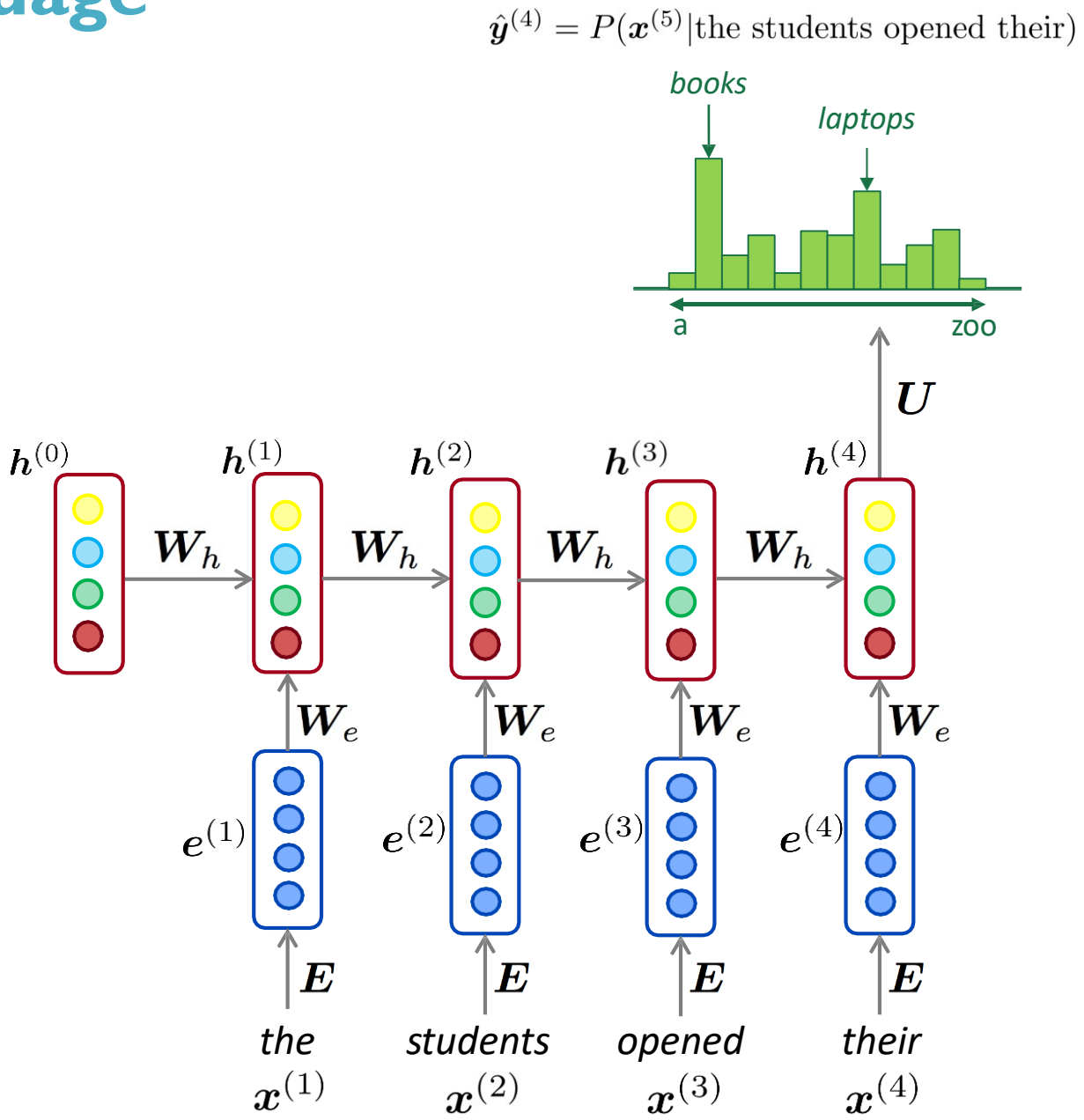
A RNN Language Model

RNN **Advantages**:

- Can process any length input
- Computation for step *t* can (in theory) use information from many steps back
- Model size doesn't increase for longer input
- Same weights applied on every timestep, so there is symmetry in how inputs are processed

RNN **Disadvantages**:

- **Recurrent computation is slow**
- **In practice, difficult to access information from many steps back**



Abigail See

Recall: Training a RNN Language Model

- Get a big corpus of text which is a sequence of words $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(T)}$
- Feed into RNN-LM; compute output distribution $\hat{\boldsymbol{y}}^{(t)}$ for *every step t*.
  - i.e. predict probability distribution of *every word*, given words so far
- Loss function on step *t* is cross-entropy between predicted probability distribution $\hat{\boldsymbol{y}}^{(t)}$, and the true next word $\boldsymbol{y}^{(t)}$ (one-hot for $\boldsymbol{x}^{(t+1)}$):

$$J^{(t)}(\theta) = CE(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)}) = -\sum_{w \in V} \boldsymbol{y}_w^{(t)} \log \hat{\boldsymbol{y}}_w^{(t)} = -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

- Average this to get overall loss for entire training set:

$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} J^{(t)}(\theta) = \frac{1}{T} \sum_{t=1}^{T} -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

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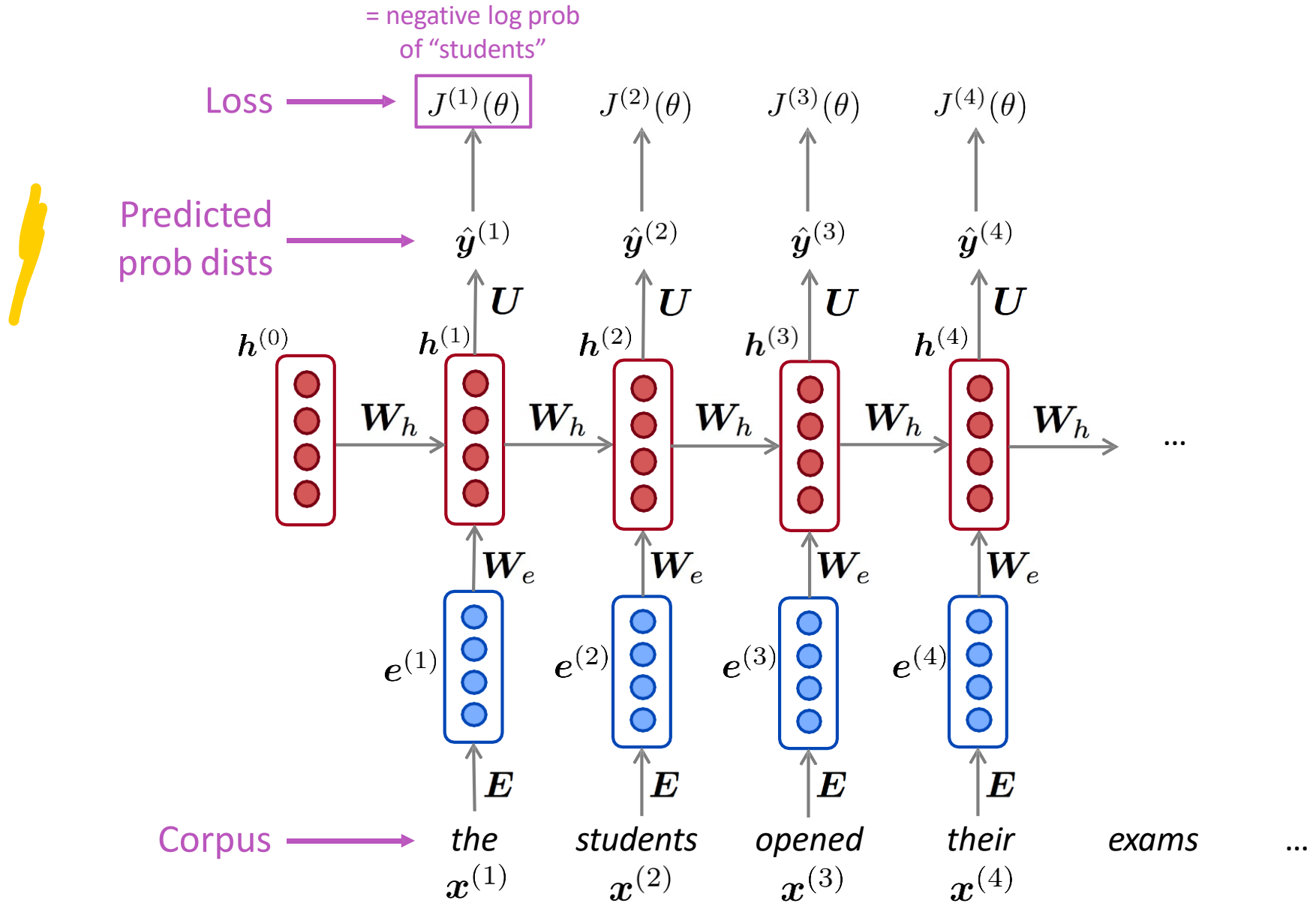
Training a RNN Language Model



