Introduction to Machine Learning

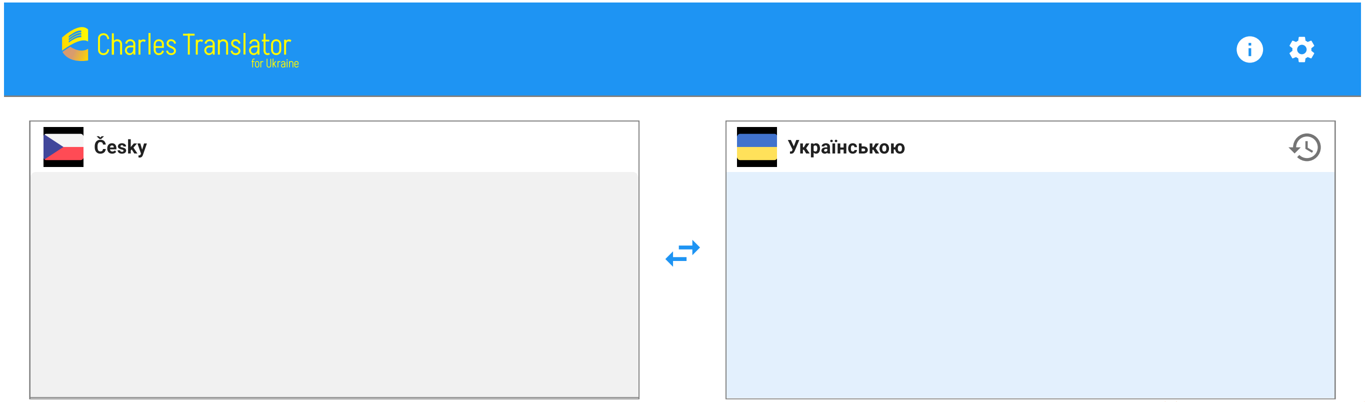
Milan Straka

October 03, 2022

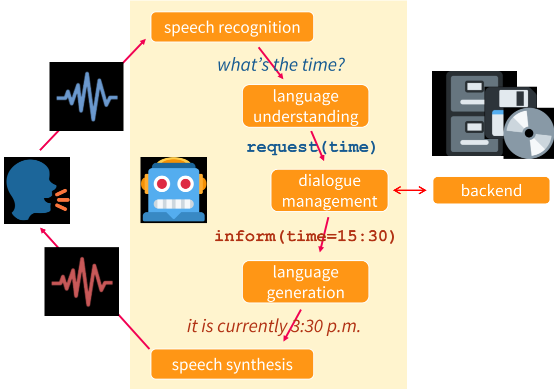
Charles University in Prague
Faculty of Mathematics and Physics
Institute of Formal and Applied Linguistics

CC BY SA
unless otherwise stated

Machine Learning



https://translator.cuni.cz/



https://ufal.mff.cuni.cz/courses/npfl123

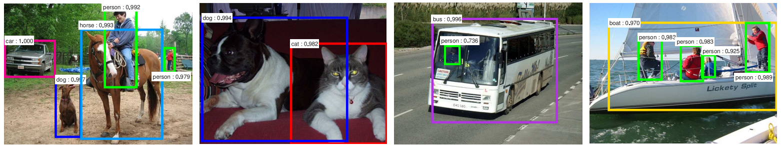


Figure 3 of "Faster R-CNN: Towards Real-Time Object Detection with Region Proposal Networks", https://arxiv.org/abs/1506.01497

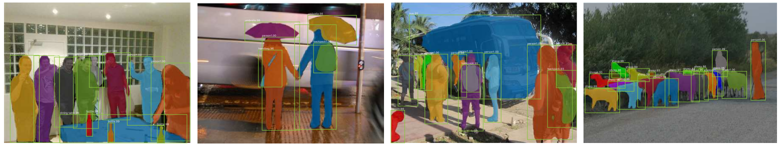


Figure 2 of "Mask R-CNN", https://arxiv.org/abs/1703.06870.

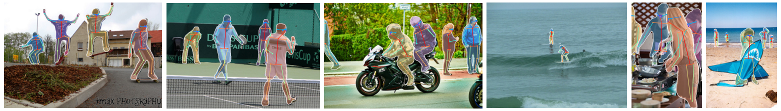
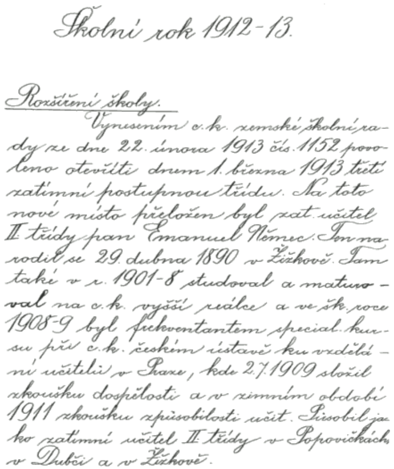


Figure 7 of "Mask R-CNN", https://arxiv.org/abs/1703.06870.



Školní rok 1912-13.

Rozšíření školy.

Vynesením c.k. zemské školní rady ze dne 22. února 1913 čís. 1152 povoleno otevříti dnem 1. března 1913 třetí zatímní postupnou třídu. Na toto nové místo přeložen byl zat. učitel II. třídy pan Emanuel Němec. Ten narodil se 29. dubna 1890 v Žižkově. Tam také v r. 1901-8 studoval a maturoval na c.k. vyšší reálce a ve šk. roce 1908-9 byl frekventantem special. kursu při c.k. českém ústavě ku vzdělání učitelů v Praze, kde 2.7.1909 složil zkoušku dospělosti a v zimním období 1911 zkoušku způsobilosti učit. Působil jako zatímní učitel II. třídy v Popovičkách, v Dubči a v Žižkově.

Figure 4.1 of diploma thesis "Adaptive Handwritten Text Recognition", https://hdl.handle.net/20.500.11956/147680

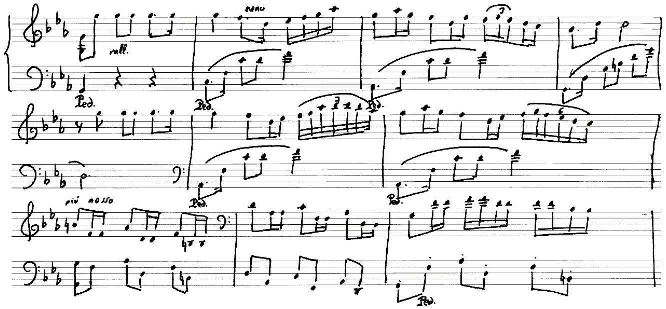


Figure 1.1 of diploma thesis "Optical Music Recognition using Deep Neural Networks", https://hdl.handle.net/20.500.11956/119393

Machine Learning

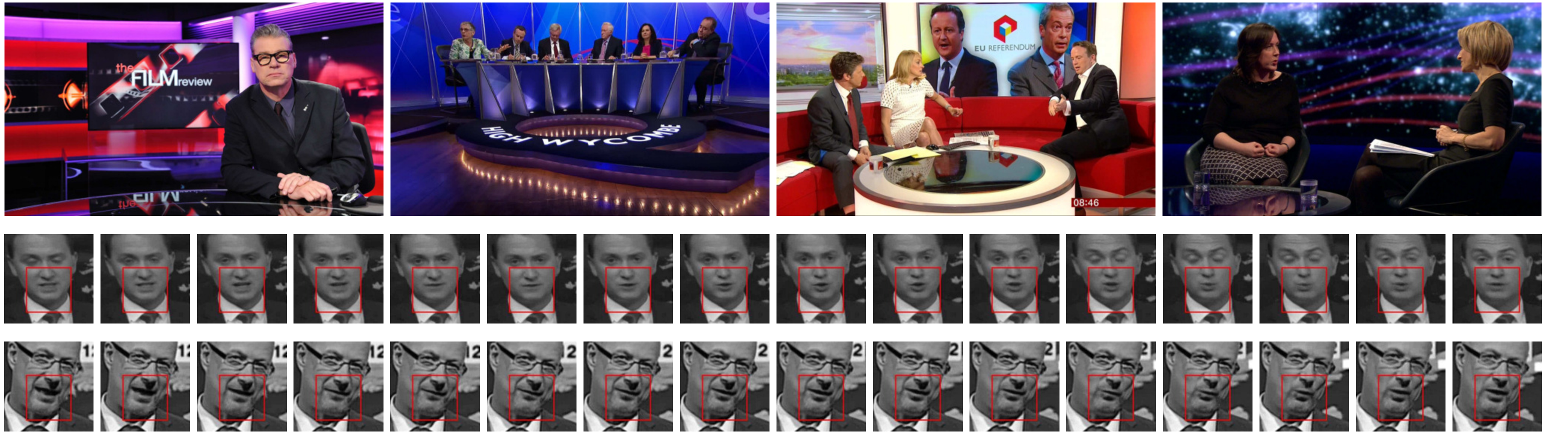


Figure 3. **Top:** Original still images from the BBC lip reading dataset – News, Question Time, Breakfast, Newsnight (from left to right). **Bottom:** The mouth motions for 'afternoon' from two different speakers. The network sees the areas inside the red squares.

Figure 3 of "Lip Reading Sentences in the Wild", https://arxiv.org/abs/1611.05358.

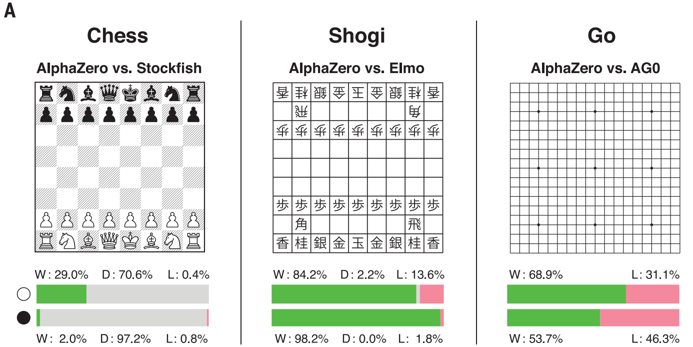


Figure 2 of "A general reinforcement learning algorithm that masters chess, shogi, and Go through self-play" by David Silver et al.

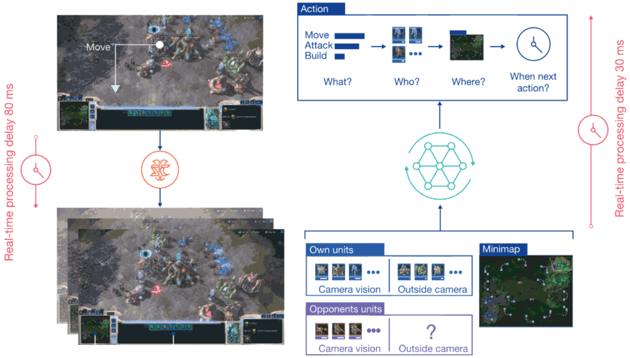
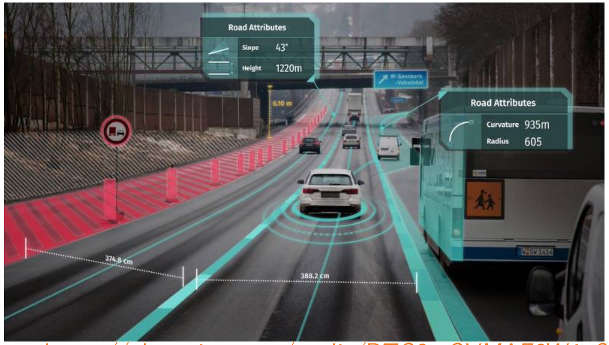
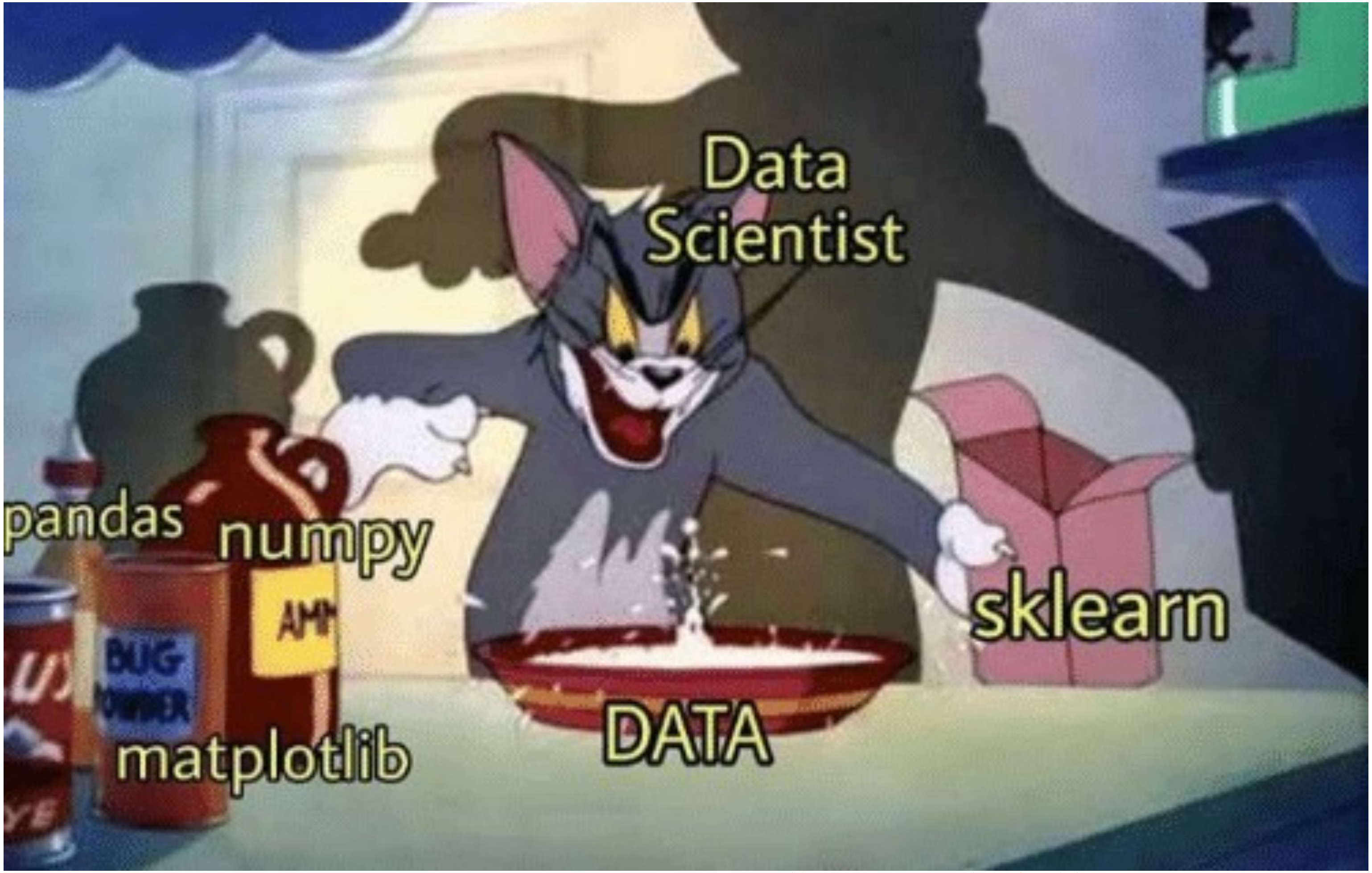


Figure 1 of "Grandmaster level in StarCraft II using multi-agent reinforcement learning" by Oriol Vinyals et al.



https://pbs.twimg.com/media/DTO2ysOVMAE2W4w?format=jpg



*https://miro.medium.com/max/640/1*kp5IPKiP7j5Q1tHEWtTcow.png*

Organization

Course Website: https://ufal.mff.cuni.cz/courses/npfl129

- Slides, recordings, assignments, exam questions

Course Repository: https://github.com/ufal/npfl129

- Templates for the assignments, slide sources.

Piazza

- Piazza will be used as a communication platform.