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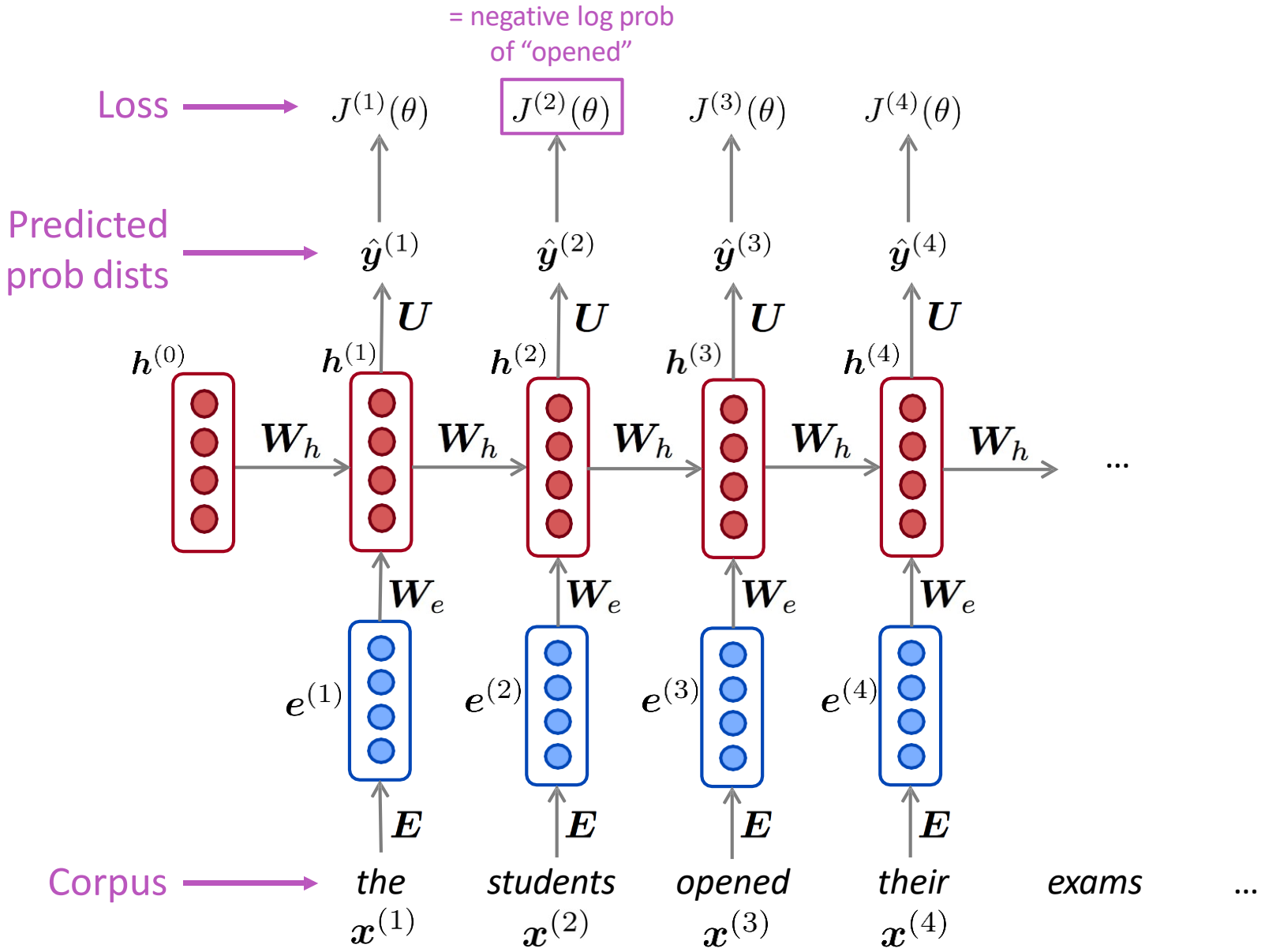
Training a RNN Language Model



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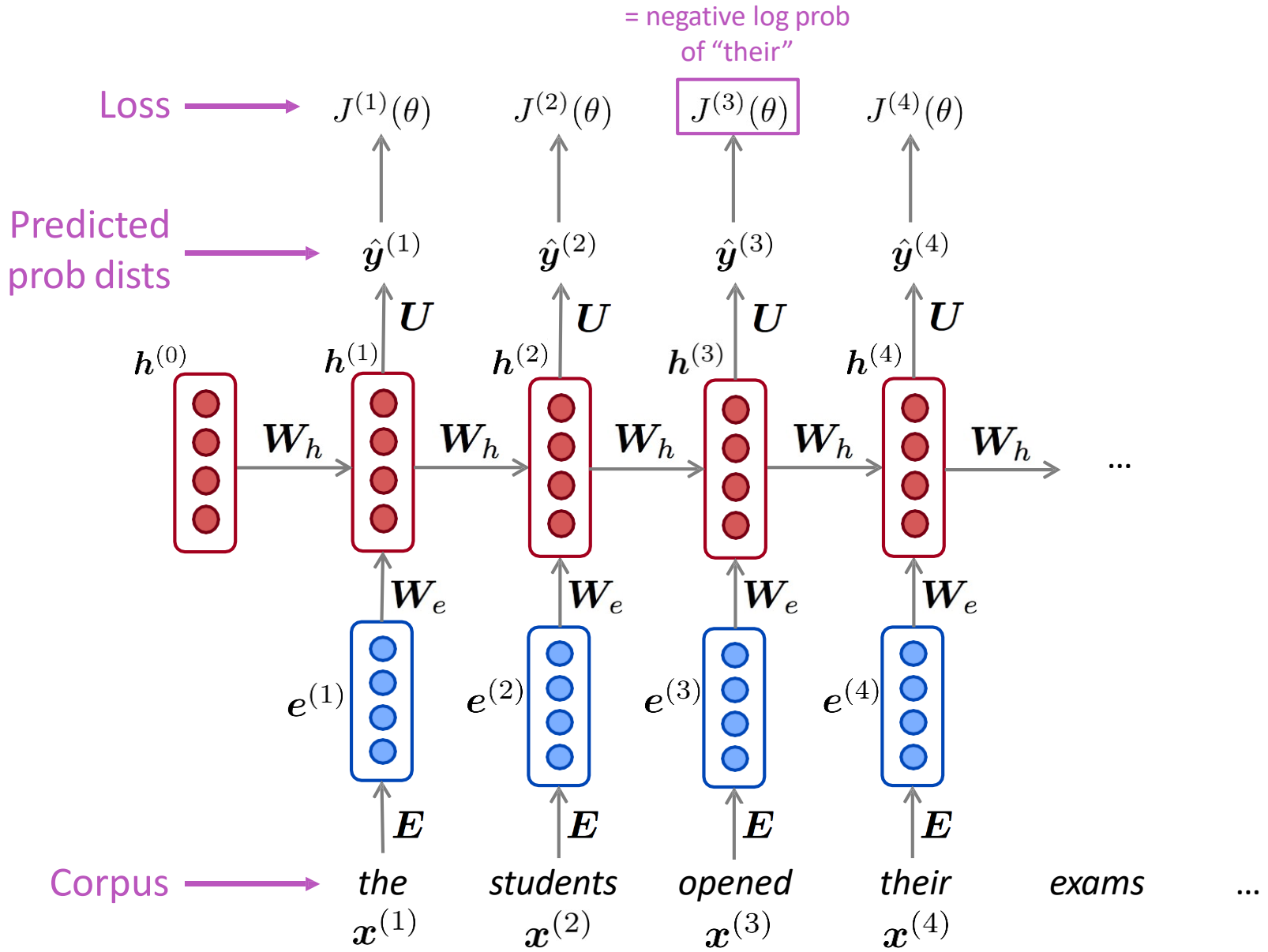
Training a RNN Language Model