  You can post questions or notes,
  - **privately** to the instructors,
  - **publicly** to everyone (signed or anonymously).
    - Other students can answer these too, which allows you to get faster response.
    - However, **do not include even parts of your source code** in public questions.
- Please use Piazza for **all communication** with the instructors.
- You will get the invite link after the first lecture.

ReCodEx

https://recodex.mff.cuni.cz

- The assignments will be evaluated automatically in ReCodEx.
- If you have a MFF SIS account, you should be able to create an account using your CAS credentials and should automatically see the right group.
- Otherwise, there will be **instructions** on **Piazza** how to get ReCodEx account (generally you will need to send me a message with several pieces of information and I will send it to ReCodEx administrators in batches).

Course Requirements

Practicals

- There will be about 2-3 assignments a week, each with a 2-week deadline.
  - There is also another week-long second deadline, but for fewer points.
- After solving the assignment, you get non-bonus points, and sometimes also bonus points.
- To pass the practicals, you need to get 80 non-bonus points. There will be assignments for at least 120 non-bonus points.
- If you get more than 80 points (be it bonus or non-bonus), they will be transferred to the exam (but at most 40 points are transferred).

Lecture

You need to pass a written exam.

- All questions are publicly listed on the course website.
- There are questions for 100 points in every exam, plus at most 40 surplus points from the practicals and plus at most 10 surplus points for **community work** (improving slides, …).
- You need 60/75/90 points to pass with grade 3/2/1.

Machine Learning

A possible definition of learning from Mitchell (1997):

> A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

- Task T
  - *classification*: assigning one of k categories to a given input
  - *regression*: producing a number $x \in \mathbb{R}$ for a given input
  - *structured prediction*, *denoising*, *density estimation*, …
- Measure P
  - *accuracy*, *error rate*, *F-score*, …
- Experience E
  - *supervised*: usually a dataset with desired outcomes (*labels* or *targets*)
  - *unsupervised*: usually data without any annotation (raw text, raw images, …)
  - *reinforcement learning*, *semi-supervised learning*, …

Supervised Machine Learning

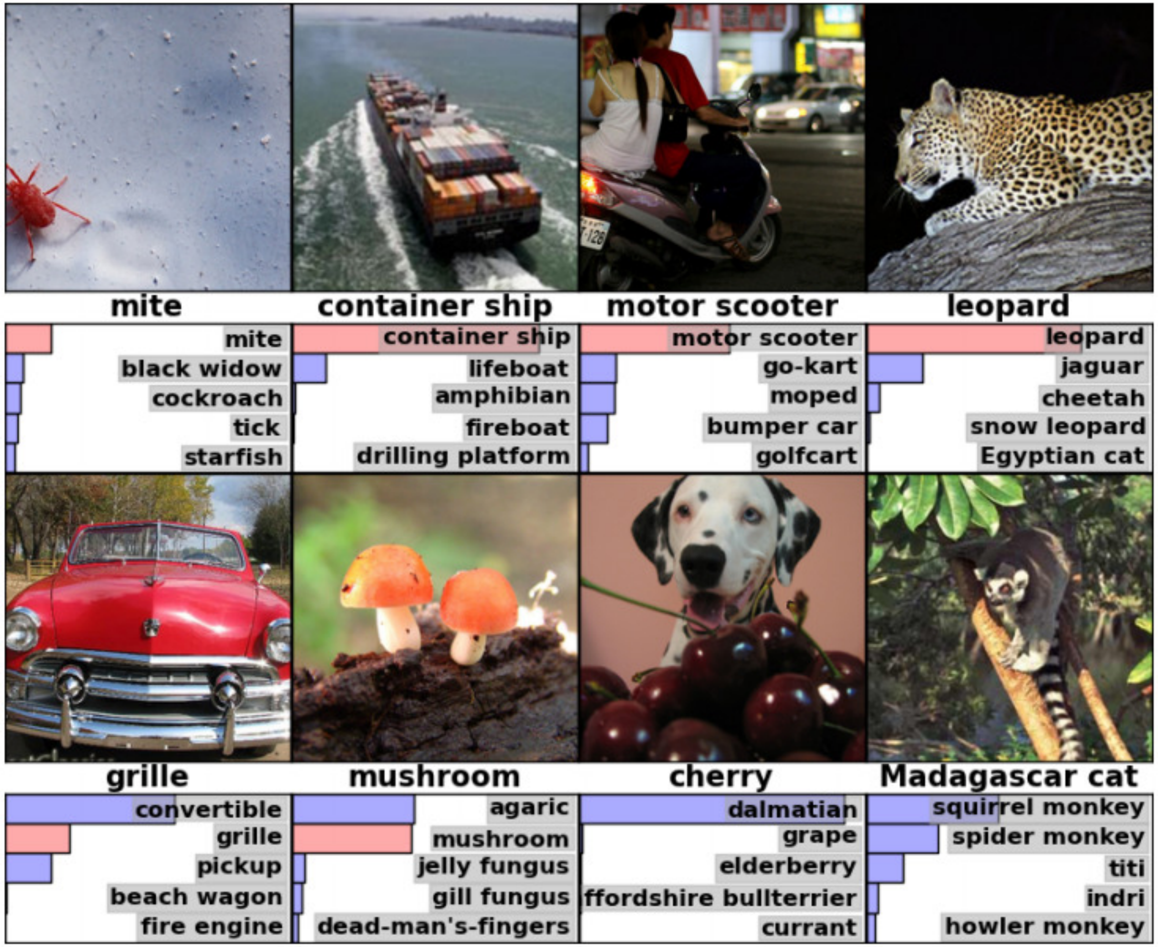
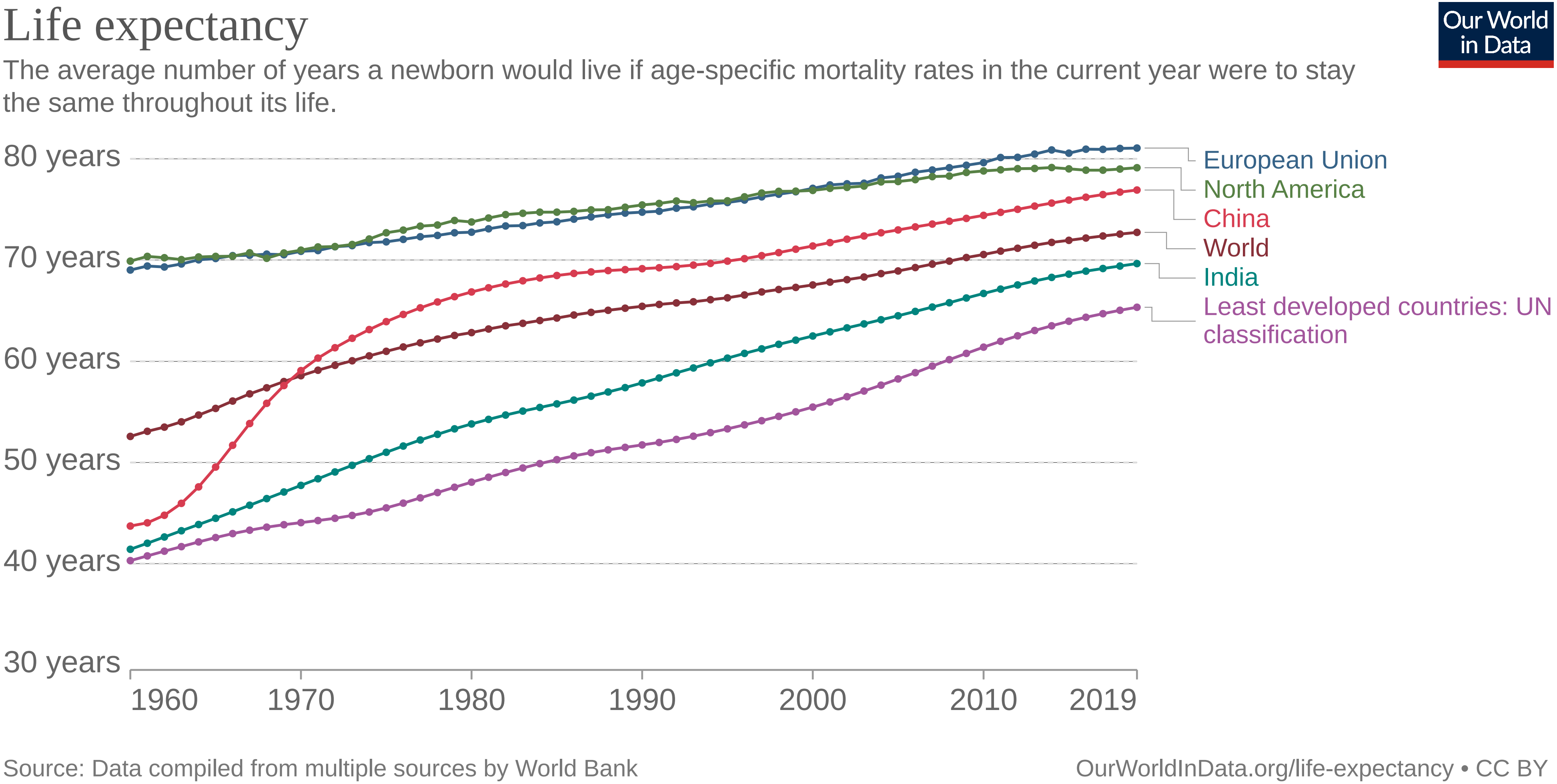