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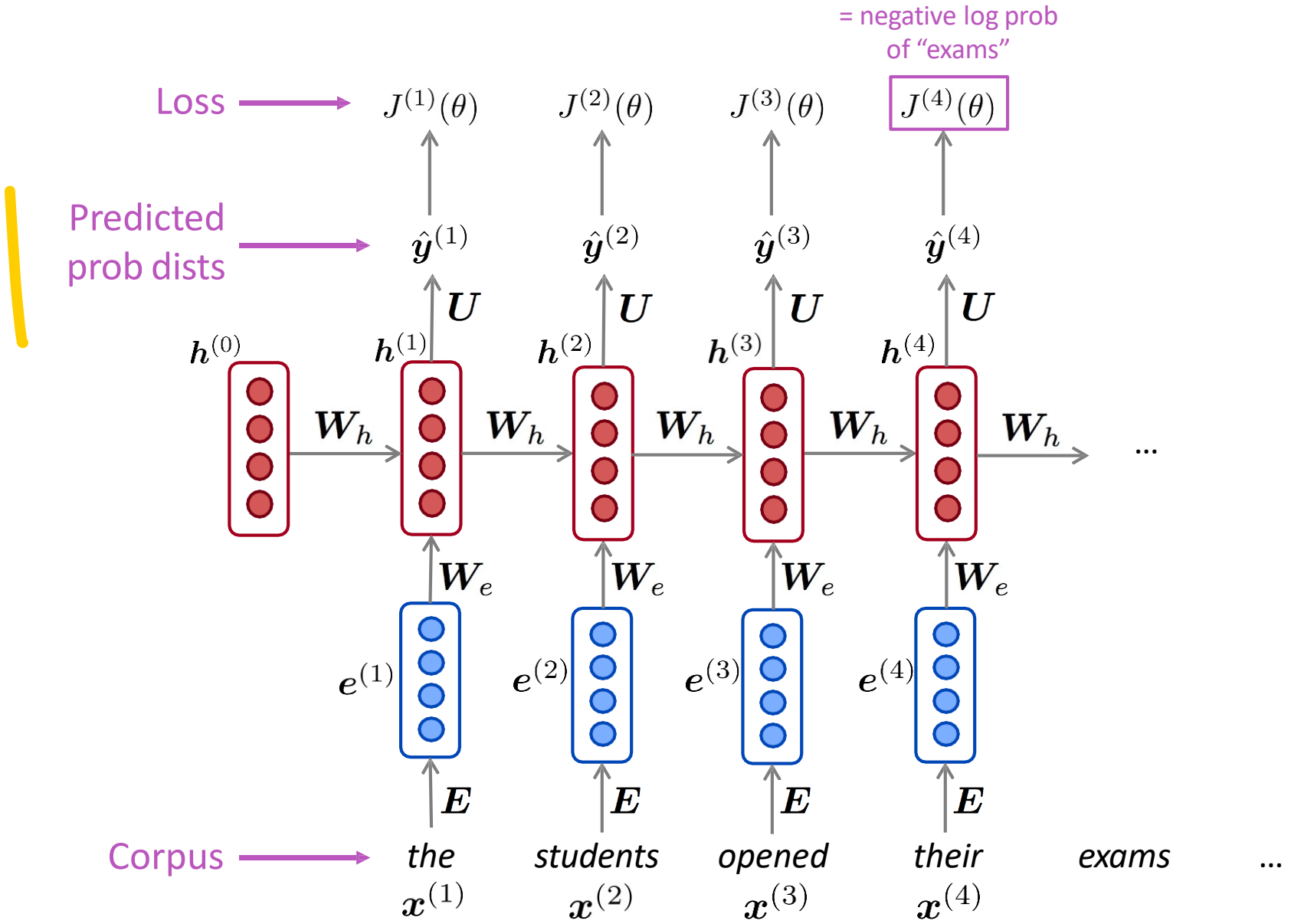
Training a RNN Language Model



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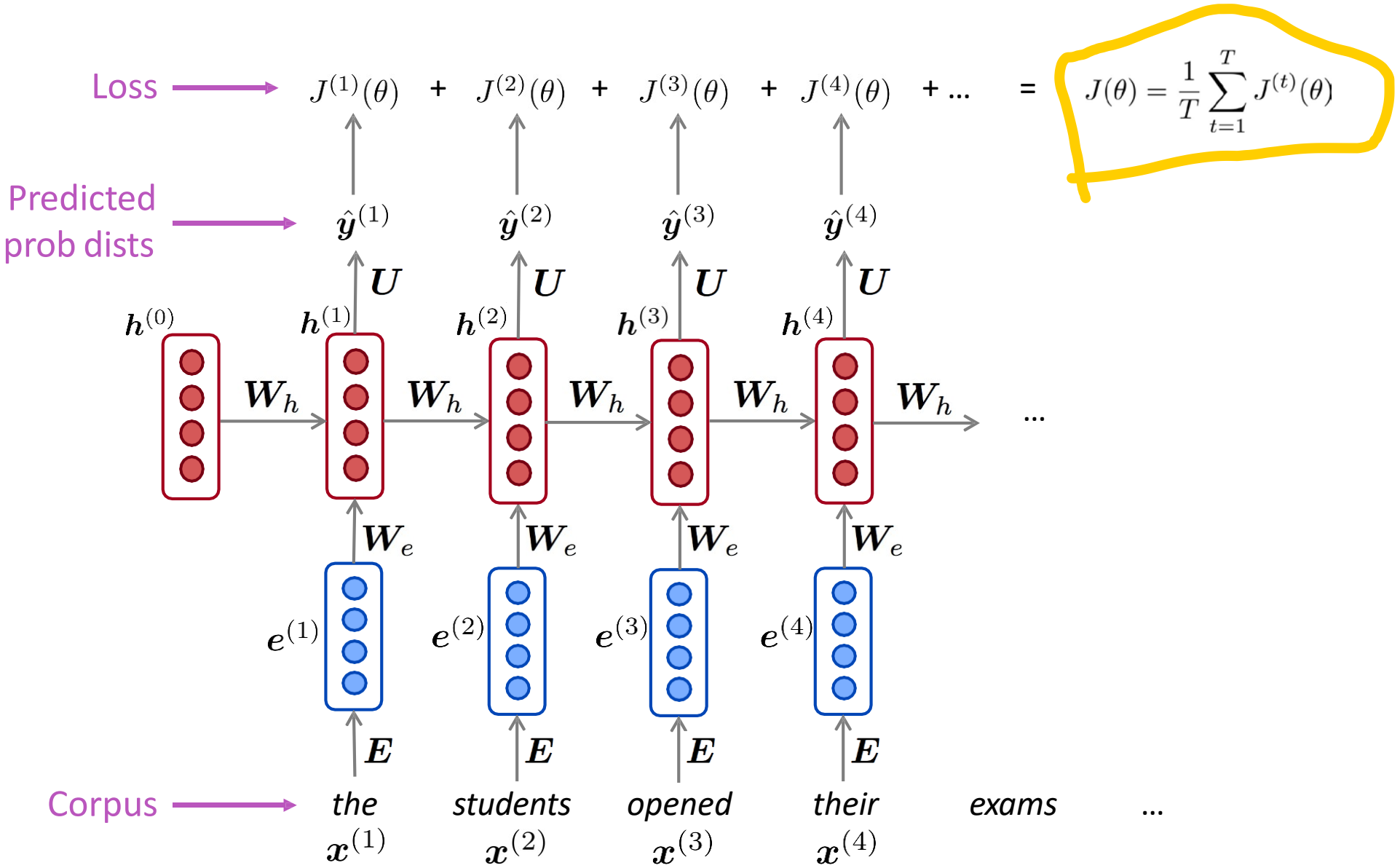
Training a RNN Language Model



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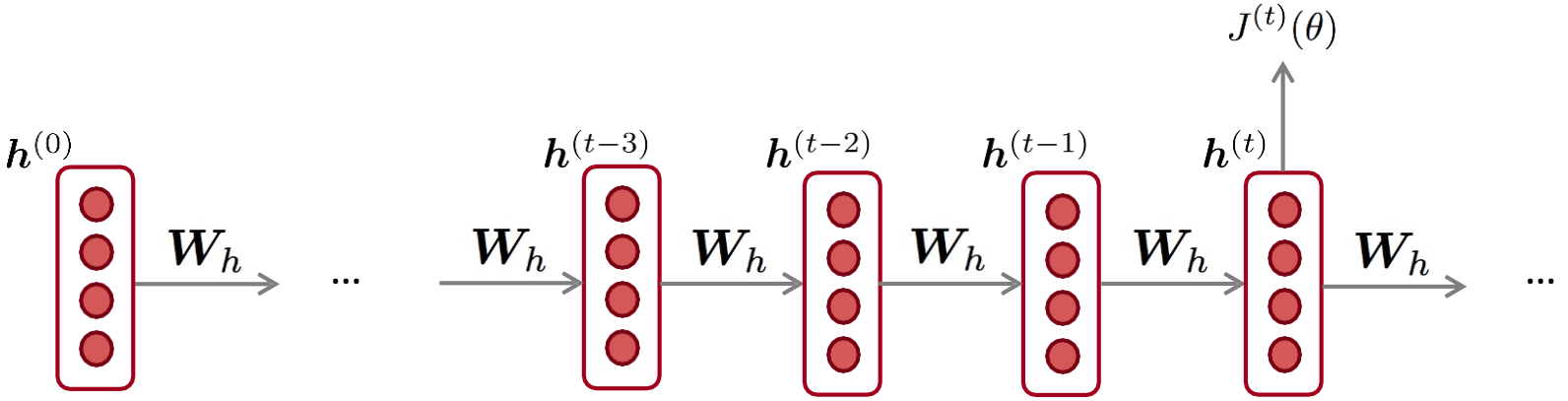
Backpropagation for RNNs



Question: What's the derivative of $J^{(t)}(\theta)$ w.r.t. the repeated weight matrix $\boldsymbol{W_h}$?

Answer: $$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \left. \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} \right|_{(i)}$$

"The gradient w.r.t. a repeated weight is the sum of the gradient w.r.t. each time it appears"

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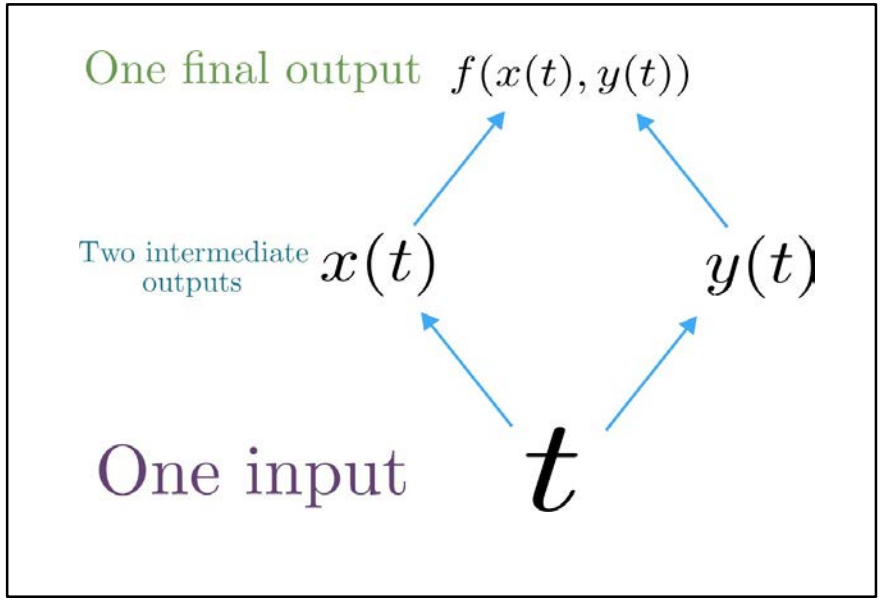
Multivariable Chain Rule

- Given a multivariable function $f(x, y)$, and two single variable functions $x(t)$ and $y(t)$, here's what the multivariable chain rule says:

$$\underbrace{\frac{d}{dt} f(x(t), y(t))}_{\text{Derivative of composition function}} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}$$



Source:
https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/differentiating-vector-valued-functions/a/multivariable-chain-rule-simple-version

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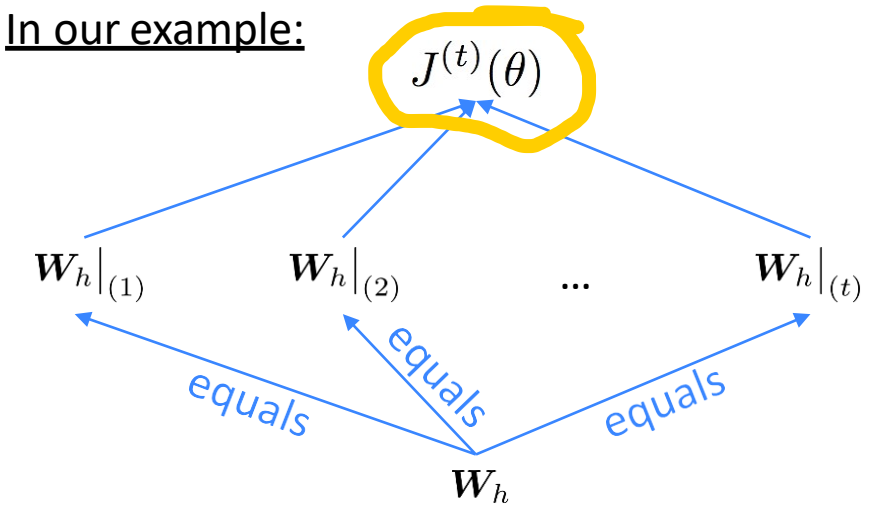
Backpropagation for RNNs: Proof sketch

- Given a multivariable function $f(x, y)$, and two single variable functions $x(t)$ and $y(t)$, here's what the multivariable chain rule says:

$$\underbrace{\frac{d}{dt} f(x(t), y(t))}_{\text{Derivative of composition function}} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}$$

In our example:



Apply the multivariable chain rule:

$$\frac{\partial J^{(t)}}{\partial W_h} = \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial W_h}\bigg|_{(i)} \frac{\partial W_h|_{(i)}}{\partial W_h}$$

= 1

$$= \sum_{i=1}^{t} \frac{\partial J^{(t)}}{\partial W_h}\bigg|_{(i)}$$

Source:
https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/differentiating-vector-valued-functions/a/multivariable-chain-rule-simple-version

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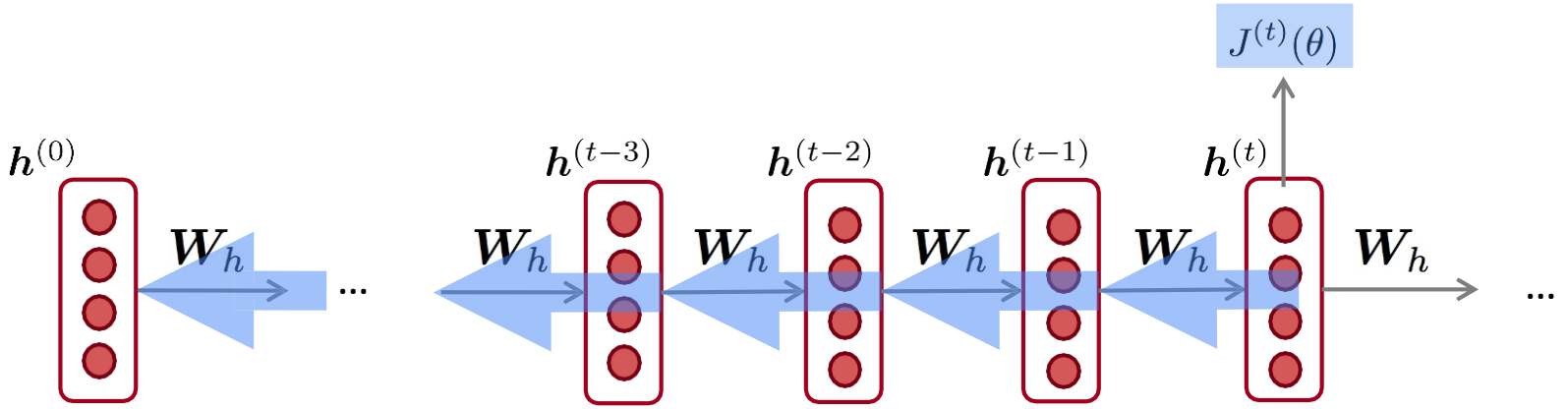
Backpropagation for RNNs