Figure 4 of "ImageNet Classification with Deep Convolutional Neural Networks" by Alex Krizhevsky et al.

Supervised Machine Learning



Life expectancy

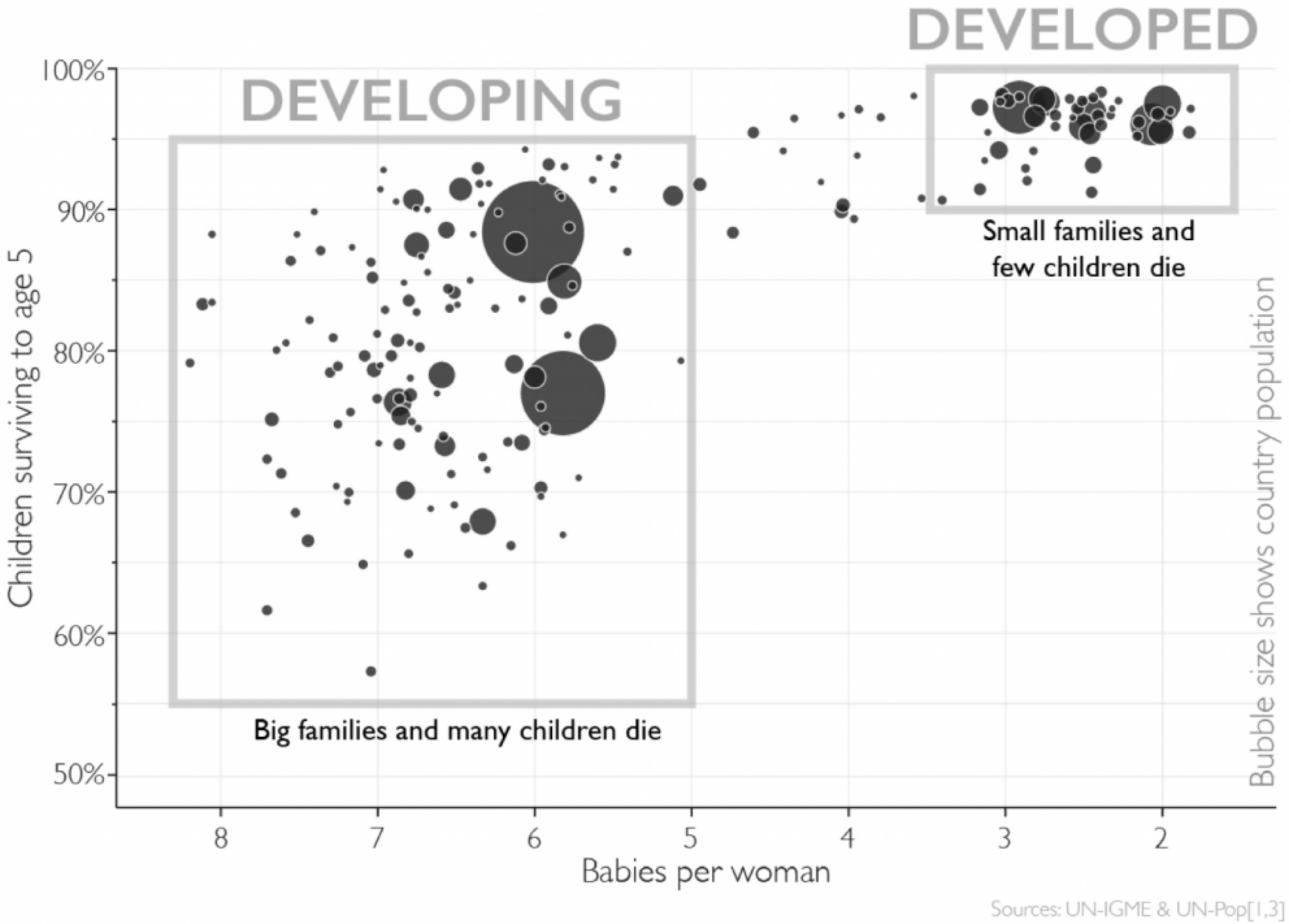
The average number of years a newborn would live if age-specific mortality rates in the current year were to stay the same throughout its life.

Source: Data compiled from multiple sources by World Bank

OurWorldInData.org/life-expectancy • CC BY

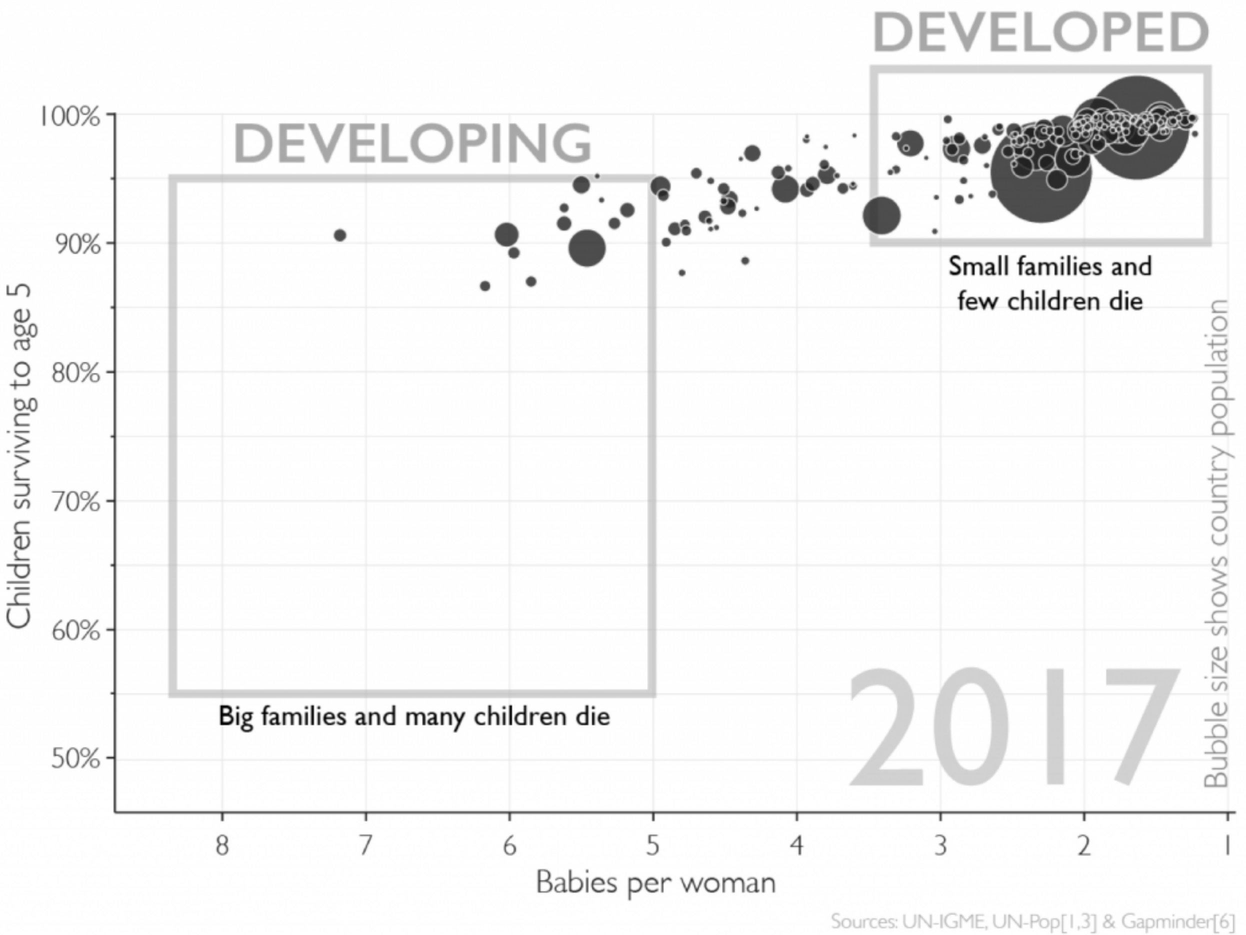
https://ourworldindata.org/life-expectancy