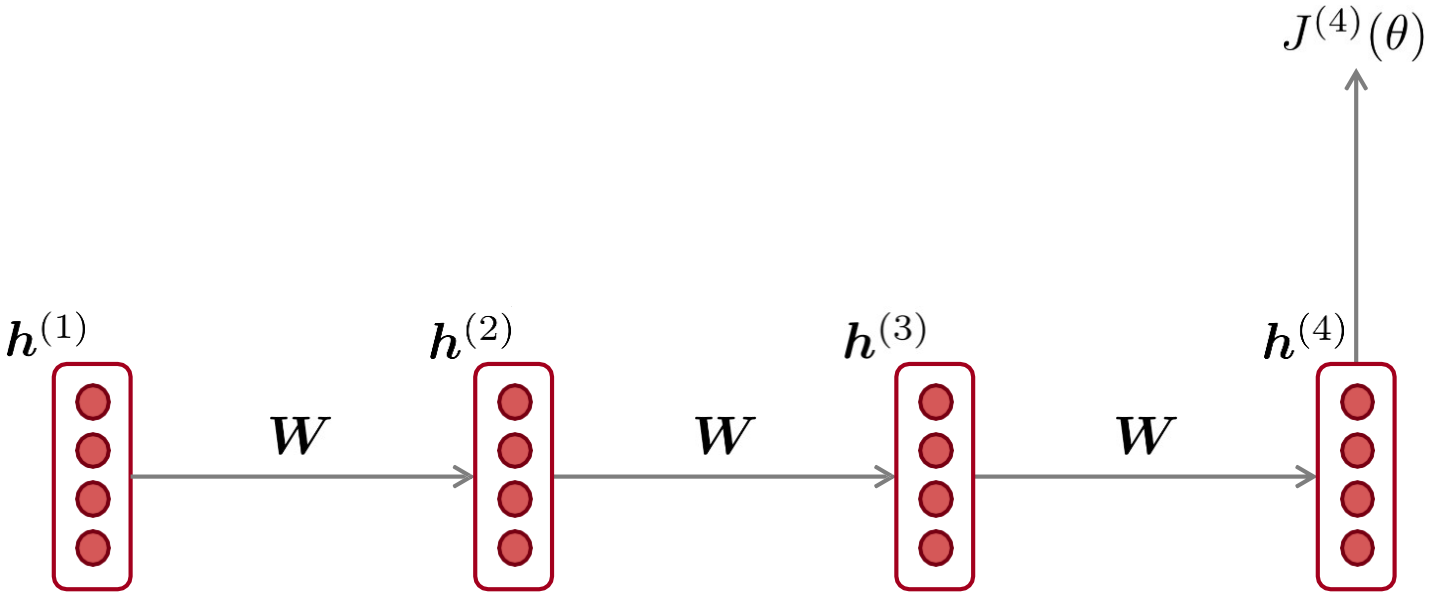


$$\frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} = \sum_{i=1}^{t} \left. \frac{\partial J^{(t)}}{\partial \boldsymbol{W_h}} \right|_{(i)}$$

Question: How do we calculate this?

Answer: Backpropagate over timesteps *i*=*t*,…,0, summing gradients as you go.
This algorithm is called
"backpropagation through time"

Vanishing gradient intuition



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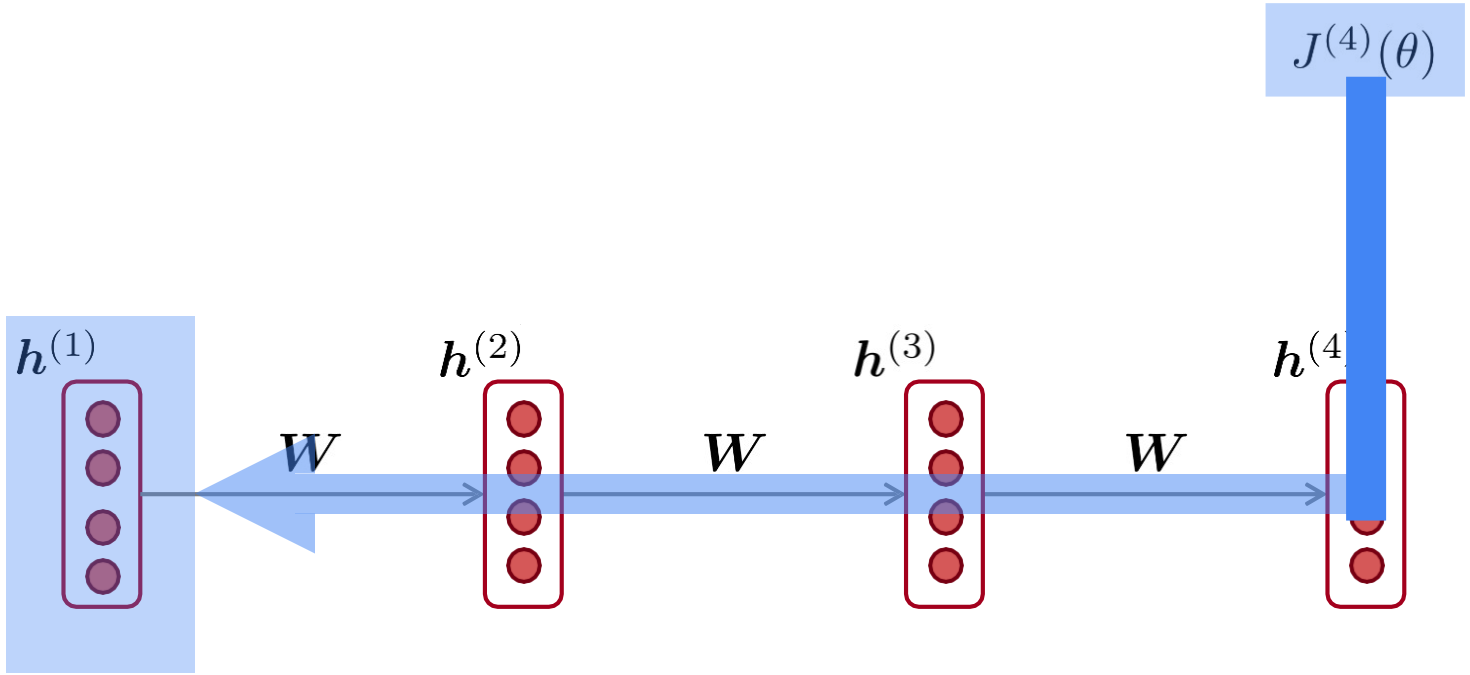
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = ?$$

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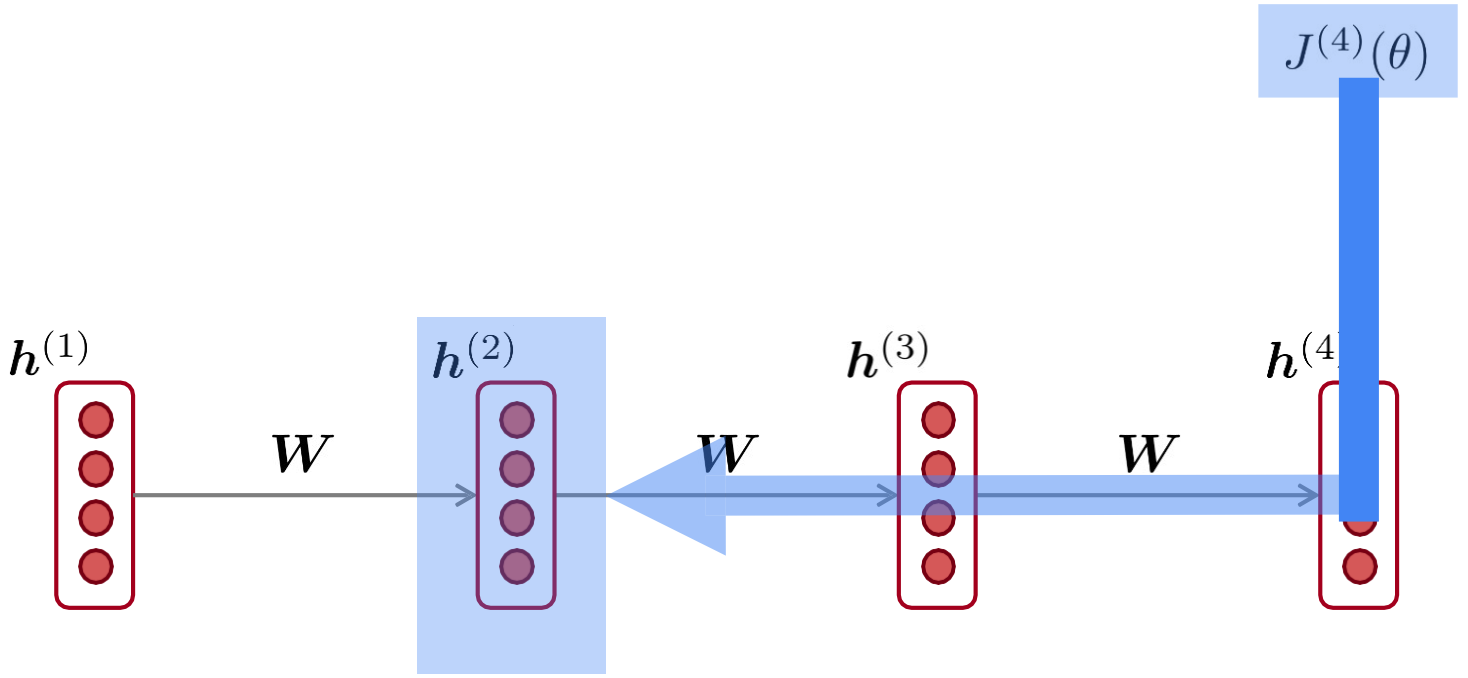
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial J^{(4)}}{\partial h^{(2)}}$$

chain rule!

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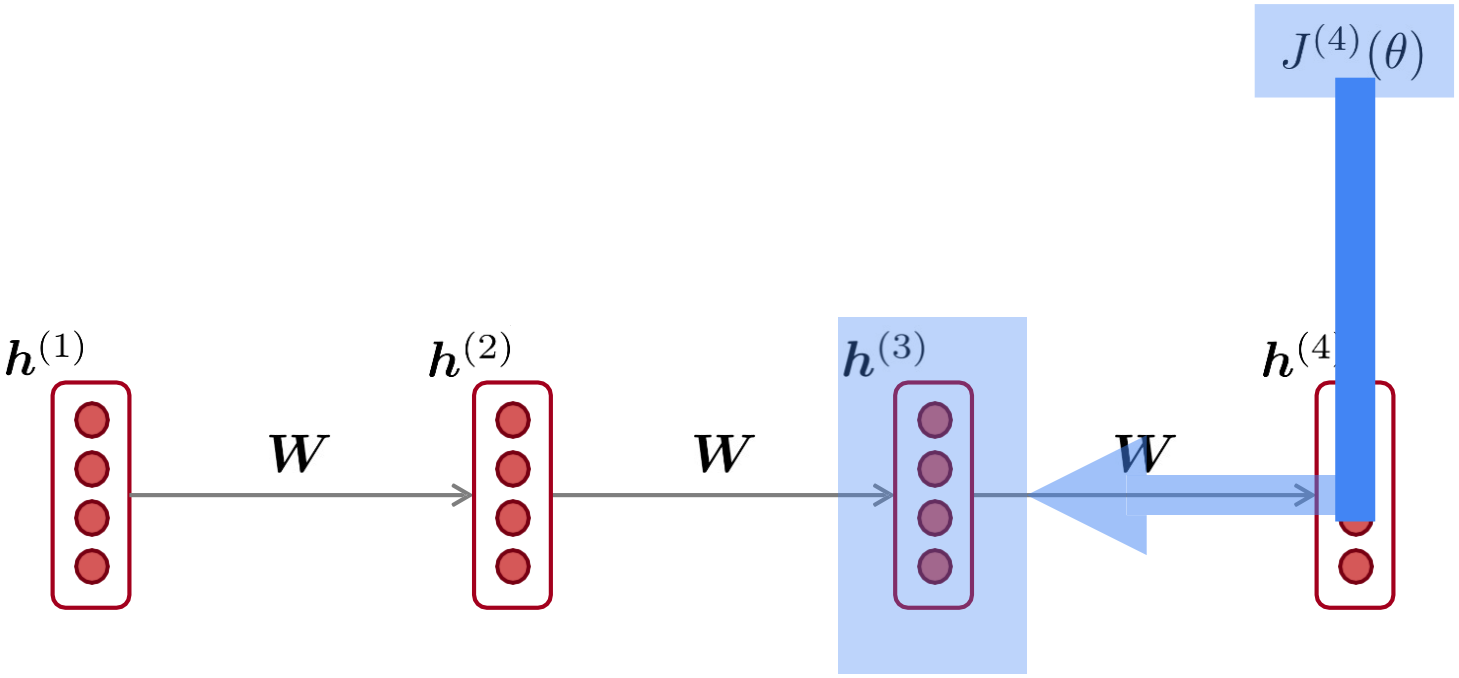
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial J^{(4)}}{\partial h^{(3)}}$$

chain rule!

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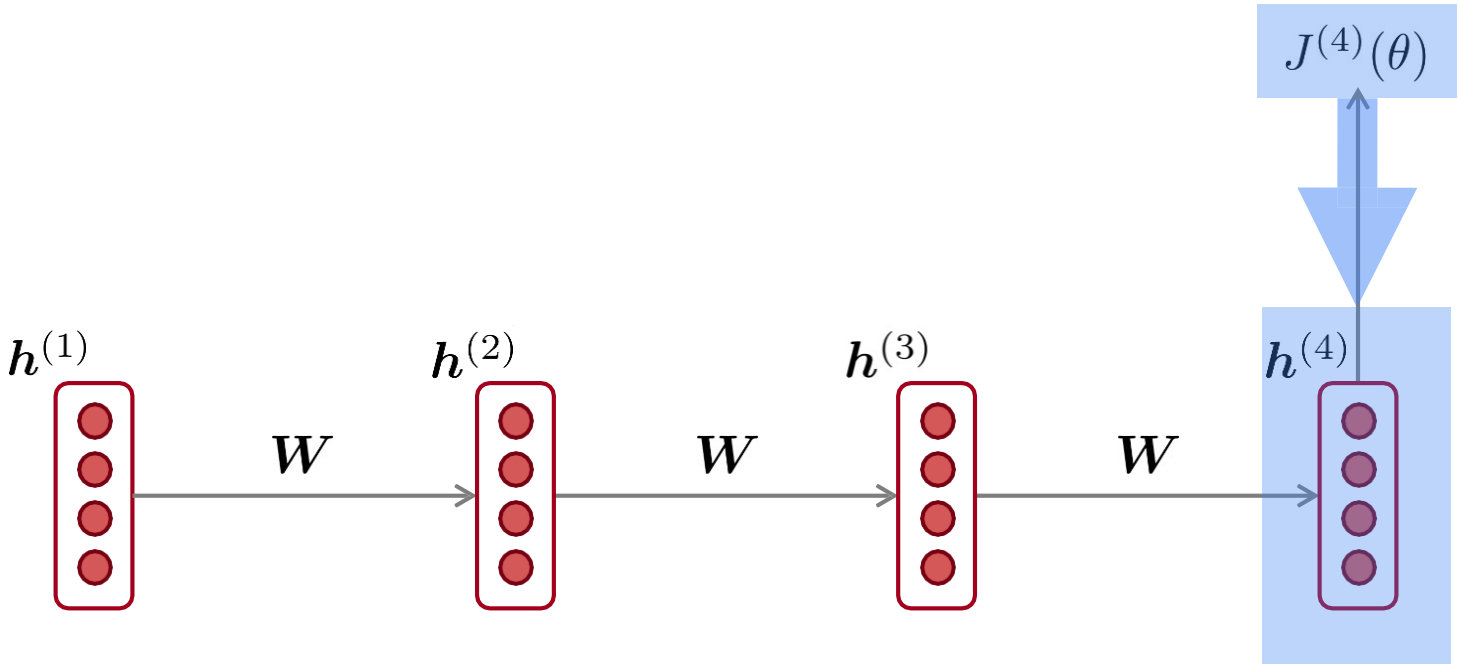
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial h^{(4)}}{\partial h^{(3)}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}$$

chain rule!

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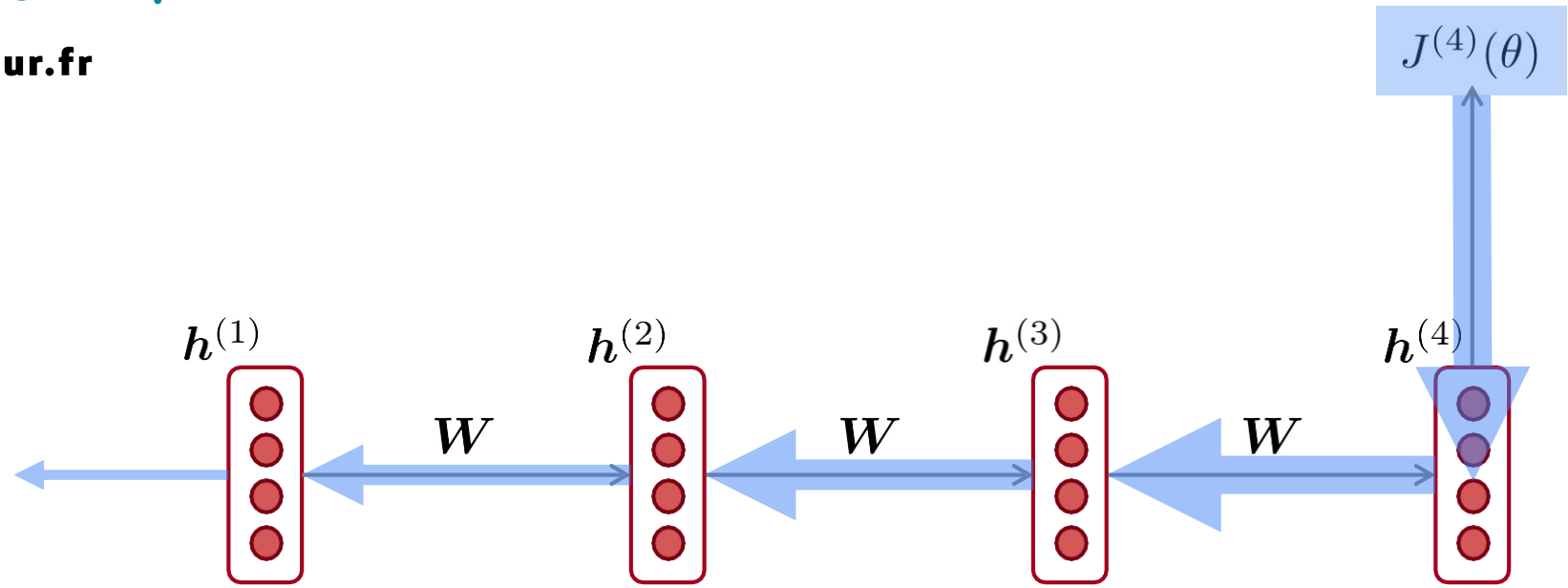
Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial h^{(4)}}{\partial h^{(3)}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}$$