Unsupervised Machine Learning – Clustering



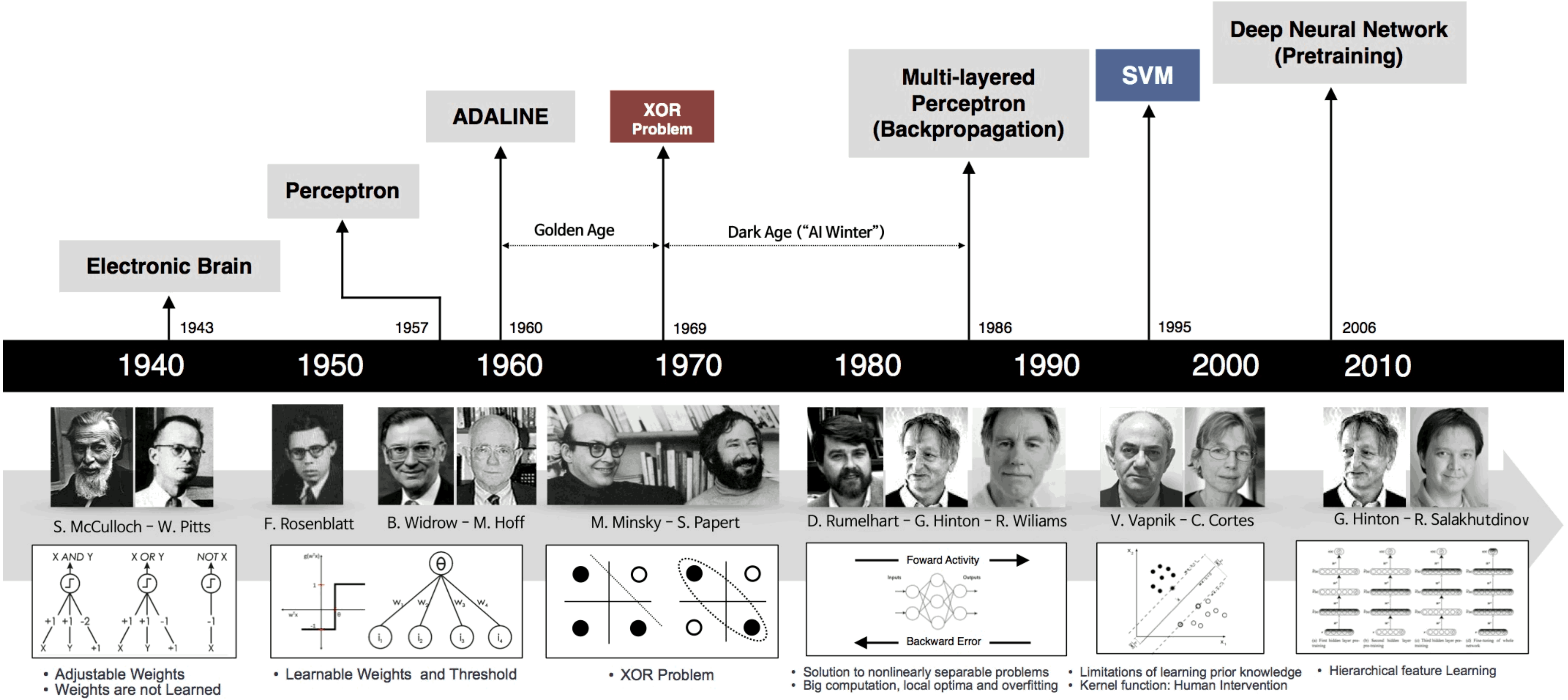
https://www.gapminder.org/topics/fertility-child-mortality/

Unsupervised Machine Learning – Clustering



https://www.gapminder.org/topics/fertility-child-mortality/

Introduction to Machine Learning History



Electronic Brain 1943

Perceptron 1957

ADALINE 1960

XOR Problem 1969

Multi-layered Perceptron (Backpropagation) 1986

SVM 1995

Deep Neural Network (Pretraining) 2006

Golden Age

Dark Age ("AI Winter")

1940 1950 1960 1970 1980 1990 2000 2010

S. McCulloch – W. Pitts
- Adjustable Weights
- Weights are not Learned

F. Rosenblatt — B. Widrow – M. Hoff
- Learnable Weights and Threshold

M. Minsky – S. Papert
- XOR Problem

D. Rumelhart – G. Hinton – R. Wiliams
- Solution to nonlinearly separable problems
- Big computation, local optima and overfitting

V. Vapnik – C. Cortes
- Limitations of learning prior knowledge
- Kernel function: Human Intervention

G. Hinton – R. Salakhutdinov
- Hierarchical feature Learning

Modified from https://www.slideshare.net/deview/251-implementing-deep-learning-using-cu-dnn/4

Basic Machine Learning Settings

Assume we have an input of $\boldsymbol{x} \in \mathbb{R}^D$. The two basic ML tasks are:

1. **regression**: The goal of regression is to predict a real-valued target variable $t \in \mathbb{R}$ for the given input.
2. **classification**: Assuming we have a fixed set of K labels, the goal of a classification is to choose a corresponding label/class for a given input.
   - We can predict the class only.
   - We can predict the whole distribution of all classes probabilities.

We usually have a **training set**, which is assumed to consist of examples of $(\boldsymbol{x}, t)$ generated independently from a **data-generating distribution**.

The goal of *optimization* is to match the training set as well as possible.

However, the goal of *machine learning* is to perform well on *previously unseen* data, to achieve the lowest **generalization error** or **test error**. We typically estimate it using a **test set** of examples independent of the training set, but generated by the same data-generating distribution.

Notation

- a, $\boldsymbol{a}$, $\boldsymbol{A}$, A: scalar (integer or real), vector, matrix, tensor
  - all vectors are always **column** vectors
  - transposition changes a column vector into a row vector, so $\boldsymbol{a}^T$ is a row vector
  - we denote the **dot (scalar) product** of the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ using $\boldsymbol{a}^T\boldsymbol{b}$
    - we understand it as matrix multiplication
  - the $\|\boldsymbol{a}\|_2$ or just $\|\boldsymbol{a}\|$ is the Euclidean (or L^2) norm
    - $\|\boldsymbol{a}\|_2 = \sqrt{\sum_i a_i^2}$
- a, $\mathbf{a}$, $\mathbf{A}$: scalar, vector, matrix random variable
- $\mathbb{A}$: set; $\mathbb{R}$ is the set of real numbers, $\mathbb{C}$ is the set of complex numbers
- $\frac{df}{dx}$: derivative of f with respect to x
- $\frac{\partial f}{\partial x}$: partial derivative of f with respect to x
- $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$: gradient of f with respect to $\boldsymbol{x}$, i.e., $\left(\frac{\partial f(\boldsymbol{x})}{\partial x_1}, \frac{\partial f(\boldsymbol{x})}{\partial x_2}, \ldots, \frac{\partial f(\boldsymbol{x})}{\partial x_n}\right)$

Example Dataset

Assume we have the following data, generated from an underlying curve by adding a small amount of noise.

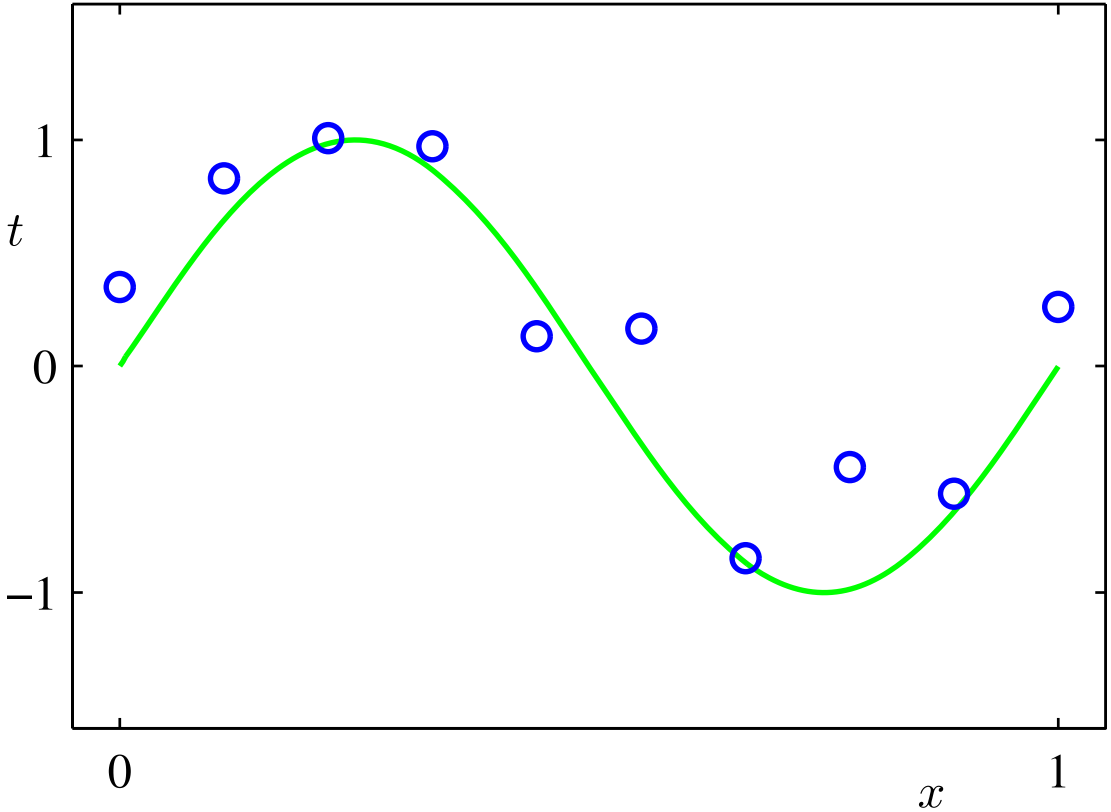


Figure 1.2 of Pattern Recognition and Machine Learning.

Input Data

Usually, our machine learning algorithms will be trained using the **train set** $\boldsymbol{X} \in \mathbb{R}^{N \times D}$, which is a collection of N instances, each represented by D real numbers.

In supervised learning, we also have a **target** $\boldsymbol{t}$ for every instance,

- a real number for regression, $\boldsymbol{t} \in \mathbb{R}^N$;
- a class for classification, $\boldsymbol{t} \in \{0, 1, \ldots, K-1\}^N$.

The input to machine learning algorithms is frequently preprocessed, i.e., the algorithms do not always work directly on the input $\boldsymbol{X}$, but on some modification of it. These preprocessed input values are called **features**.

In literature, the collection of the processed inputs is called a **design matrix** $\boldsymbol{\Phi} \in \mathbb{R}^{N \times M}$. However, we will denote the inputs to algorithms always as $\boldsymbol{X}$, be it the original training data or processed features.

Linear Regression

Given an input value $\boldsymbol{x} \in \mathbb{R}^D$, one of the simplest models to predict a target real value is **linear regression**:

$$y(\boldsymbol{x}; \boldsymbol{w}, b) = x_1 w_1 + x_2 w_2 + \ldots + x_D w_D + b = \sum_{i=1}^{D} x_i w_i + b = \boldsymbol{x}^T \boldsymbol{w} + b.$$

The $\boldsymbol{w}$ are usually called *weights* and b is called *bias*.

Sometimes it is convenient not to deal with the bias separately. Instead, we might enlarge the input vector $\boldsymbol{x}$ by padding a value 1, and consider only $\boldsymbol{x}^T \boldsymbol{w}$, where the role of a bias is accomplished by the last weight. Therefore, when we say “weights”, we usually mean both weights and biases.

Separate Bias vs. Padding $\boldsymbol{X}$ with Ones

Using an explicit bias term in the form of $y(x) = \boldsymbol{x}^T\boldsymbol{w} + b$.

$$\begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ & \vdots & \\ x_{n1} & x_{n2} \end{bmatrix} \cdot \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} + b = \begin{bmatrix} w_1 x_{11} + w_2 x_{12} + b \\ w_1 x_{21} + w_2 x_{22} + b \\ \vdots \\ w_1 x_{n1} + w_2 x_{n2} + b \end{bmatrix}$$

With extra 1 padding in $\boldsymbol{X}$ and an additional b weight representing the bias.

$$\begin{bmatrix} x_{11} & x_{12} & 1 \\ x_{21} & x_{22} & 1 \\ & \vdots & \\ x_{n1} & x_{n2} & 1 \end{bmatrix} \cdot \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix} = \begin{bmatrix} w_1 x_{11} + w_2 x_{12} + b \\ w_1 x_{21} + w_2 x_{22} + b \\ \vdots \\ w_1 x_{n1} + w_2 x_{n2} + b \end{bmatrix}$$

Linear Regression

Assume we have a dataset of N input values $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ and targets $t_1, \ldots, t_N$.

To find the values of weights, we usually minimize an **error function** between the real target values and their predictions.

A popular and simple error function is *mean squared error*:

$$\mathrm{MSE}(\boldsymbol{w}) = \frac{1}{N} \sum_{i=1}^{N} \big(y(\boldsymbol{x}_i; \boldsymbol{w}) - t_i\big)^2.$$

Often, *sum of squares*

$$\frac{1}{2} \sum_{i=1}^{N} \big(y(\boldsymbol{x}_i; \boldsymbol{w}) - t_i\big)^2$$

is used instead, because minimizing it is equal to minimizing MSE, but the math comes out nicer.

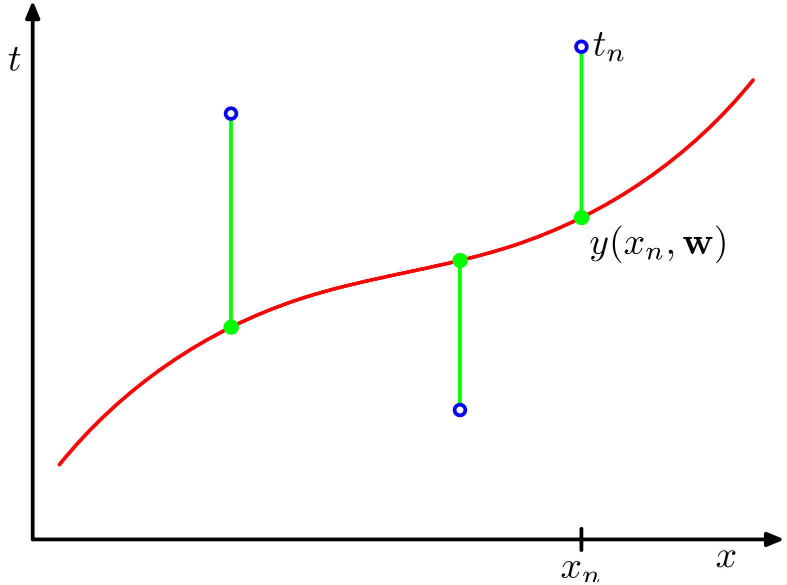


Figure 1.3 of Pattern Recognition and Machine Learning.