What happens if these are small?

Vanishing gradient problem:
When these are small, the gradient signal gets smaller and smaller as it backpropagates further

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Vanishing gradient proof sketch

- Recall: $$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)$$

- Therefore: $$\frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}} = \operatorname{diag}\left(\sigma'\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)\right) \boldsymbol{W}_h$$ (chain rule)

- Consider the gradient of the loss $J^{(i)}(\theta)$ on step *i*, with respect to the hidden state $\boldsymbol{h}^{(j)}$ on some previous step *j*.

$$\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(j)}} = \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \prod_{j<t\leq i} \frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}}$$ (chain rule)

$$= \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boldsymbol{W}_h^{(i-j)} \prod_{j<t\leq i} \operatorname{diag}\left(\sigma'\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)\right)$$ (value of $\frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}}$)

If W_h is small, then this term gets vanishingly small as *i* and *j* get further apart

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf

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Vanishing gradient proof sketch

- Consider matrix L2 norms:

$$\left\|\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(j)}}\right\| \leq \left\|\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}}\right\| \|\boldsymbol{W}_h\|^{(i-j)} \prod_{j<t\leq i} \left\|\operatorname{diag}\left(\sigma'\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)\right)\right\|$$

- Pascanu et al showed that that if the largest eigenvalue of W_h is less than 1, then the gradient $\left\|\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(j)}}\right\|$ will shrink exponentially

- There's a similar proof relating a largest eigenvalue >1 to exploding gradients

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013.
http://proceedings.mlr.press/v28/pascanu13.pdf

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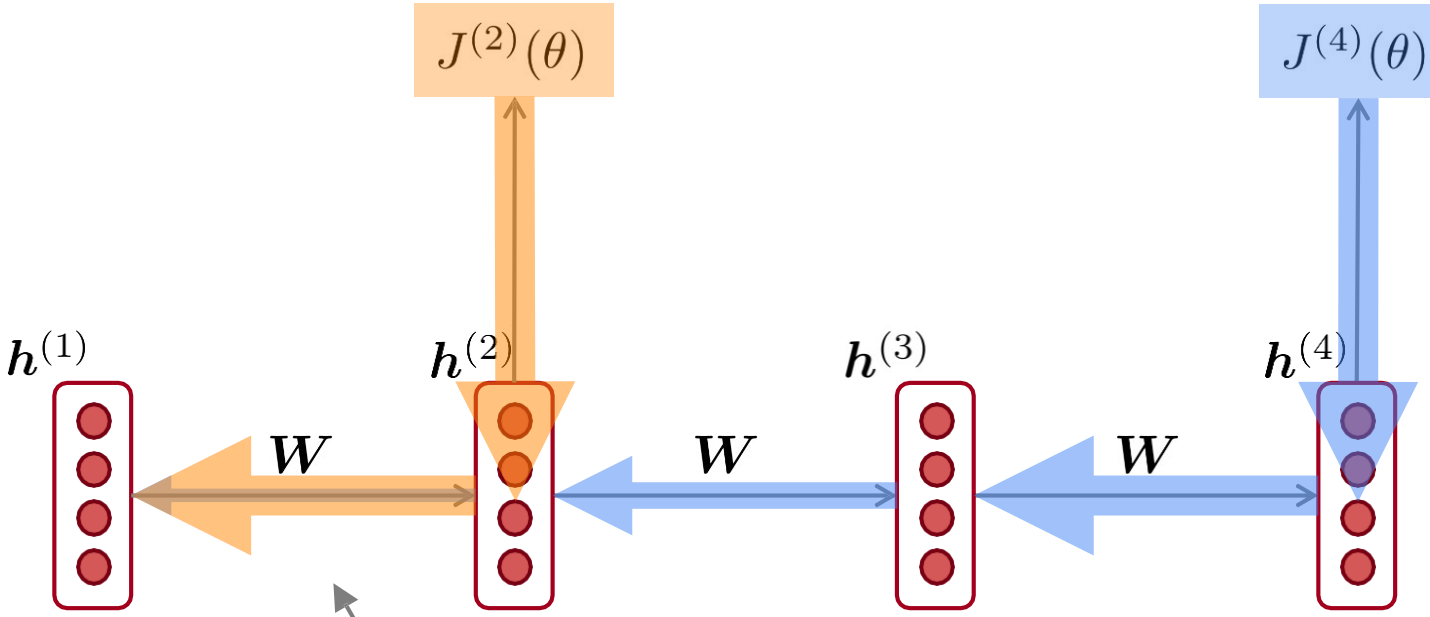
Why is vanishing gradient a problem?



Gradient signal from faraway is lost because it's much smaller than gradient signal from close-by.

So model weights are only updated only with respect to near effects, not long-term effects.

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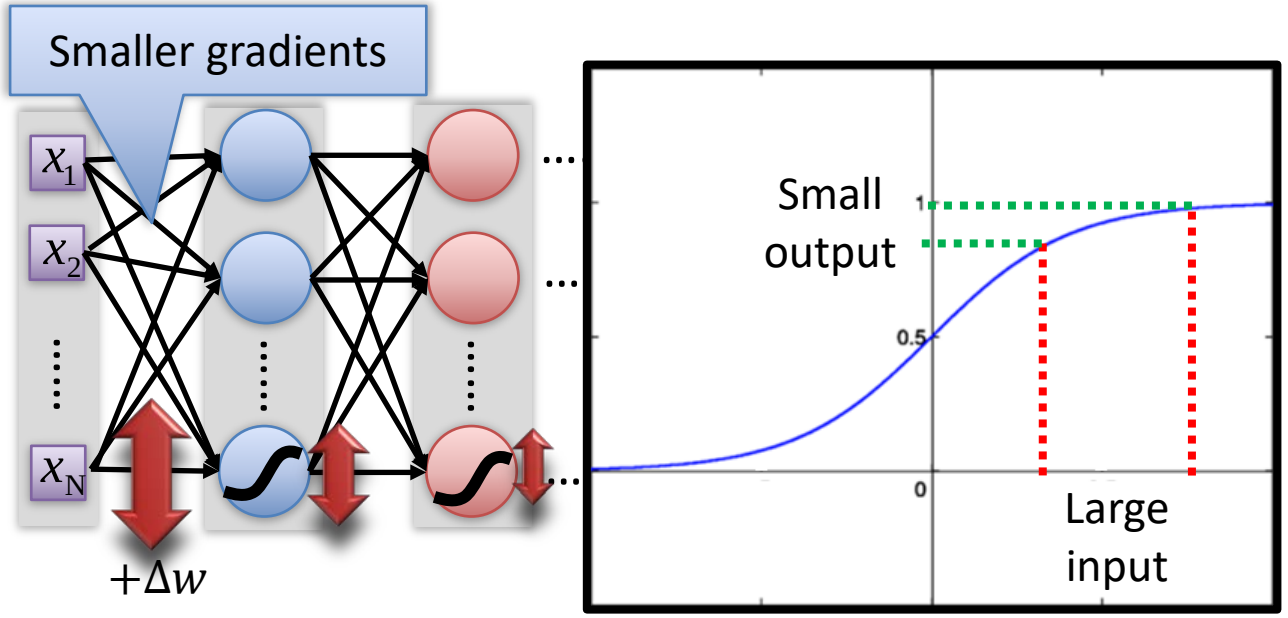
Recipe of Deep Learning