Linear Regression

There are several ways how to minimize the error function, but in the case of linear regression and sum of squares error, there exists an explicit solution.

Our goal is to minimize the following quantity:

$$\frac{1}{2}\sum_i^N(\boldsymbol{x}_i^T\boldsymbol{w} - t_i)^2.$$

If we denote $\boldsymbol{X} \in \mathbb{R}^{N\times D}$ the matrix of input values with $\boldsymbol{x}_i$ on a row $\boldsymbol{i}$ and $\boldsymbol{t} \in \mathbb{R}^N$ the vector of target values, we can rewrite the minimized quantity as

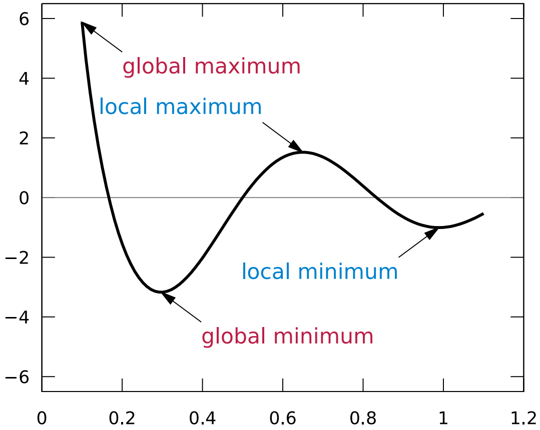
$$\frac{1}{2}\|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{t}\|^2,$$

because

$$\|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{t}\|^2 = \sum_i \big((\boldsymbol{X}\boldsymbol{w} - \boldsymbol{t})_i\big)^2 = \sum_i \big((\boldsymbol{X}\boldsymbol{w})_i - t_i)\big)^2 = \sum_i(\boldsymbol{x}_i^T\boldsymbol{w} - t_i)^2.$$

Minimization – Unconstrained, Single Real Variable

Assume we have a function and we want to find its minimum.



https://commons.wikimedia.org/wiki/File:Extrema_example_original.svg

We usually use the Fermat's theorem (interior extremum theorem):

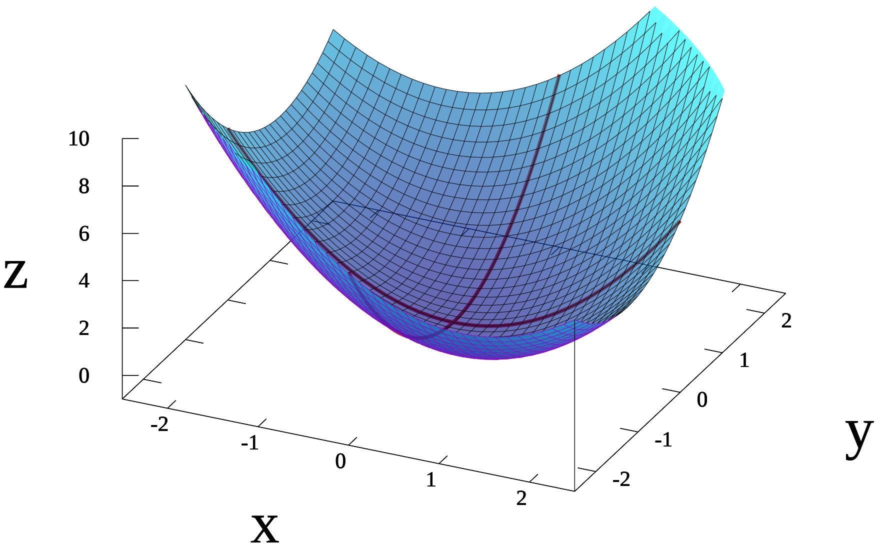
Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a function. If it has a minimum (or a maximum) in x and if it has a derivative in x, then

$$\frac{\partial f}{\partial x} = 0.$$

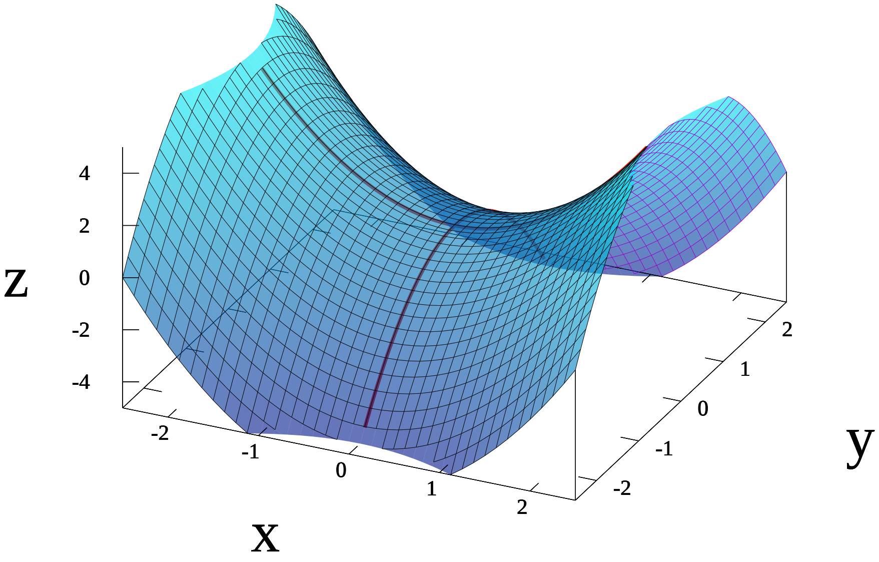
Minimization – Unconstrained, Multiple Real Variables

The previous theorem can be generalized to the multivariate case:

Let $f: \mathbb{R}^D \rightarrow \mathbb{R}$ be a function. If it has a minimum or a maximum in $\boldsymbol{x} = (x_1, x_2, \ldots, x_D)$ and if it has a derivative in $\boldsymbol{x}$, then for all i, $\frac{\partial f}{\partial x_i} = 0$. In other words, $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \mathbf{0}$.



https://commons.wikimedia.org/wiki/File:Partial_func_eg.svg



https://commons.wikimedia.org/wiki/File:Partial_func_eg.svg

Linear Regression

In order to find a minimum of $\frac{1}{2}\sum_i^N(\boldsymbol{x}_i^T\boldsymbol{w}-t_i)^2$, we can inspect values where the derivative of the error function is zero, with respect to all weights w_j.

$(a^2)' = 2a \cdot a'$

$Xw - t$

$$\frac{\partial}{\partial w_j}\frac{1}{2}\sum_i^N(\boldsymbol{x}_i^T\boldsymbol{w}-t_i)^2 = \frac{1}{2}\sum_i^N\Big(2(\boldsymbol{x}_i^T\boldsymbol{w}-t_i)x_{ij}\Big) = \sum_i^N x_{ij}(\boxed{\boldsymbol{x}_i^T\boldsymbol{w}}-t_i)$$

Therefore, we want for all j that $\sum_i^N x_{ij}(\boldsymbol{x}_i^T\boldsymbol{w}-t_i)=0$.

We can rewrite the explicit sum into $\boldsymbol{X}_{*,j}^T(\boldsymbol{X}\boldsymbol{w}-\boldsymbol{t})=0$, then write the equations for all j together using matrix notation as $\boldsymbol{X}^T(\boldsymbol{X}\boldsymbol{w}-\boldsymbol{t})=\boldsymbol{0}$, and finally, rewrite to

$$\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} = \boldsymbol{X}^T\boldsymbol{t}.$$

pokud není, je nejlepší přidat šum,
pak často je regulární

The matrix $\boldsymbol{X}^T\boldsymbol{X}$ is of size $D \times D$. If it is regular, we can compute its inverse and therefore

$$\boldsymbol{w} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{t}.$$

Linear Regression

Input: Dataset ($\boldsymbol{X} \in \mathbb{R}^{N\times D}$, $\boldsymbol{t} \in \mathbb{R}^N$).
Output: Weights $\boldsymbol{w} \in \mathbb{R}^D$ minimizing MSE of linear regression.

- $\boldsymbol{w} \leftarrow (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{t}$.

The algorithm has complexity $\mathcal{O}(ND^2)$, assuming $N \geq D$.

When the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is singular, we can solve $\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} = \boldsymbol{X}^T\boldsymbol{t}$ using SVD, which will be demonstrated in the next lecture.

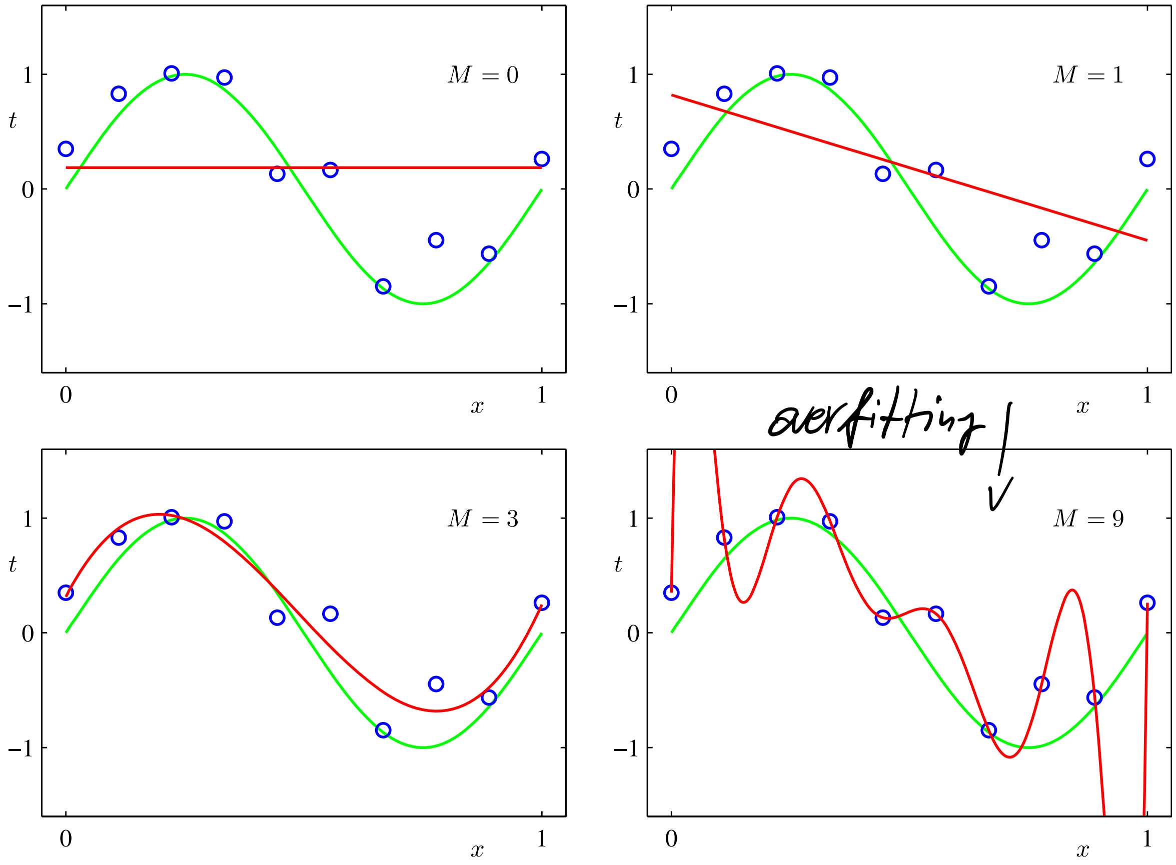
Linear Regression Example

Assume we want to predict a $t \in \mathbb{R}$ for a given $x \in \mathbb{R}$. If we train the linear regression with "raw" input vectors $\boldsymbol{x} = (x)$, only straight lines could be modeled.

However, if we consider input vectors $\boldsymbol{x} = (x^0, x^1, \ldots, x^M)$ for a given $M \geq 0$, the linear regression is able to model polynomials of degree M, because the prediction is then computed as

$$w_0 x^0 + w_1 x^1 + \ldots + w_M x^M.$$

Therefore, the weights are the coefficients of a polynomial of degree M.



overfitting!

Linear Regression Example

To plot the error, the *root mean squared error* $\mathrm{RMSE} = \sqrt{\mathrm{MSE}}$ is frequently used.

The displayed error nicely illustrates two main challenges in machine learning:

- *underfitting*
- *overfitting*

největší problém a strašák

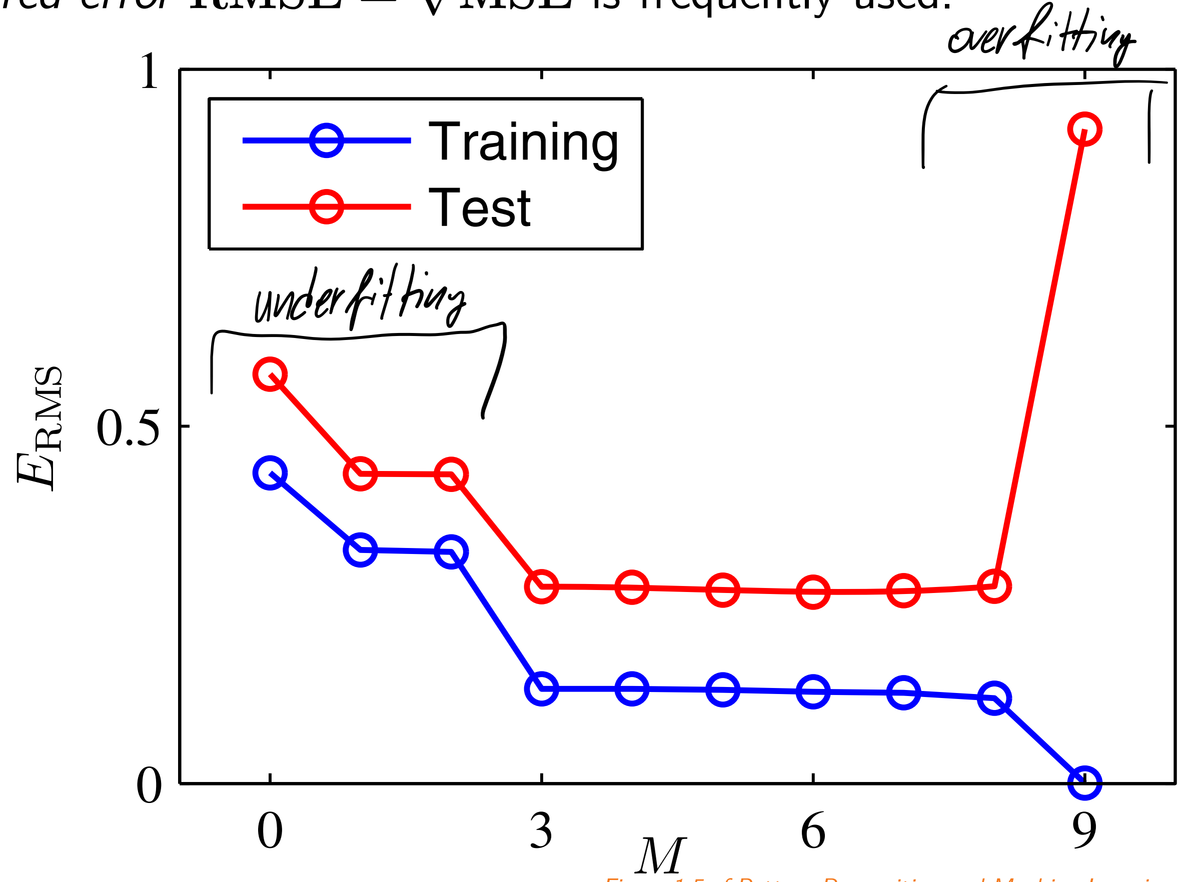


Figure 1.5 of Pattern Recognition and Machine Learning.