- ***Vanishing Gradient Problem***



Intuitive way to compute the derivatives …

$$\frac{\partial l}{\partial w} =? \frac{\Delta l}{\Delta w}$$

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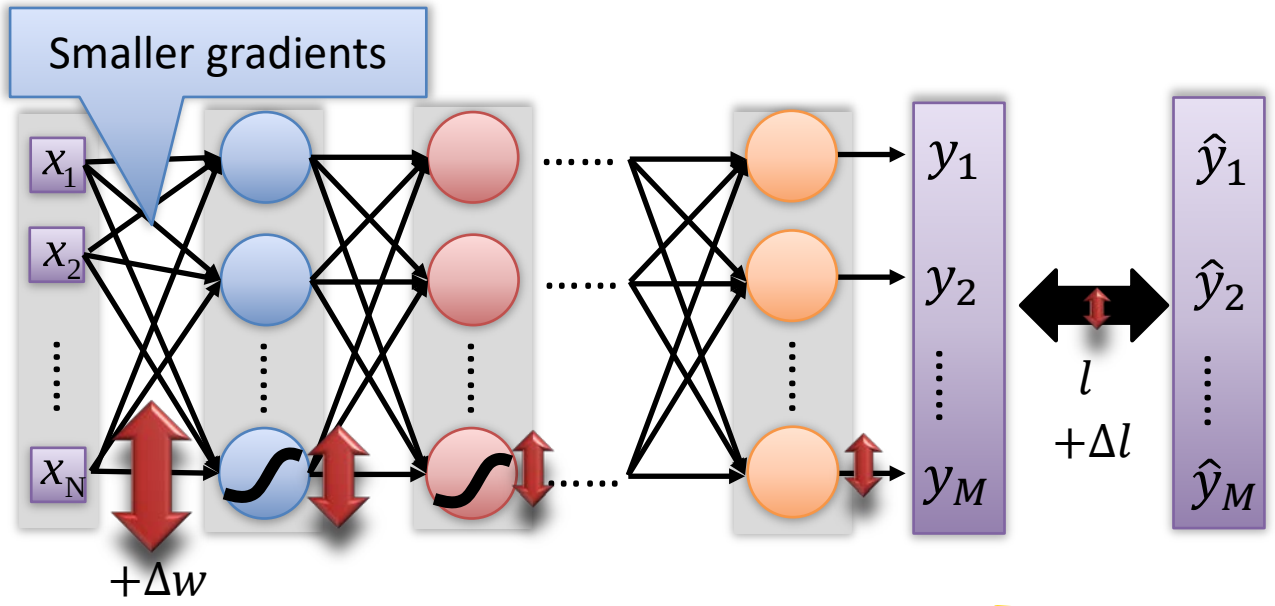
Recipe of Deep Learning

- ***Vanishing Gradient Problem***



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Recipe of Deep Learning

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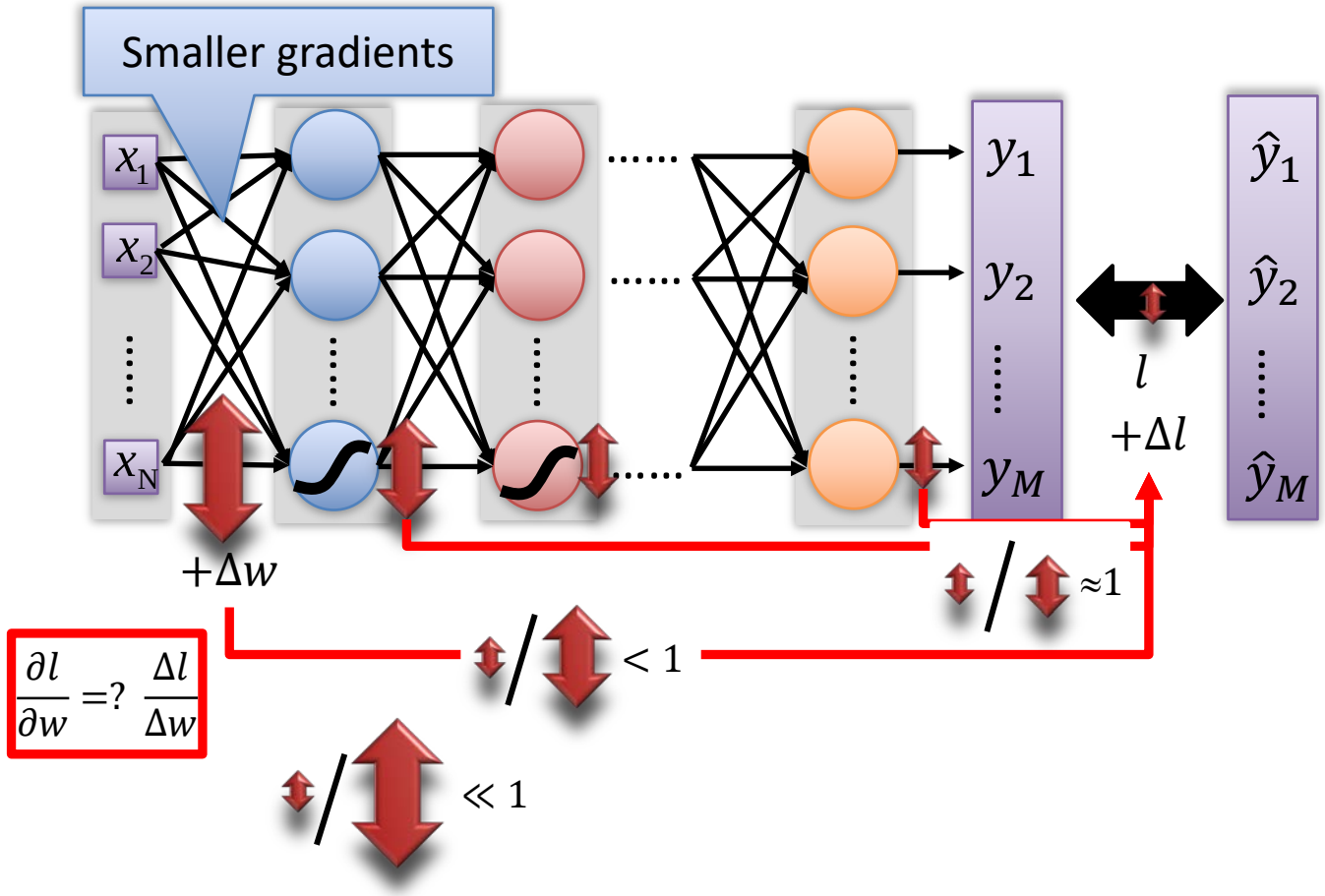

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Effect of vanishing gradient on RNN-LM

- **LM task:** *When she tried to print her _____, she found that the printer was out of toner. She went to the stationery store to buy more toner. It was very overpriced. After installing the toner into the printer, she finally printed her tickets.*

- To learn from this training example, the RNN-LM needs to model the dependency between *"tickets"* on the 7th step and the target word *"tickets"* at the end.

- But if gradient is small, the model can't learn this dependency
  - So the model is unable to predict similar long-distance dependencies at test time

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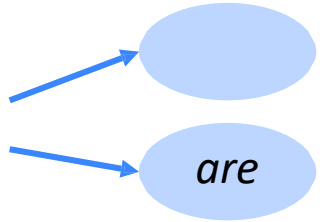
Effect of vanishing gradient on RNN-LM

- **LM task:** *The writer of the books* ____



- **Correct answer**: *The writer of the books <u>is</u> planning a sequel*
- **Syntactic recency:** *The <u>writer</u> of the books <u>is</u>* (correct)
- **Sequential recency:** *The writer of the <u>books</u> <u>are</u>* (incorrect)
- Due to vanishing gradient, RNN-LMs are better at learning from sequential recency than syntactic recency, so they make this type of error more often than we'd like [Linzen et al 2016]

"Assessing the Ability of LSTMs to Learn Syntax-Sensitive Dependencies", Linzen et al, 2016. https://arxiv.org/pdf/1611.01368.pdf

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Why is exploding gradient a problem?

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \underbrace{\alpha}_{\text{learning rate}} \underbrace{\nabla_\theta J(\theta)}_{\text{gradient}}$$

- This can cause bad updates: we take too large a step and reach a bad parameter configuration (with large loss)

- In the worst case, this will result in Inf or NaN in your network (then you have to restart training from an earlier checkpoint)

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Gradient clipping: solution for exploding gradient

- Gradient clipping: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

Algorithm 1 Pseudo-code for norm clipping

$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**
  $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$
end if

- Intuition: take a step in the same direction, but a smaller step

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf