Machine learning and (geo)physical modelling-1

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NERSC

`https://github.com/brajard/MAT330`

Overview of the next lectures

1. Lecture 1 (Tuesday 21 Oct. 2023):
   Generalities and Principles of Machine Learning
2. Lecture 2 (Wednesday 23 Oct. 2023):
   Neural networks, deep learning, training
3. Lecture 3 (Tuesday 30 Oct. 2023):
   Practical work

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References

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  Simon and Schuster, 2021.
  https://d2l.ai/index.html.
- Ian Goodfellow, Yoshua Bengio, and Aaron Courville.
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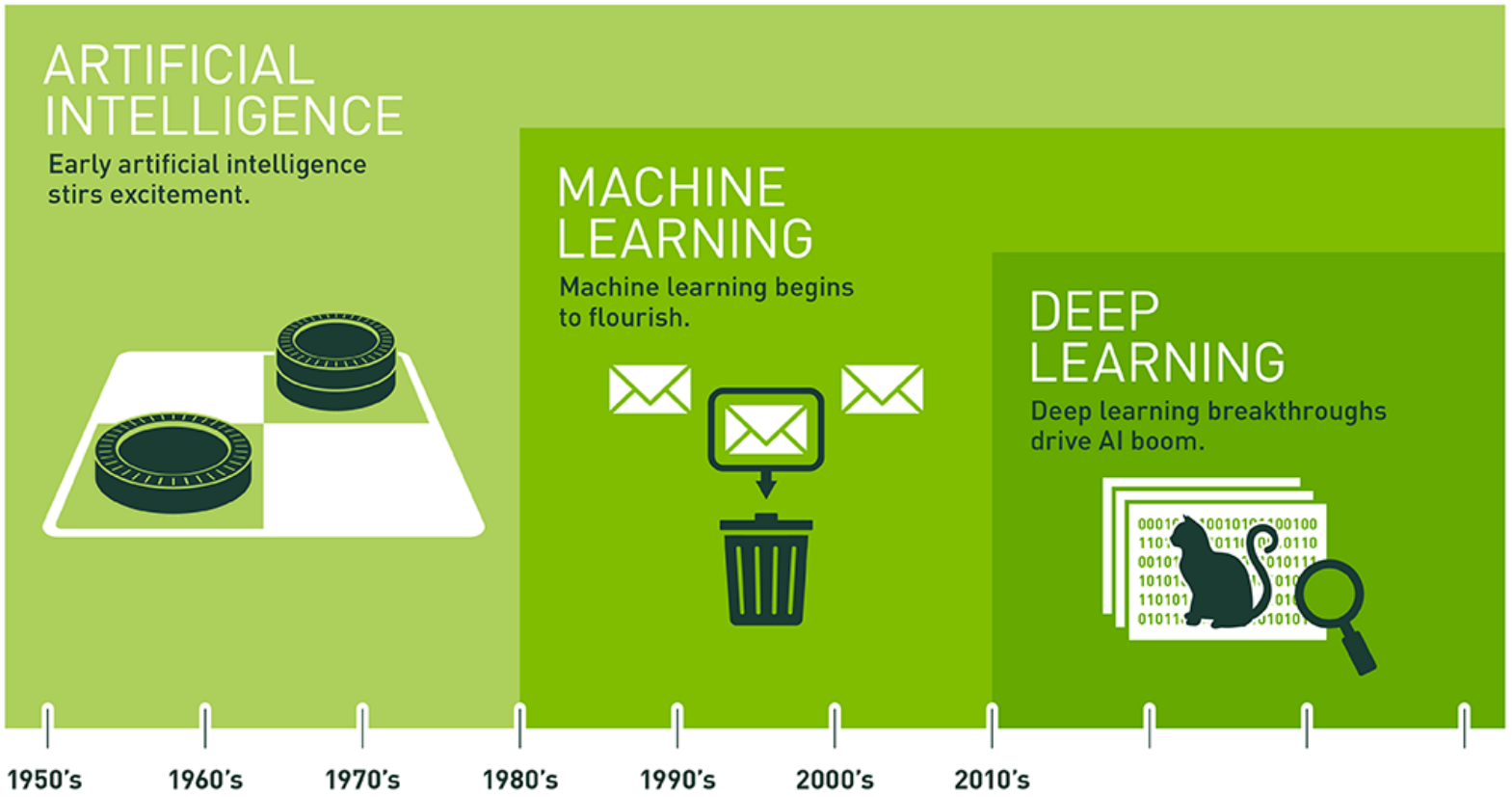
  MIT Press, 2016.
  http://www.deeplearningbook.org.
- Jake VanderPlas.
  Python Data Science Handbook: Essential Tools for Working with Data.
  O'Reilly Media, Inc., 1st edition, 2016.
  https://jakevdp.github.io/PythonDataScienceHandbook/.
- Aston Zhang, Zachary C Lipton, Mu Li, and Alexander J Smola.
  Dive into deep learning.
  Cambridge University Press, 2023.
  https://d2l.ai/index.html.

Table of contents

Introduction

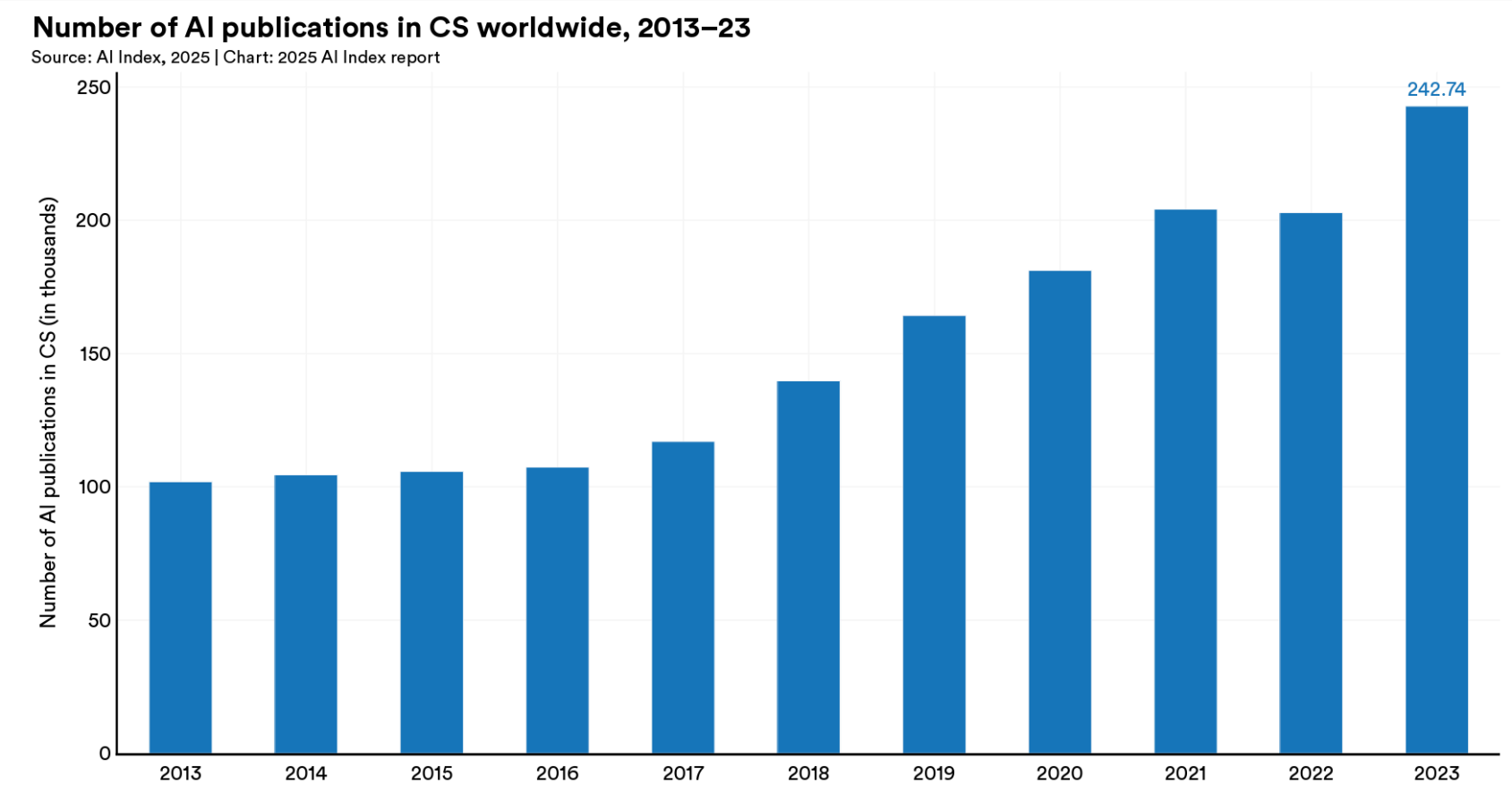
Scope of the lecture: Machine Learning



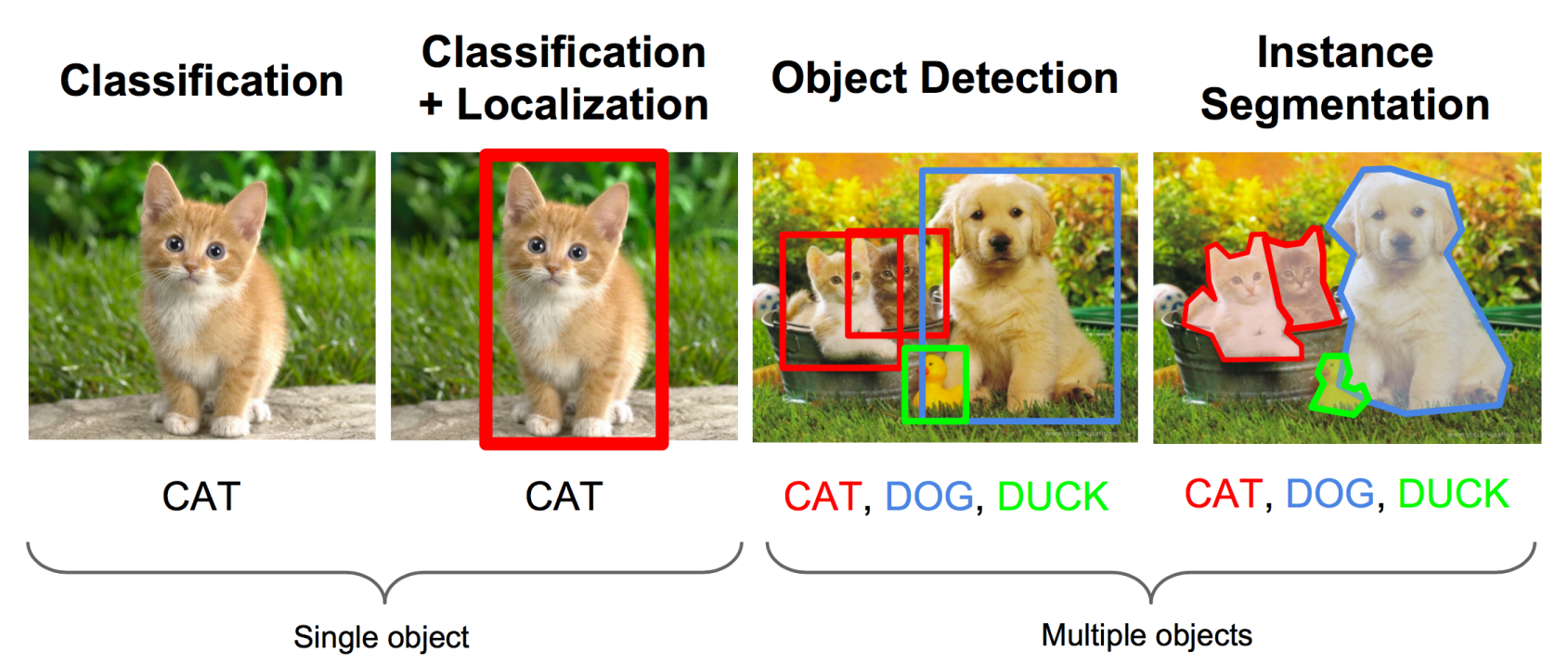
Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

Source: NVidia

A (very) active field



Example 1: Computer Vision



Li, Karpathy and Johnson, 2016, Stanford CS231n course

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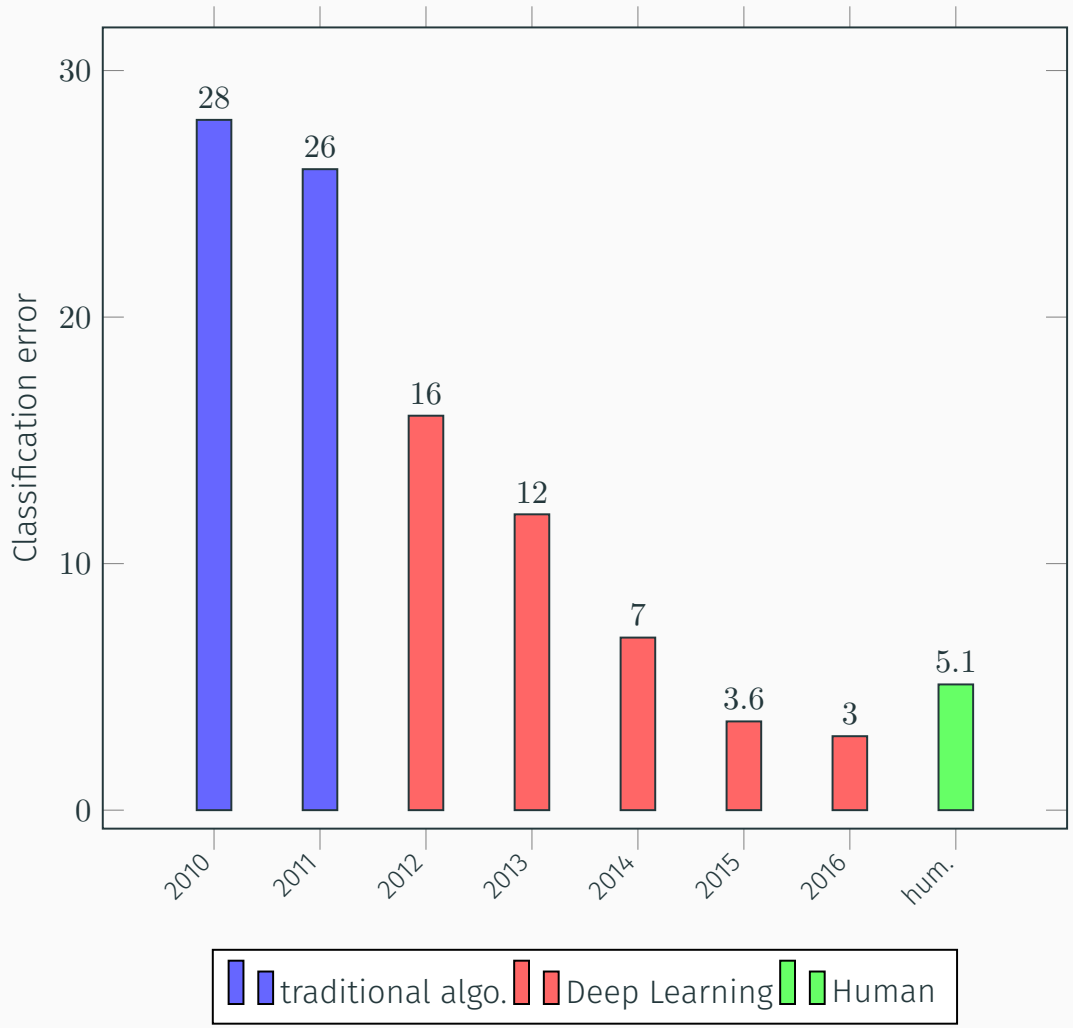

Deep learning architectures were based on Convolutional Neural Networks (CNN).

Example 2: Playing Games

- **1997**: Deep Blue defeats Kasparov at Chess.
- **2016**: AlphaGo's victory again Lee Sedol at Go.

  - **2017**: AphaGo Zero learns how to play Go only by playing against itself. It outperformed previous AlphaGo version (Reinforcement learning)
  - **2017**: DeepStack beats professional human poker players.

Example 3: Text to image

Objective: Generate an image from a textual description.

- **2021**: DALL·E
- **2022**: Midjourney and Stable diffusion
- Since **2022**: all over the place

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photography style with a 22mm lens of a handsome redheaded biker man with a short beard.

Text to image - Progress in free tools

A test on:

`https://deepai.org/machine-learning-model/text2img`

Prompt: *“students attending a machine learning course”*

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Example 4: Large language models (LLM)

Examples: GPT-5 (OpenAI), LLaMA 4(Meta AI), Gemini 2.5 (Google DeepMind), DeepSeek3.2 (DeepSeek).

How I tried to delegate my job

I have to give 6 hours of an introduction course to machine learning to master students. The objective is to undersrtand the main concepts of machine learning from a practical point of view. Can you suggest an outline?

Copilot

That sounds like a great opportunity to give students a solid foundation in machine learning! For a 6-hour introductory course aimed at master's students with a practical focus, here's a suggested outline that balances theory, intuition, and hands-on experience:

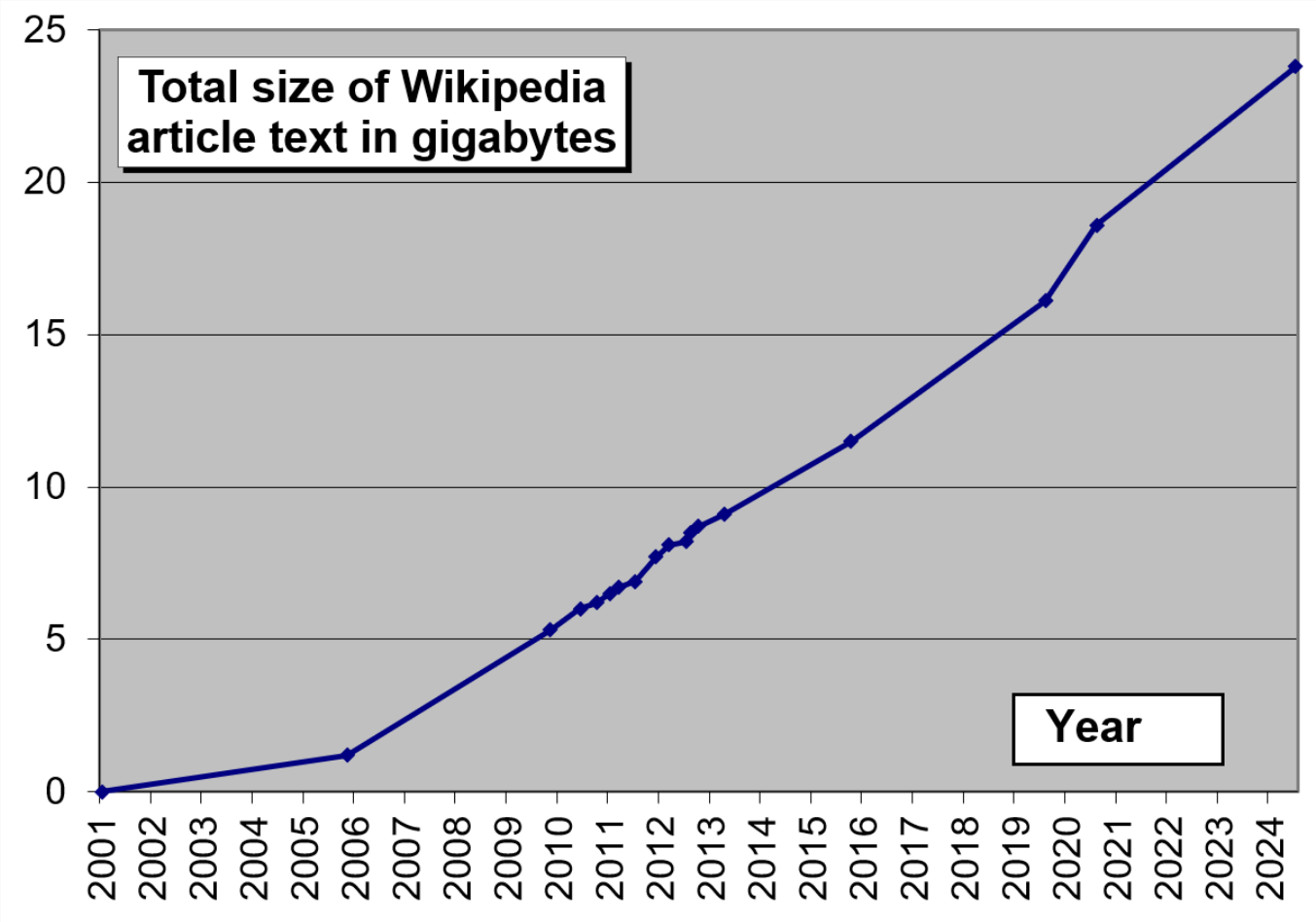
🧠 Machine Learning Introduction Course Outline (6 Hours)

Session 1: Foundations of Machine Learning (1 hour)

- **What is Machine Learning?**
  - Definitions and types: Supervised, Unsupervised, Reinforcement Learning
  - ML vs. traditional programming
- **Key Concepts**
  - Features, labels, models, training, testing
  - Overfitting vs. underfitting
- **Real-world Applications**

Reasons for these recent achievements?

- Increasing of the datasets in size and quality



source: wikimedia.org

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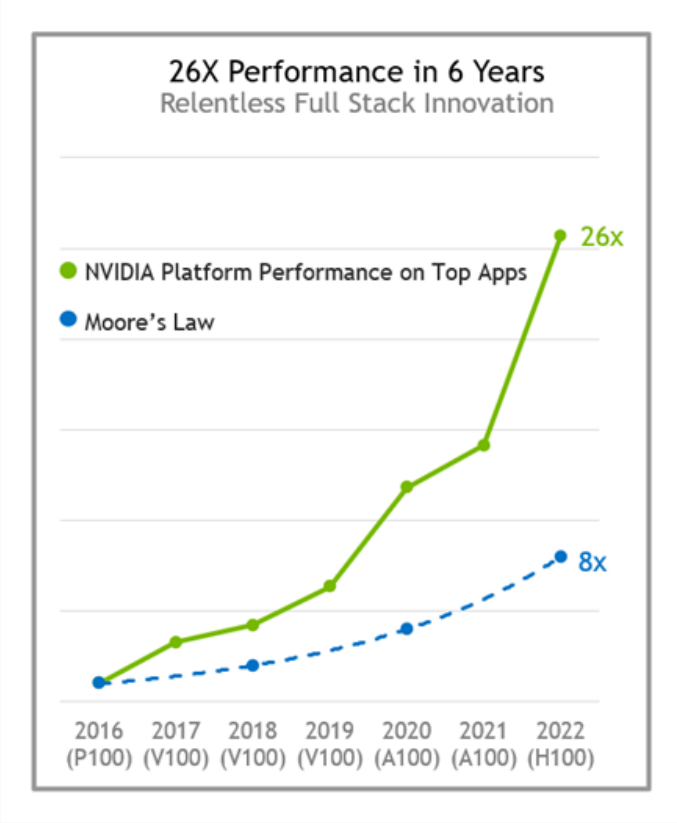

source: NVDIA

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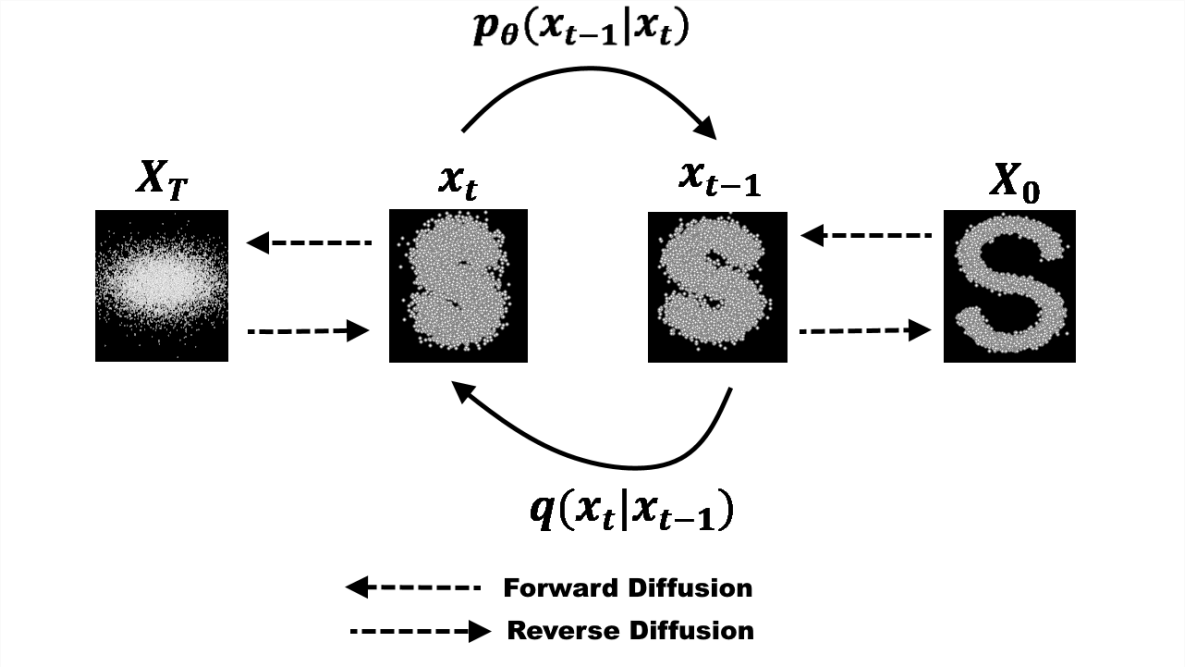

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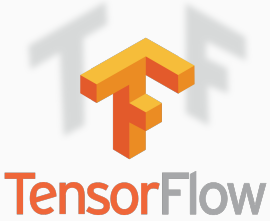

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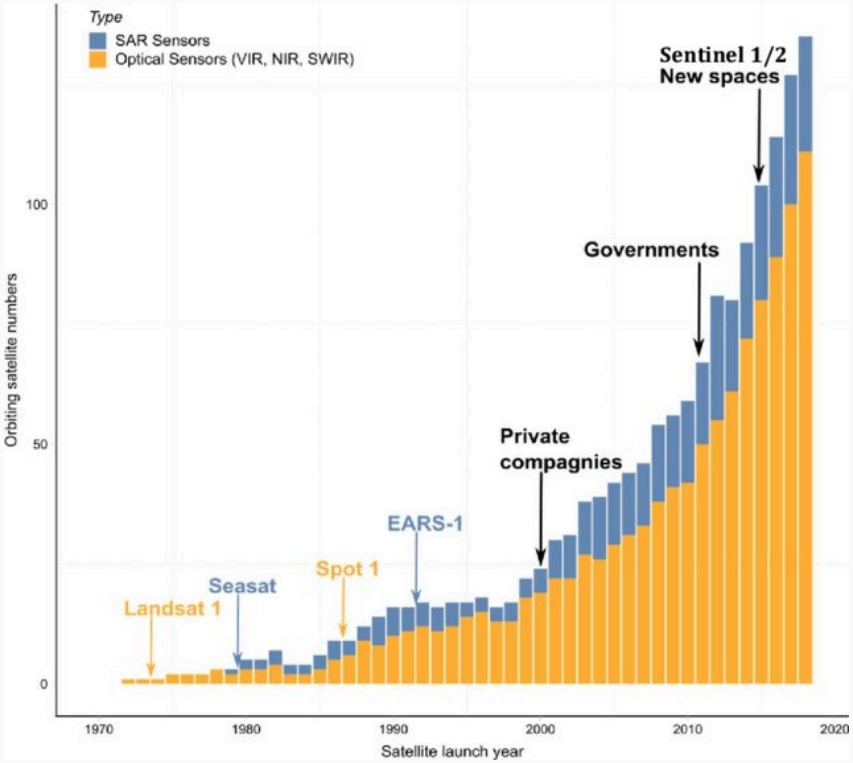
- Scientific research on new algorithms (e.g adapted to image processing)
- Very efficient software (GPU, cloud computing, automatic differentiation, ...)
- Free software and open data culture.

Apply Machine-Learning to physical (Earth-system) modelling?

Why is it a good idea?

- A increasing number of geophysical data (one spatial mission: 24 TB/day)



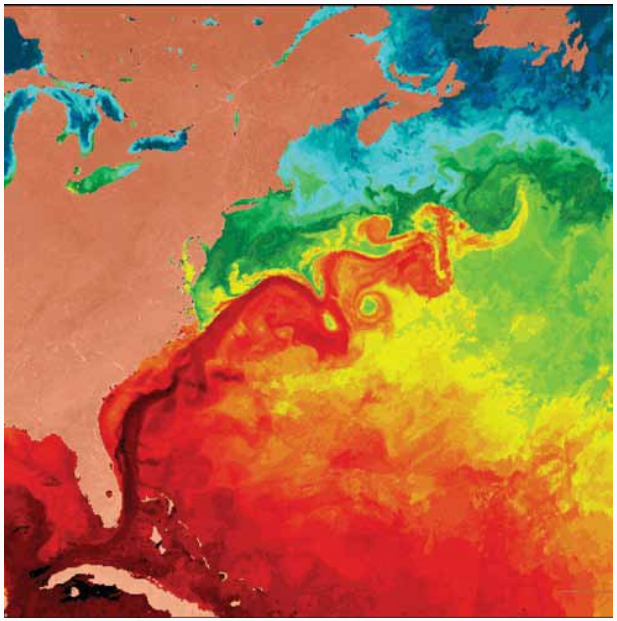
Earth System observavtion satellites

source: Tonneau et al. (2020)

Apply Machine-Learning to physical (Earth-system) modelling?

Why is it a good idea?

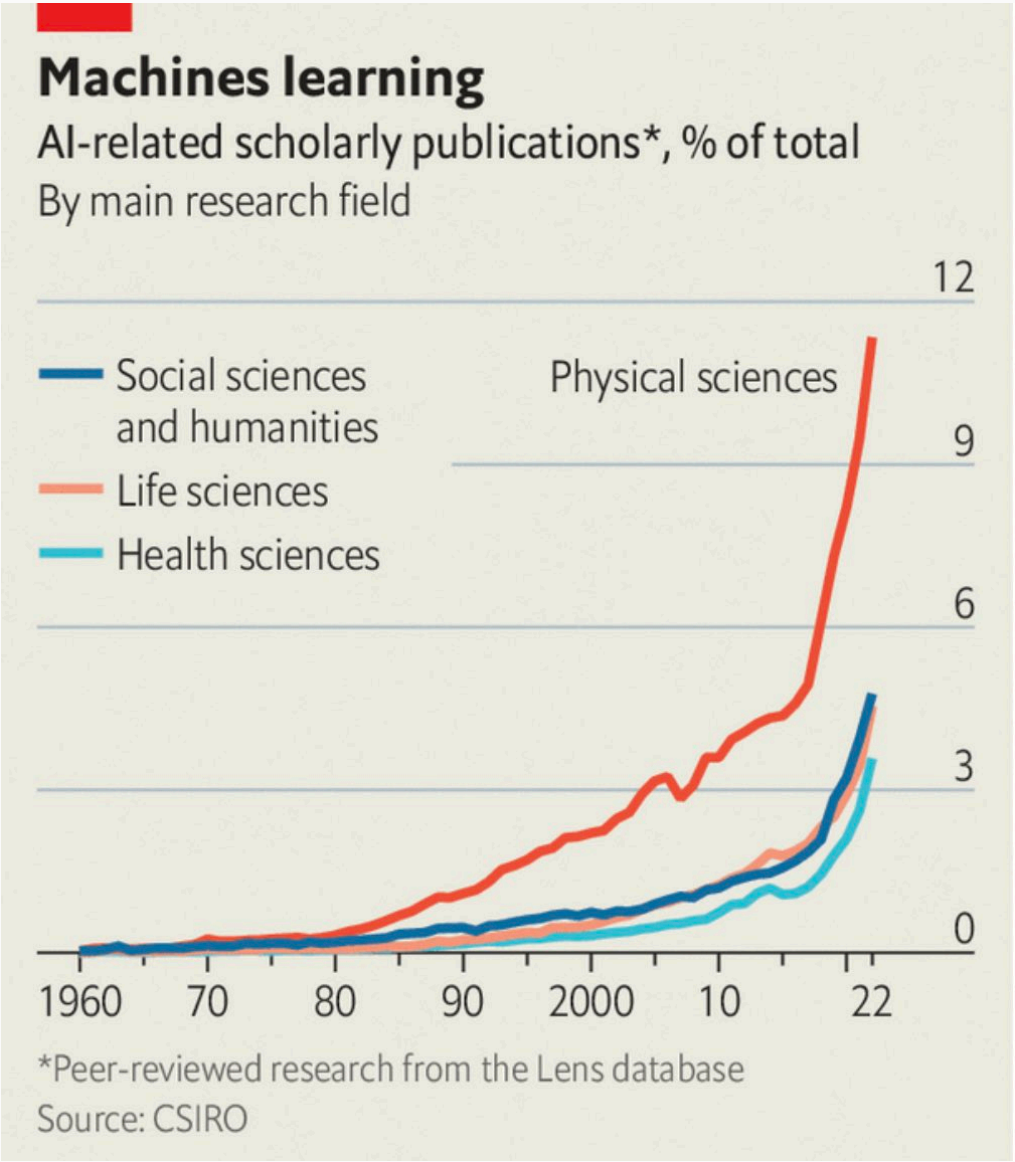
- A increasing number of geophysical data (one spatial mission: 24 TB/day)
- Data with highly significant spatial patterns



Sea Surface temperature of the gulf stream

source: Talley (2000)

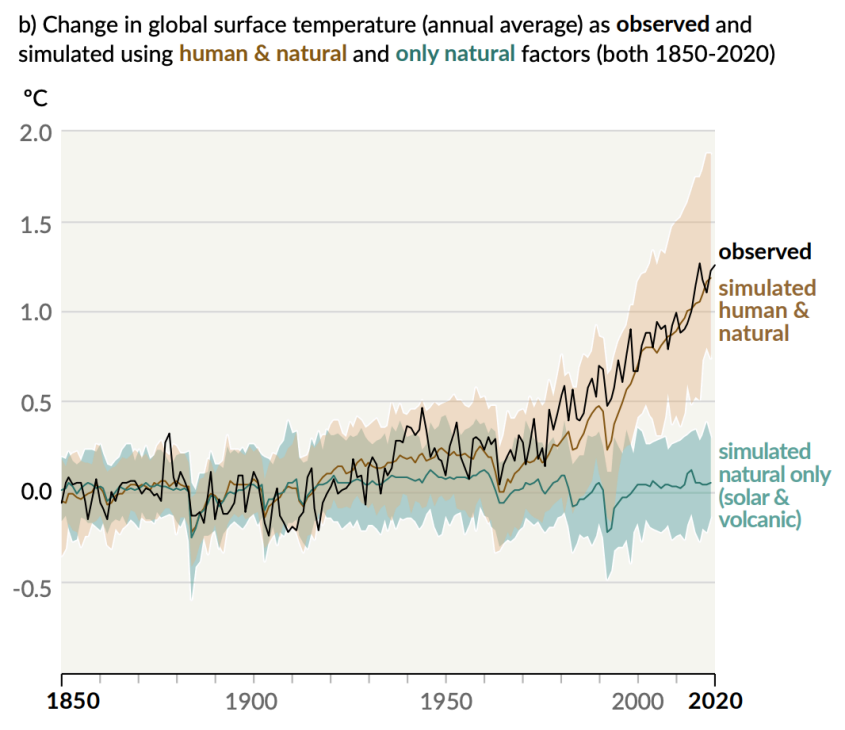
AI in physical sciences



Why is physical modelling specific?

NASDAQ Composite sock market index over the last 10 years

Figure 1: IPCC, AR6, WG1



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Mostly unknown dynamical processes

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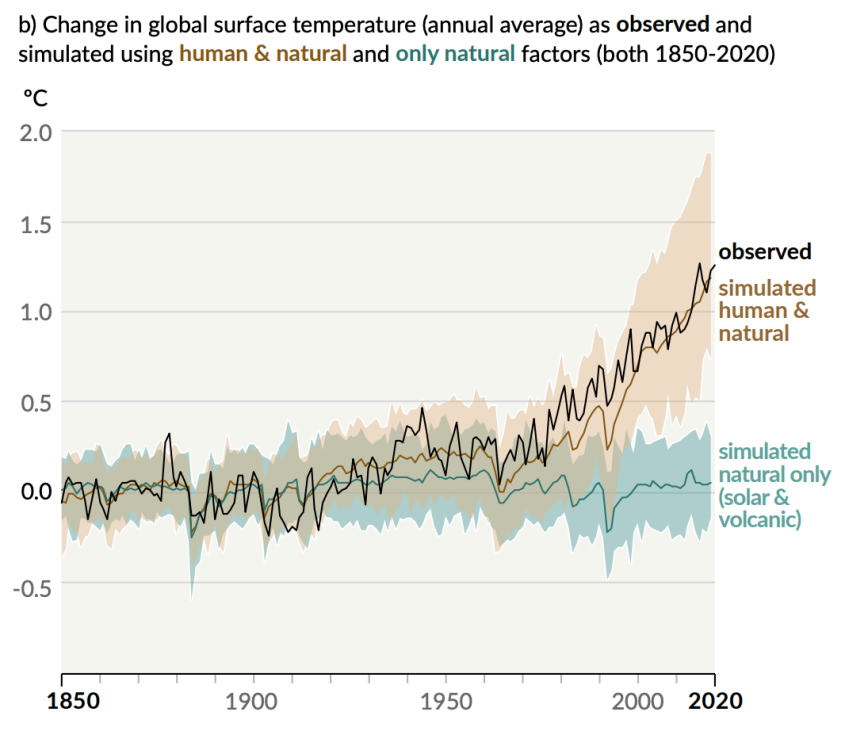

Mostly known dynamical processes (based on physical principles)

What about data assimilation?

Machine learning and data assimilation are closely linked.

- Cheng, Sibo, et al., 2023. Machine learning with data assimilation and uncertainty quantification for dynamical systems: a review. *IEEE/CAA Journal of Automatica Sinica* 10.6:1361-1387.
- Geer, A.J., 2021. Learning earth system models from observations: machine learning or data assimilation?. *Philosophical Transactions of the Royal Society A*, 379(2194)
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- Abarbanel, H.D., Rozdeba, P.J. and Shirman, S., 2018. Machine learning: Deepest learning as statistical data assimilation problems. *Neural computation, 30(8).*

Generalities on Machine Learning

What is this about ?

Can we extract knowledge, make some predictions, determine a ”model” using this large amount of data ?

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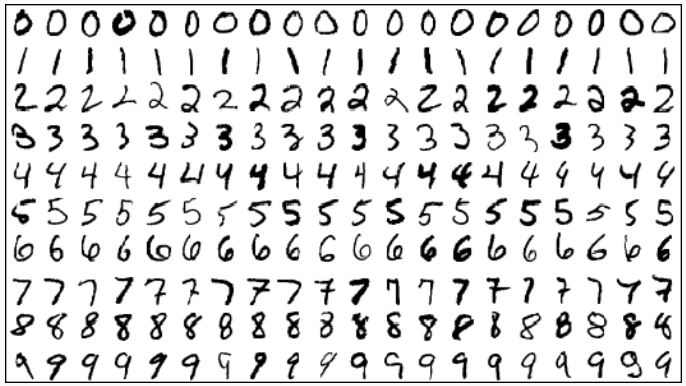

Base of images

$\longrightarrow$ Digit$\in \{0, \ldots, 9\}$

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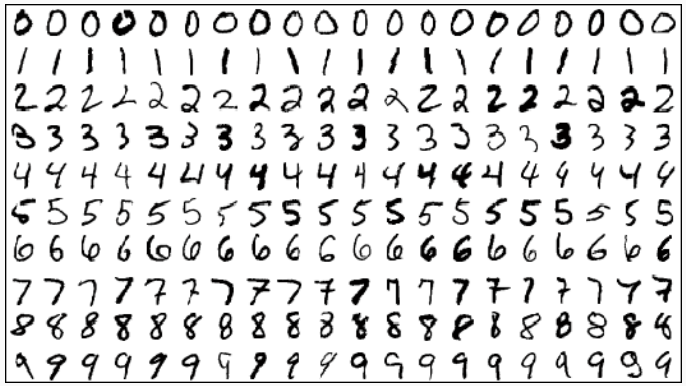
Can we extract knowledge, make some predictions, determine a "model" using this large amount of data ?



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- From high dimensional data (thousands to millions dimensions) to reduced dimensional data (less than 100)
- From disorganized data to organized information
- Can we teach a machine how to do that ?

Two types of settings

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    - Playing a chess game.

Two classes of (self)-supervised learning problems

1. Regression: Determination of a quantitative variable from a set of data
    - The price of a building from various predictors (Surface, ...)
    - A physical value (Temperature, humidity, ...) in the future knowing the past
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   - ...
2. Classification: Determination of a class
   - A digit from a image
   - Identification of the content of an image
   - ...

Formally

A Machine

$$y = \mathcal{M}(x, \theta)$$

- x: input
- y: output
- $\mathcal{M}$: a model (named "machine")
- θ : parameters of the model $\mathcal{M}$.

Machine learning consists in optimizing θ using a set of data.
This is the training process.

The Machine Learning recipe

A Machine

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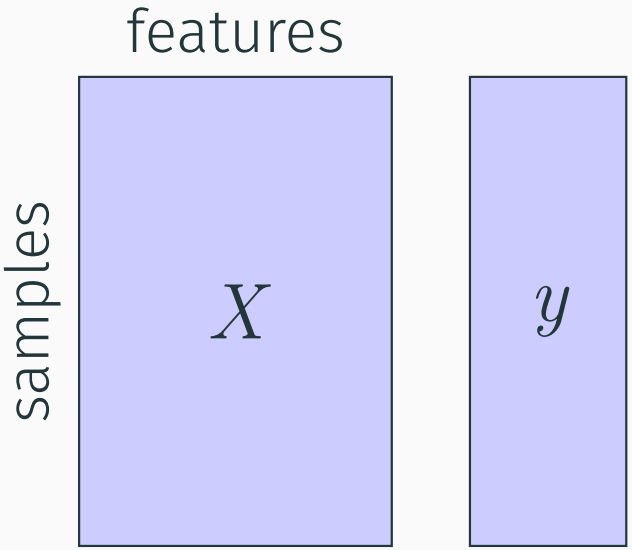
- A learning process
  - Estimation of θ

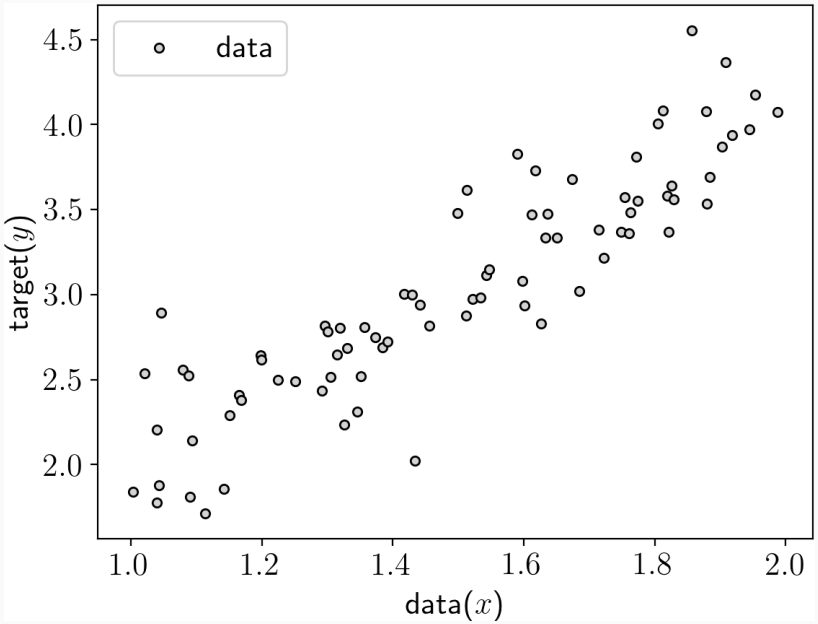
Multidimensional data

Generally, we have multidimensional data X and a one-dimensional target y.



An illustration

- Some Data



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  - y is quantitative: regression

An illustration

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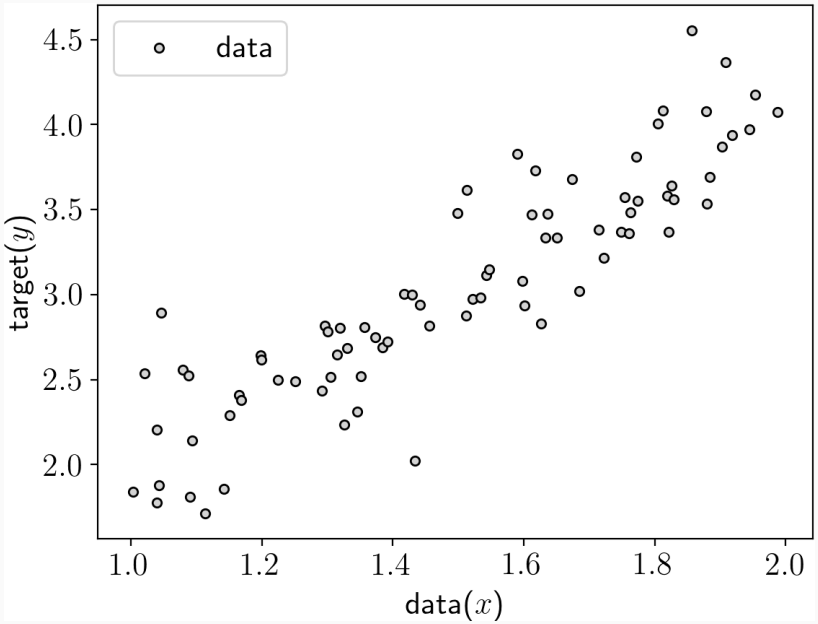

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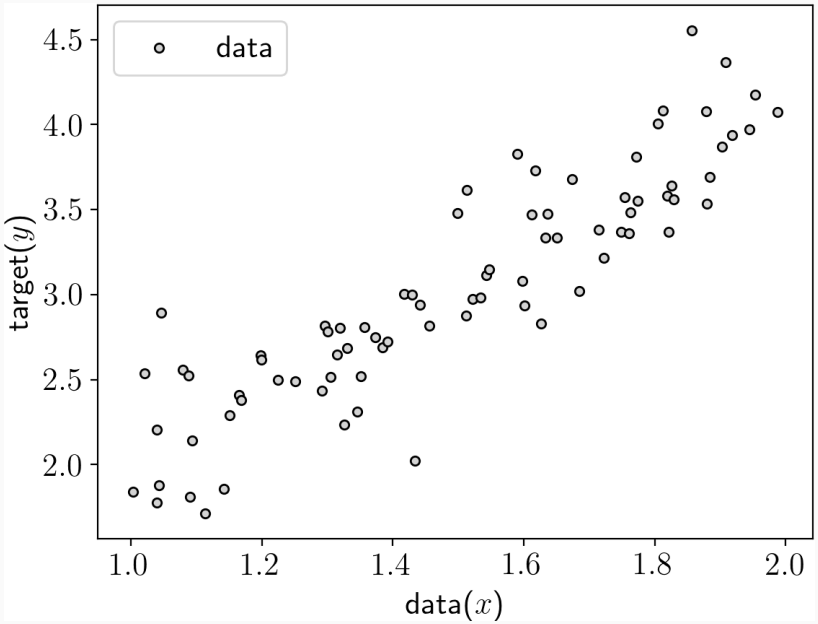

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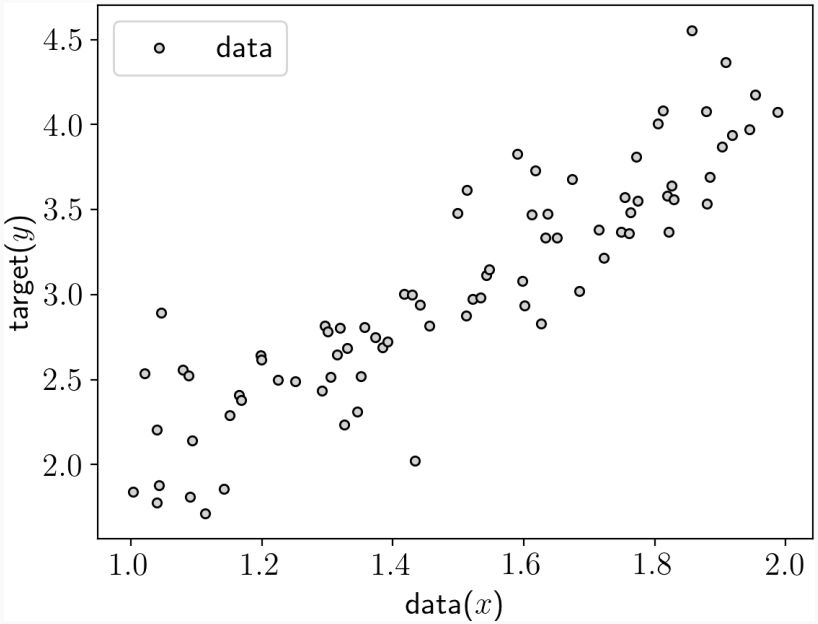

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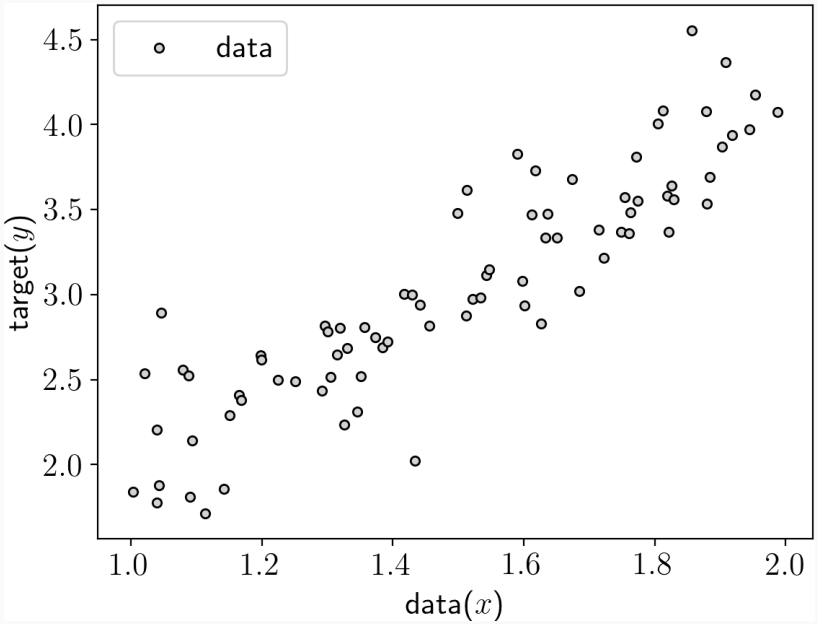

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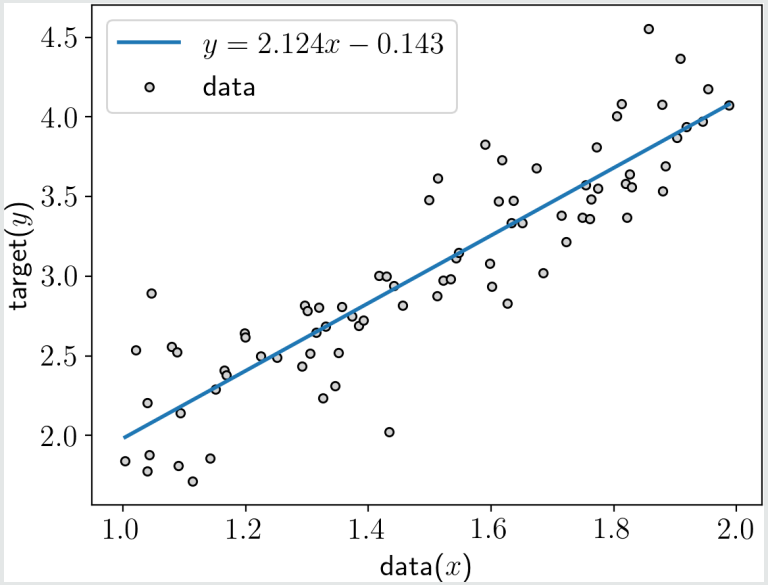
Result



Model selection/validation

Choice of the model

Polynomial regression

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d = \sum_{i=0}^{d} \theta_i X^i$$

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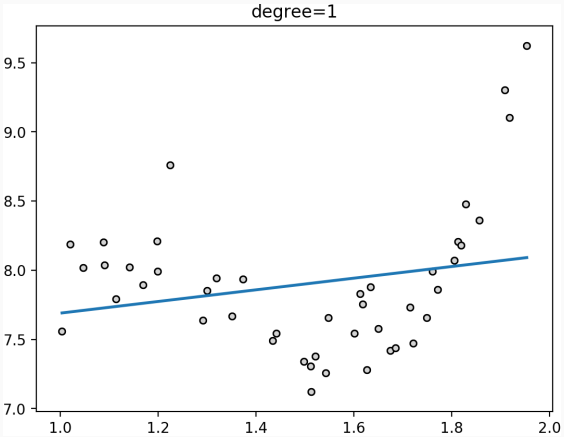

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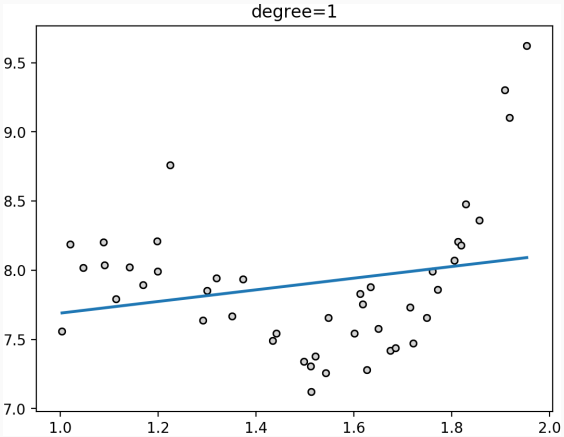
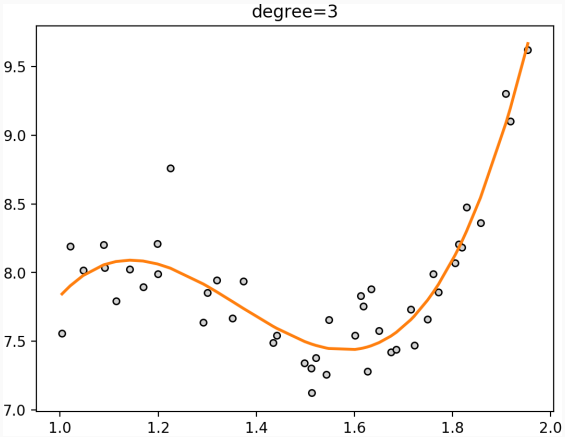


degree = 3



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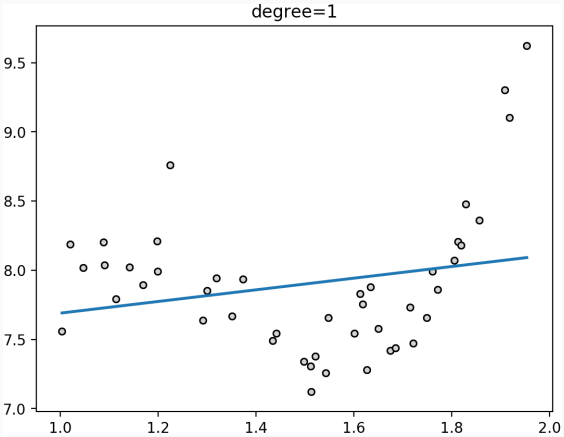
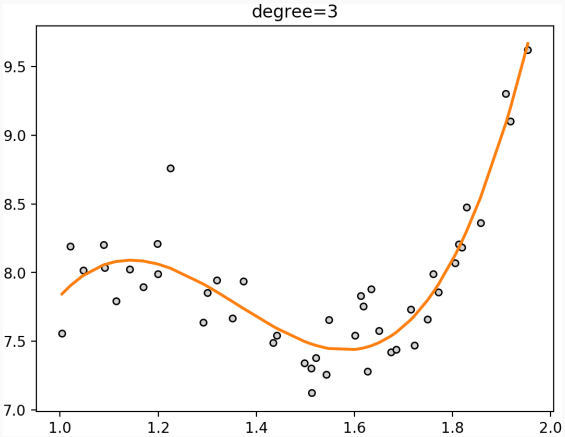
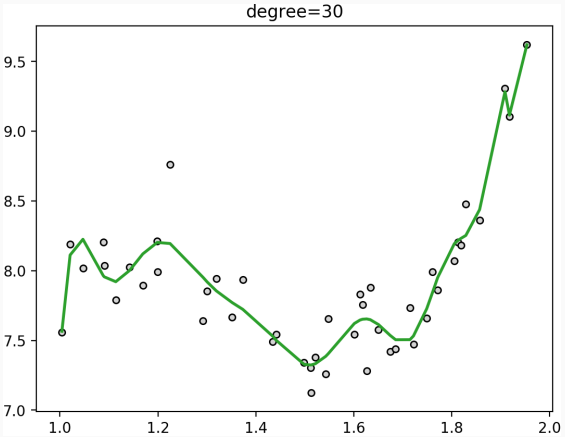


degree = 3



degree = 30



What is the best model?

Train/Validation split

The idea

Evaluate a score on an independent dataset

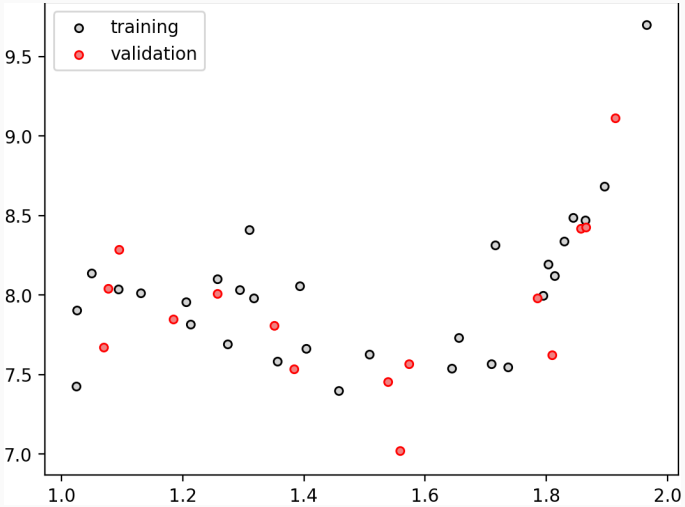
Train/Validation split

The idea

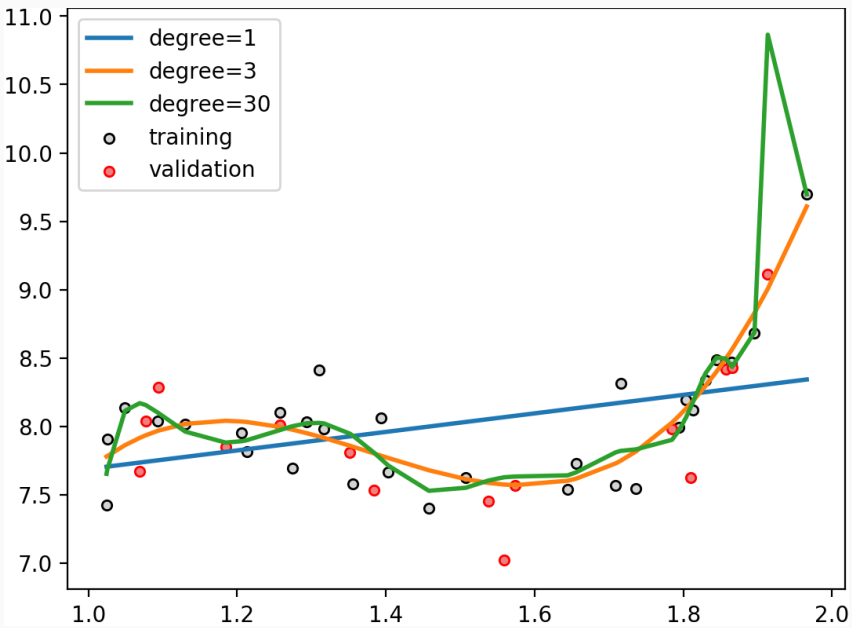
Evaluate a score on an independent dataset

In our example we can randomly divide (X, y) in two datasets:

- The training dataset X_{train}, y_{train} used to fit the model.
- The validation dataset X_{val}, y_{val} used to compute the score (e.g., correlation, mean-squared error)



Choice of the model



Score: Mean Square Error (MSE)

Deg.	Train Score	Val. Score
1	0.17	0.23
3	0.045	0.062
30	0.035	0.27

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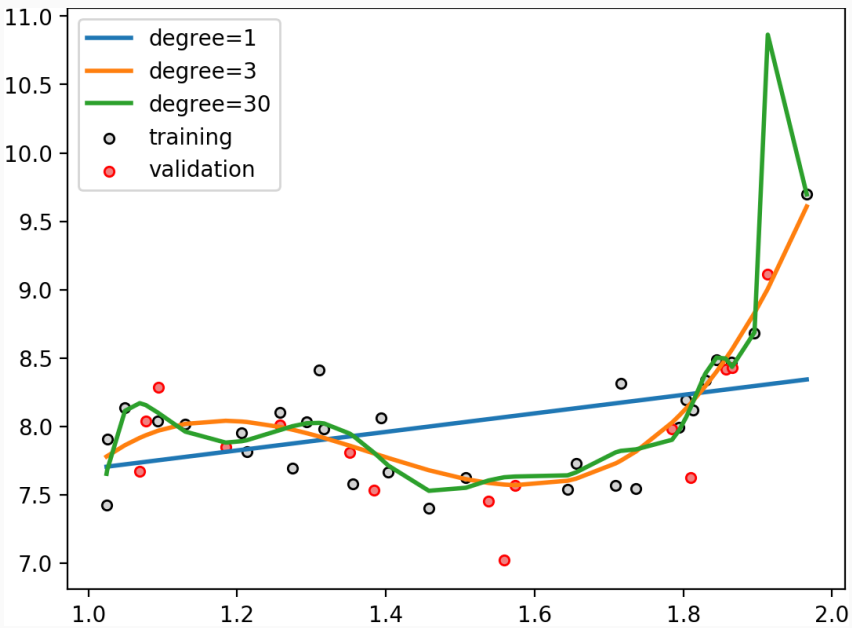

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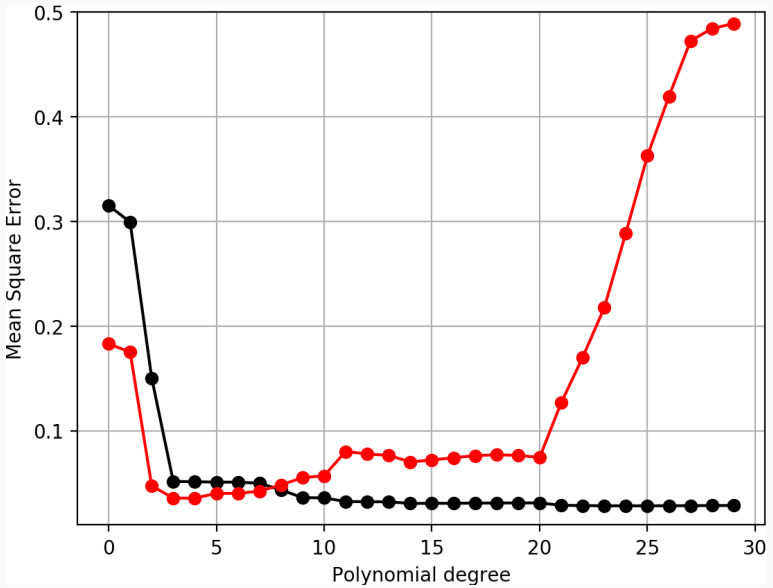

Choice of the model

Polynomial regression

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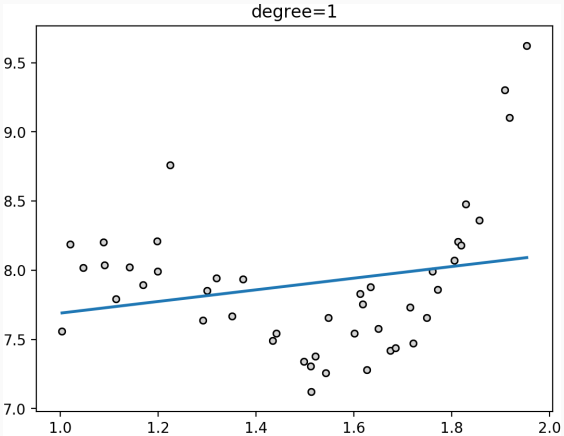
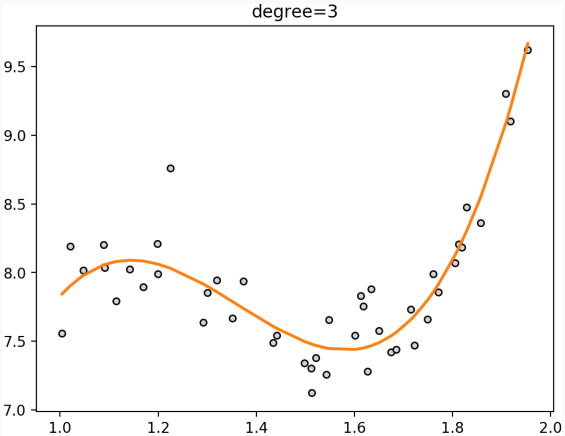


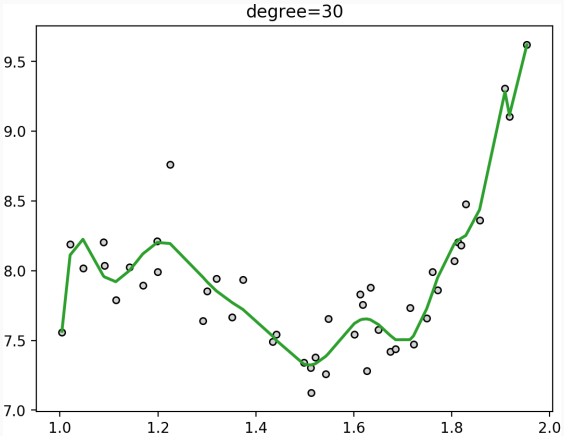
underfitting

degree = 3



good fit

degree = 30



overfitting

Train/Validation split

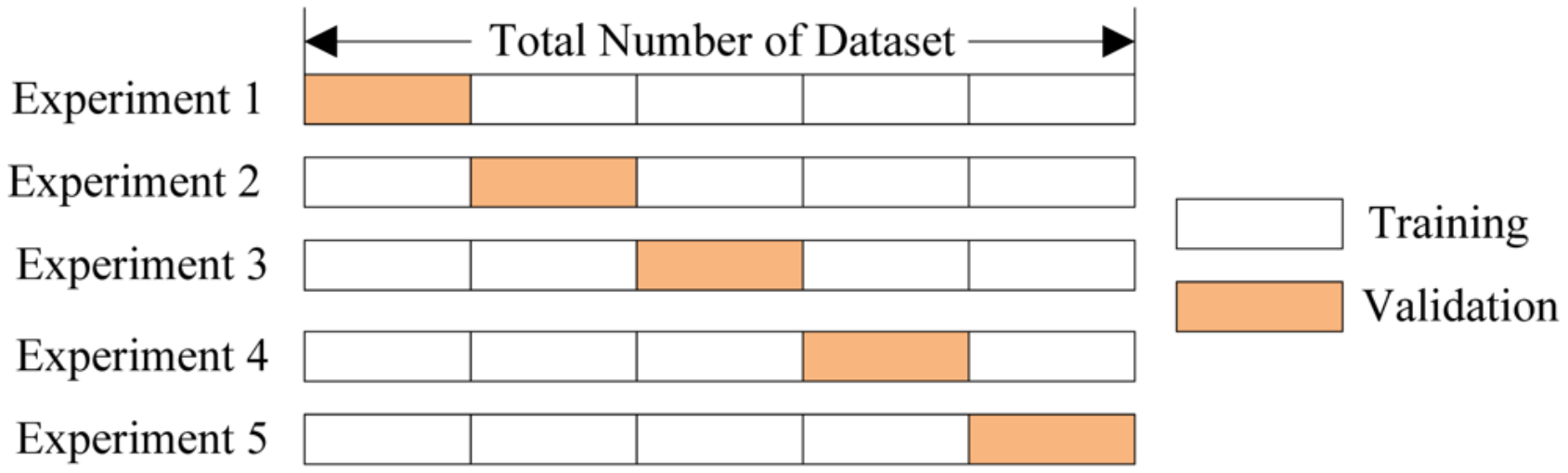
Drawbacks

- drastically reduces the number of samples that can be used for learning the model
- Results can depend on a particular random choice for the pair of (train, validation) sets.

More Robust: cross validation

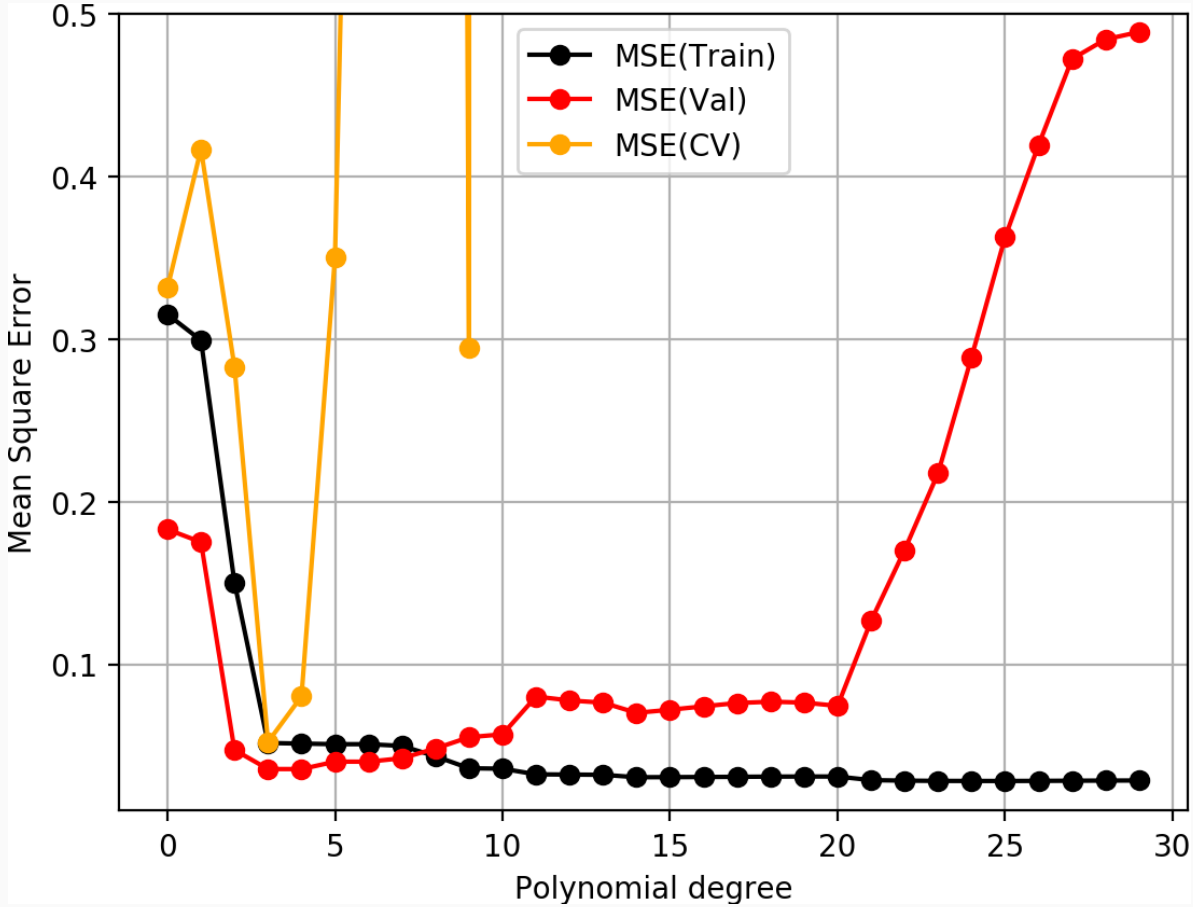
The idea

- Dividing the data in n folds,
- Learning n model (each time with a different training set),
- Compute the mean score over n validation set.



Cross-Validation

Fold	MSE
1	0.052
2	0.043
3	0.137
4	0.025
5	0.048
6	0.144
7	0.011
8	0.025
9	0.010
10	0.028
Mean	0.05



Wrapping up

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More on that in next lecture...

Steps of a machine learning process

Steps

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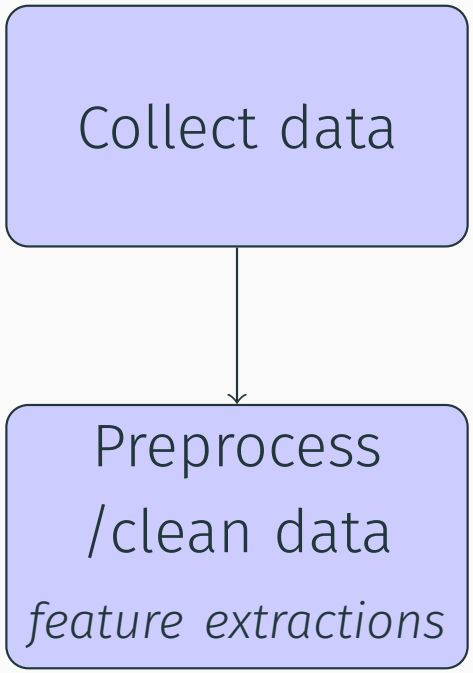

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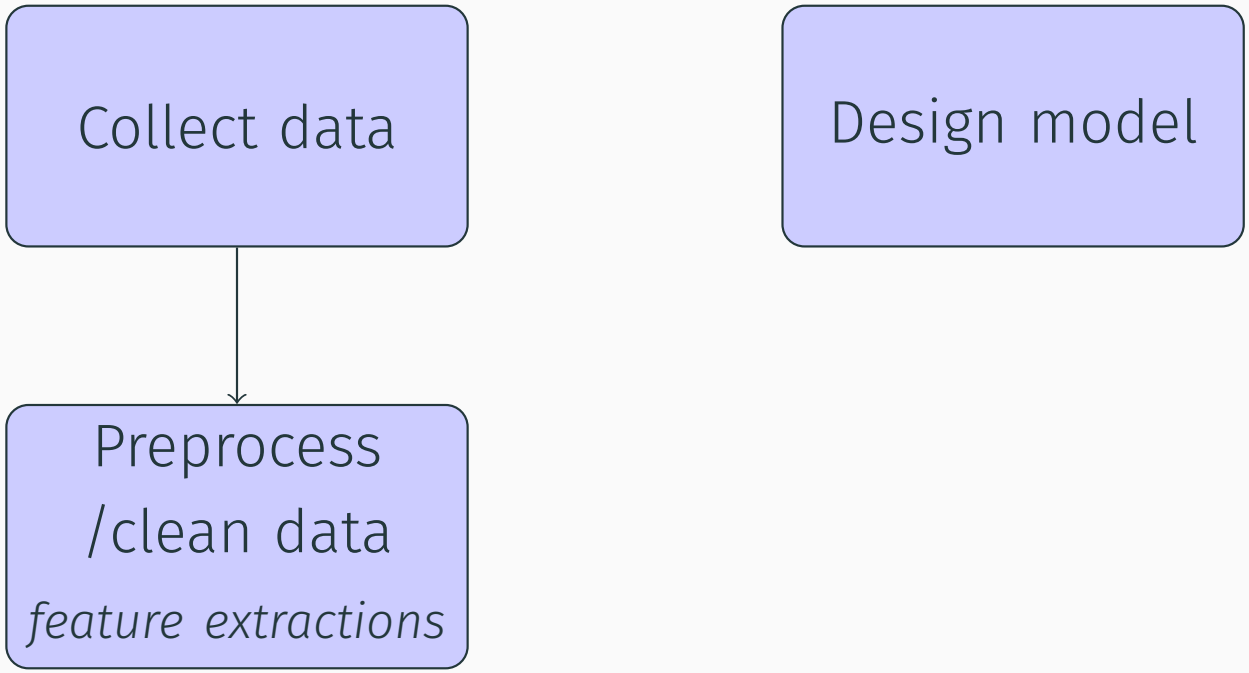
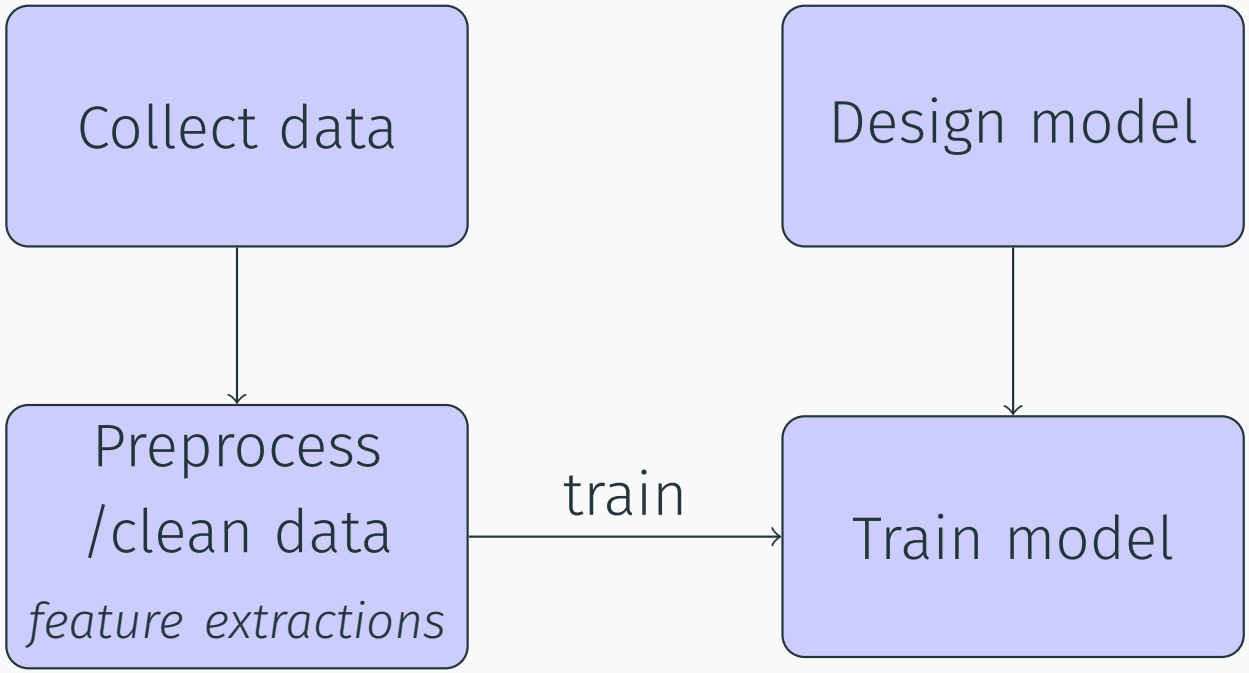

Collect data
Preprocess
/clean data
feature extractions
Design model

Steps


Collect data
Design model
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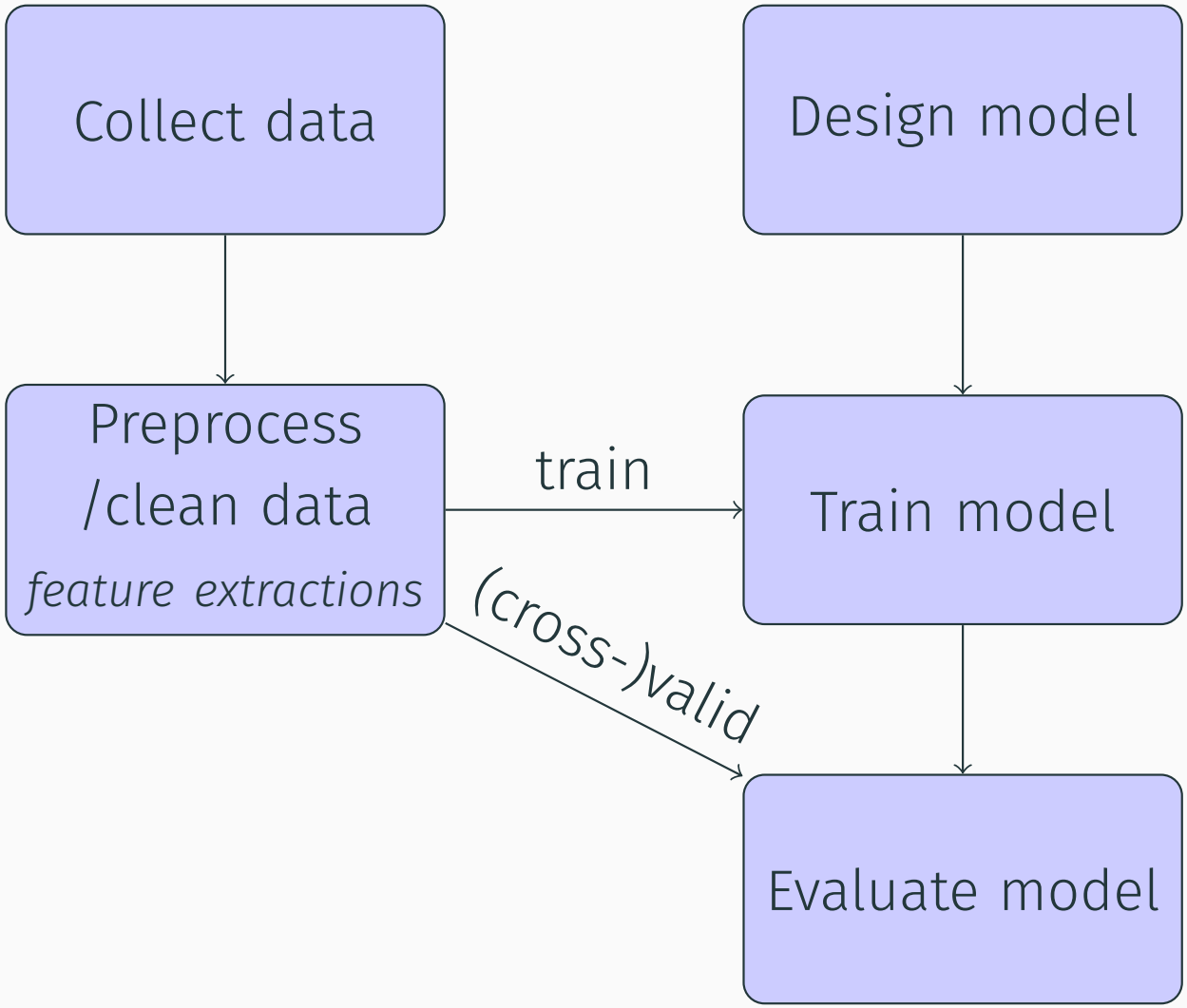
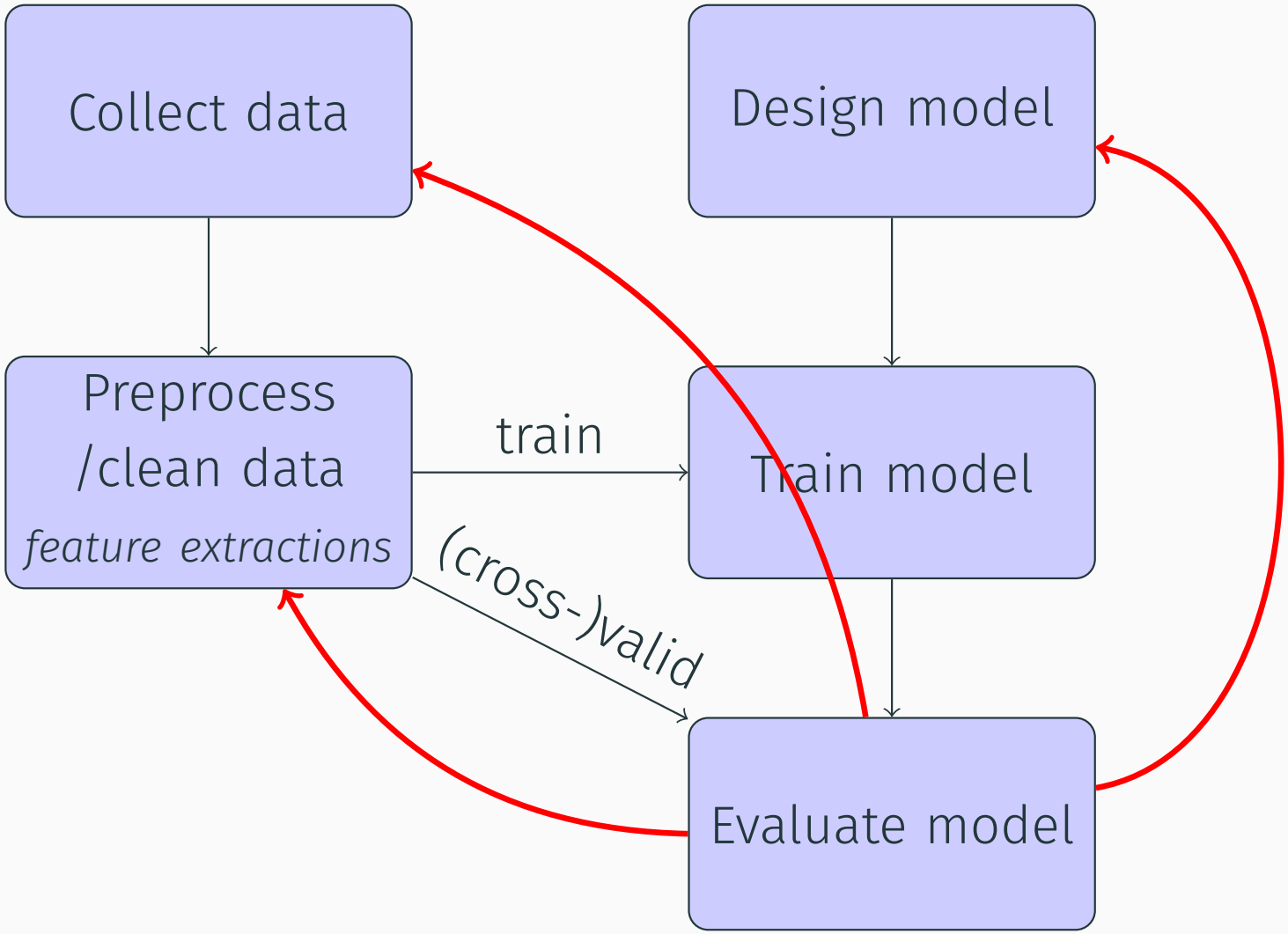
train
Train model

Steps


Collect data
Design model
Preprocess
/clean data
feature extractions
train
Train model
(cross-)valid
Evaluate model

Steps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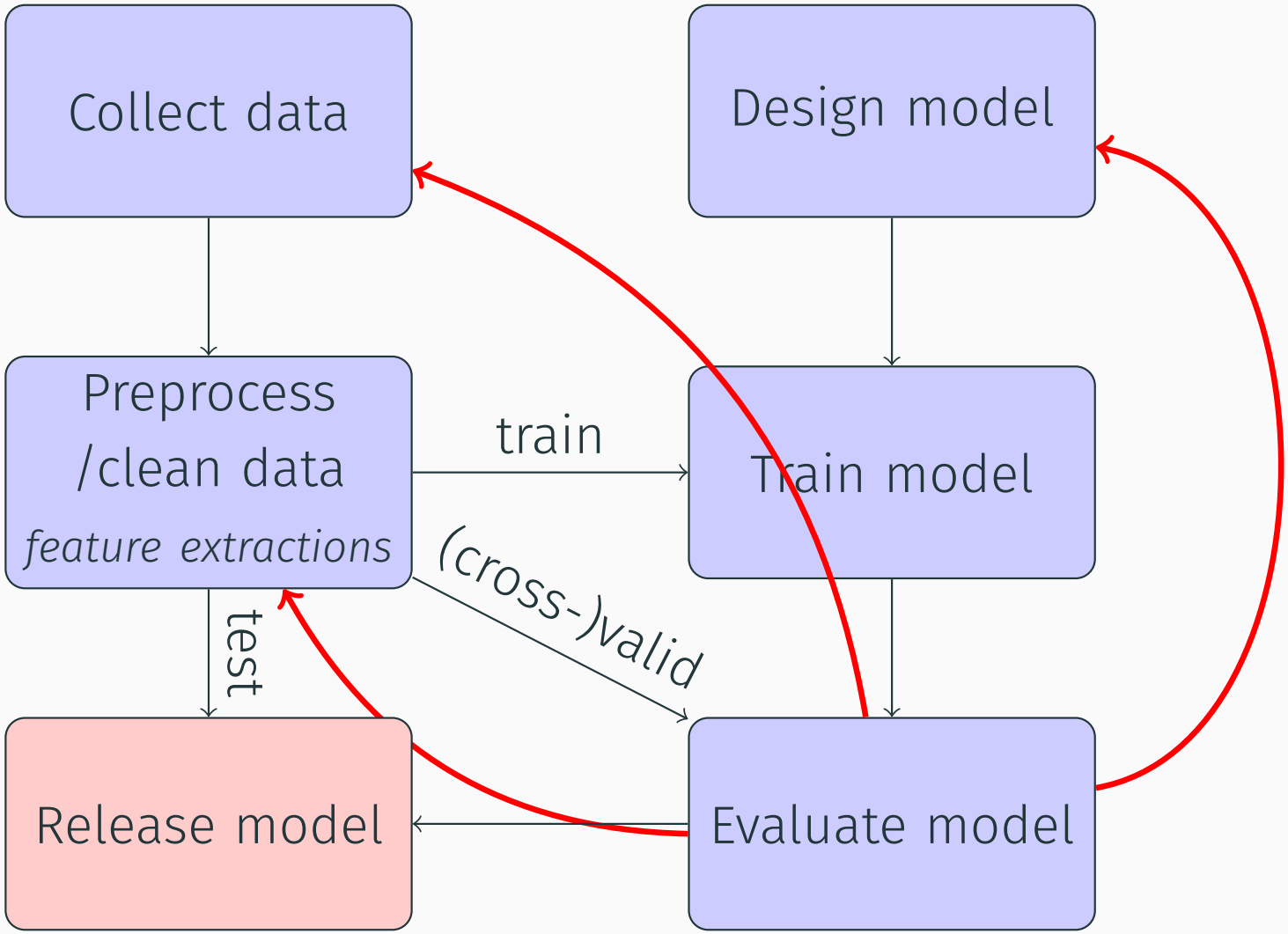
Collect data
Design model
Preprocess
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feature extractions
train
Train model
(cross-)valid
test
Release model
Evaluate model

In summary

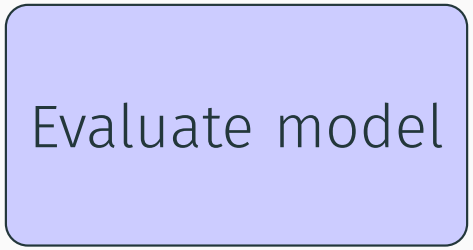
From one dataset, 3 sub-datasets have to be extracted:

- A training dataset
- A validation dataset

Can be done iteratively in a cross-validation procedure.
Some parameters of the model (e.g. polynomial order in a polynomial regression) were determined from the validation dataset.

- A test dataset (independent from the two others) to estimate the final performance of the model.

Additional Comments



Model evaluation is a critical step in the machine learning pipeline. Key considerations include:

- Is the dataset and evaluation metric unbiased? Do they accurately reflect the desired model performance?
- Is there a simpler model that performs sufficiently well? Avoid proposing complex machine learning solutions when a simpler approach is more effective.

Adequate metric

A typical metric for classification problems is the **accuracy**:

$$\text{acc} = \frac{TP + TN}{T + N}$$

TP: True Positive (number of positive results correctly classified)

TN: True Negative (number negative results correctly classified)

P: Number of positive examples

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Example of Credit Card Fraud Detection

Objective: Predict if a credit card operation is fraudulent

In the dataset, frauds (positive class) are **0.172%** of the cases.

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Other metric:

$$\text{recall} = \frac{TP}{P}$$

Always define a baseline

Example: Weather Forecast

Imagine we have a model predicting ”rain” or ”no-rain” the day after with an accuracy of 75%.

Is it good?

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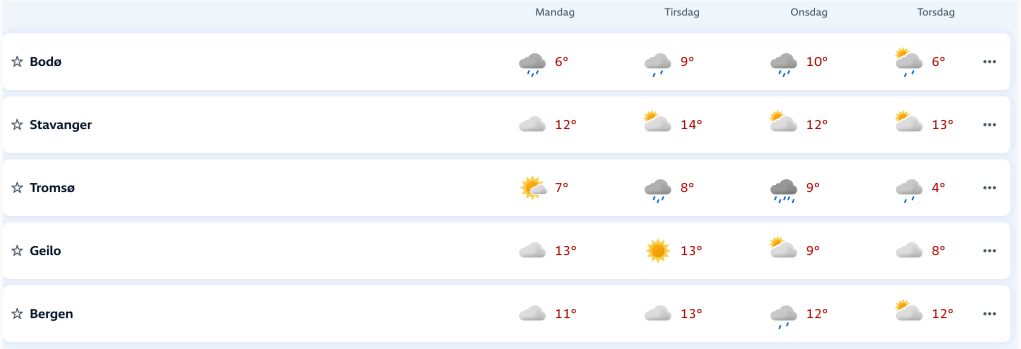

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Predict that the day after is the same as the day before

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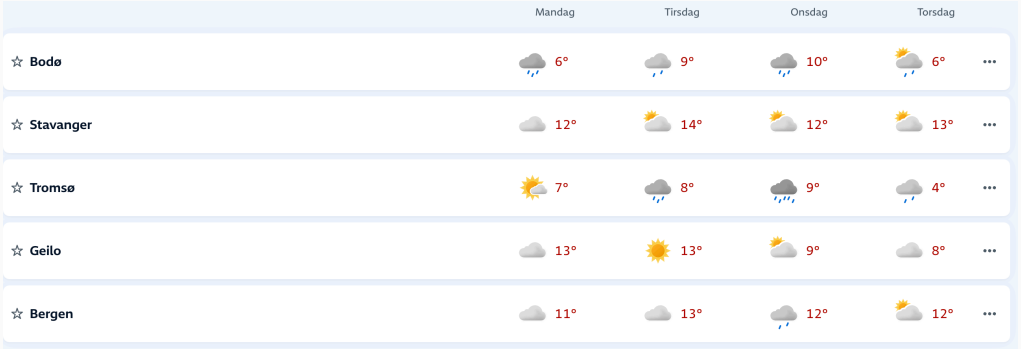

A very simple baseline: the persistence.

Predict that the day after is the same as the day before

Accuracy of persistence: 80%

In this case, a ML model should do better than 80% to be considered.


Kahoot!

Feature processing

Structure of the features

What is a feature?

It is a measurable property of the data.

Orgnisation of the features:

Scalar	Image/Tensor	Sequence	Unstructured
number of room of a house, profession, ...	values of a pixel in a image	time series, text	available paths in a city map

Type of features

- quantitative/continuous features (e.g. distance to employment centers, temperature)

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Encoding of the features?

Feature encoding

Type	Examples		Encoding
Quantitative	distance	$\{1.2, 2.3, 0.1\}$	$\{1.2, 2.3, 0.1\}$
Ordinal	rooms	$\{2, 3, 4\}$	$\{2, 3, 4\}$
Qualitative	Ocean	$\{\text{Atlantic}, \text{Indian}, \text{Pacific}\}$	$\{[1, 0, 0], [0, 1, 0], [0, 0, 1]\}$

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Qualitative variable: one-hot encoding.

- You must not encode qualitative features with integer $1, 2, 3$, it would mean that Pacific > Indian > Atlantic.
- In $\mathrm{sklearn}$ there is a function that makes the one-hot encoding: $\mathrm{OneHotEncoder}()$
- If the number of modalities (number of different features) is high, encoding qualitative feature produces a big-sized vector.

Embedding

A common way to deal with features with a lot of modalities: Embedding

Principle of embedding

Let's consider a qualitative variable with n modalities, represented by the n-dimensional binary vector $\mathbf{x}$

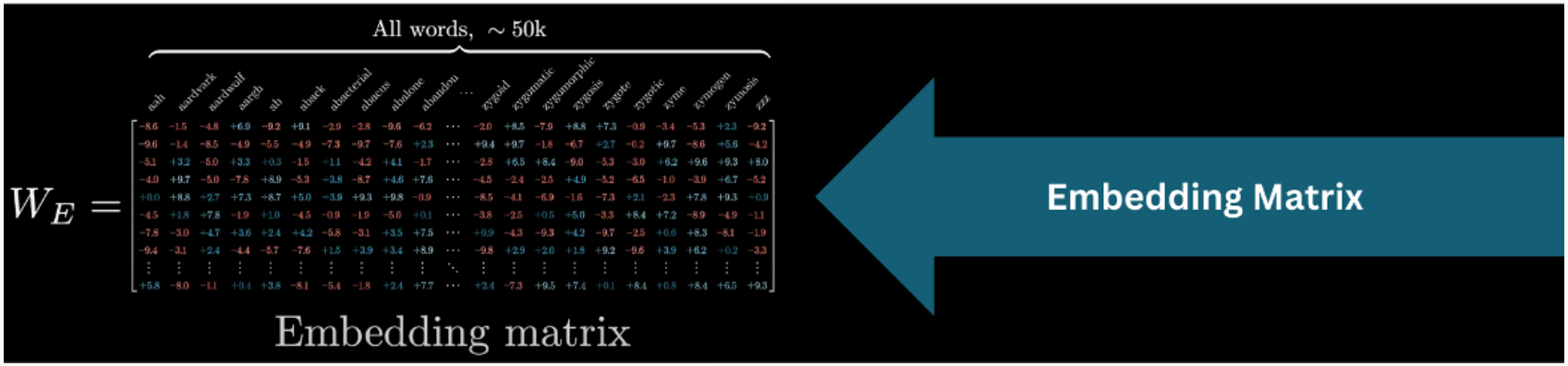
Embedding consists in representing this variable by a vector $\mathbf{v} \in \mathbb{R}^p, p << n$

The embedding is represented by a matrix $\mathbf{M} \in \mathbb{R}^{n \times p}$ such as:

$$\mathbf{v} = \mathbf{M} \cdot \mathbf{x}$$

Coefficients of $\mathbf{M}$ have to be optimized given an objective criteria (that depends on your problem)

Embedding for Large Language Models (LLM)



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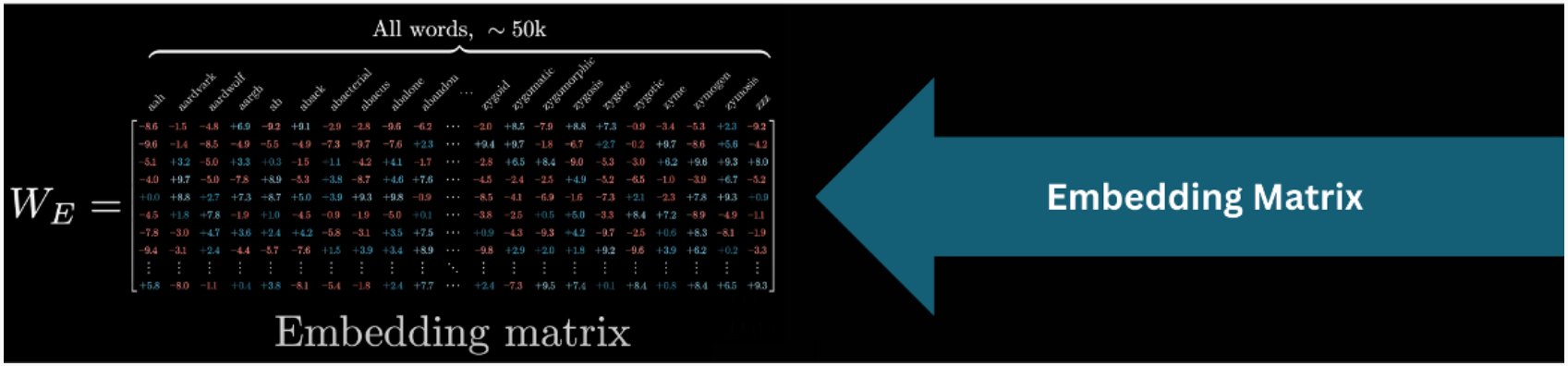

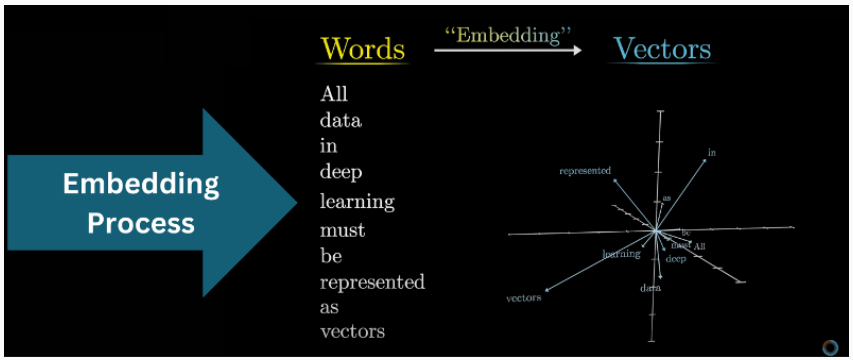

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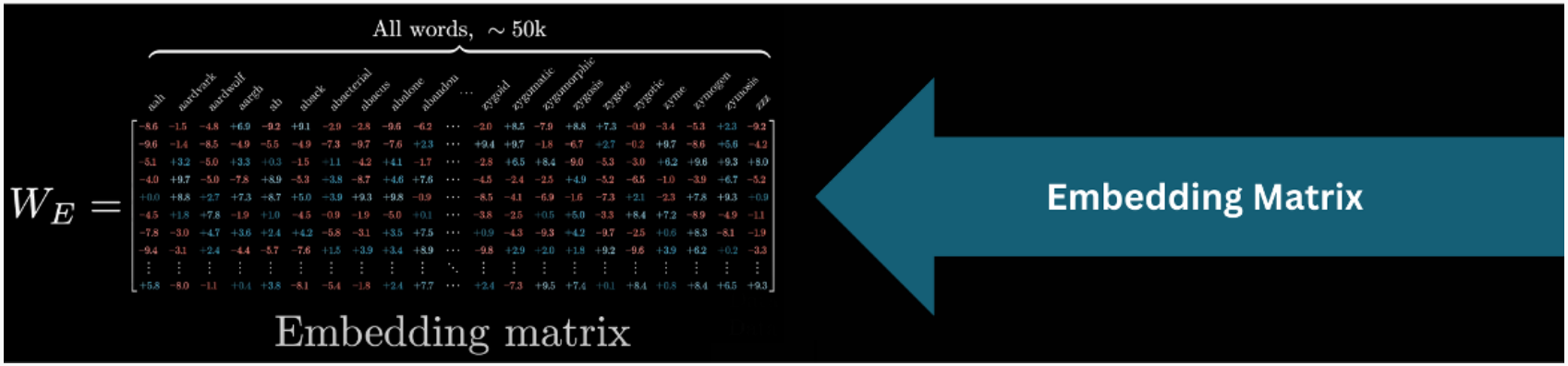
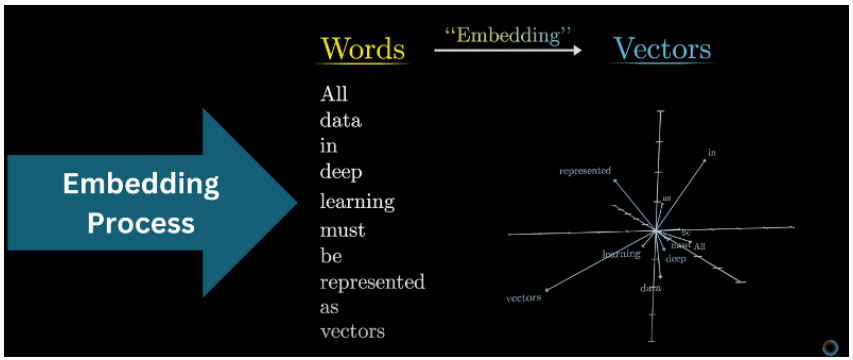
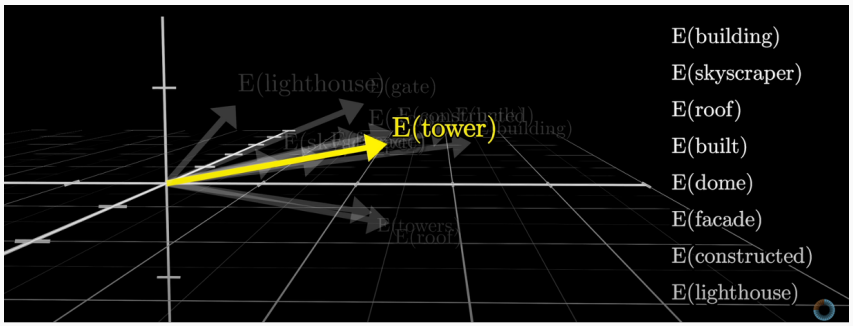


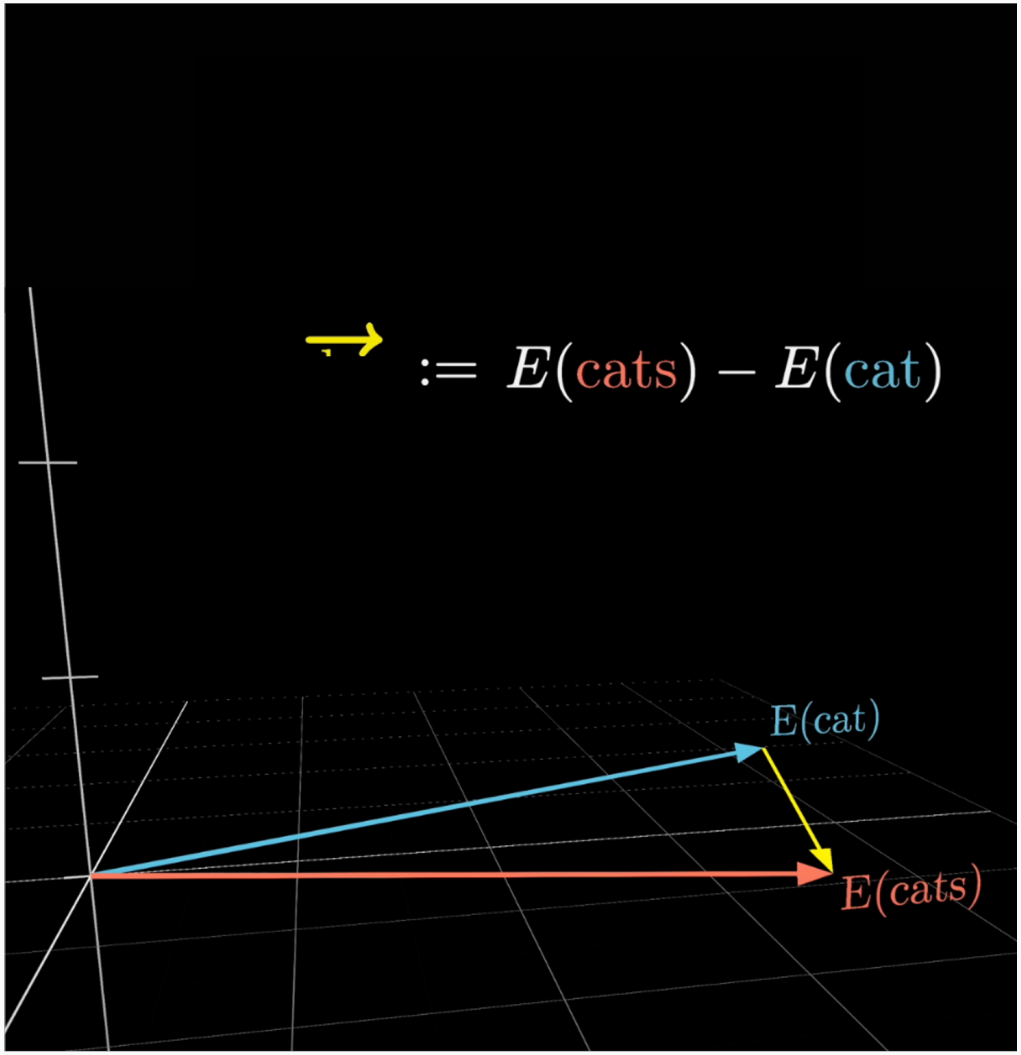


Embeddings of similar words are close:



https://www.3blue1brown.com/lessons/gpt

The notion of direction



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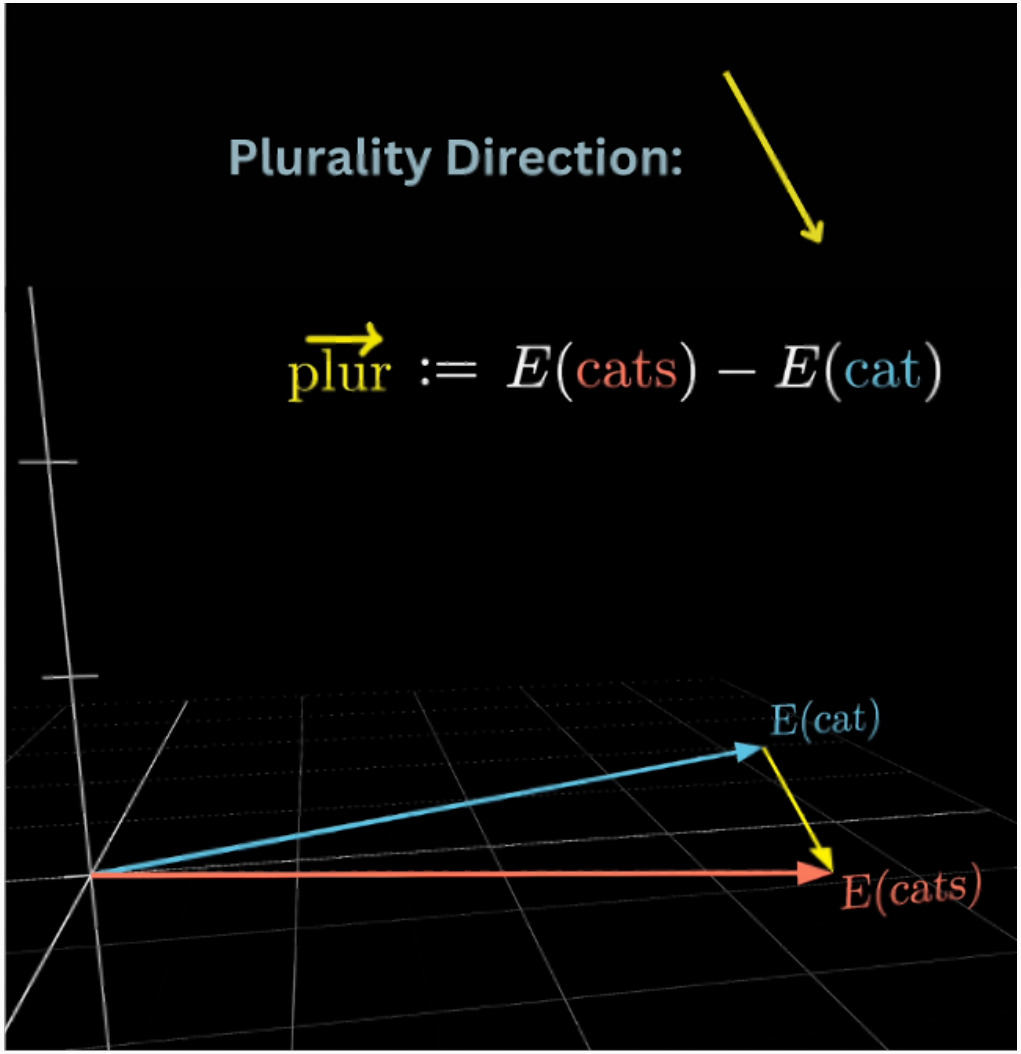

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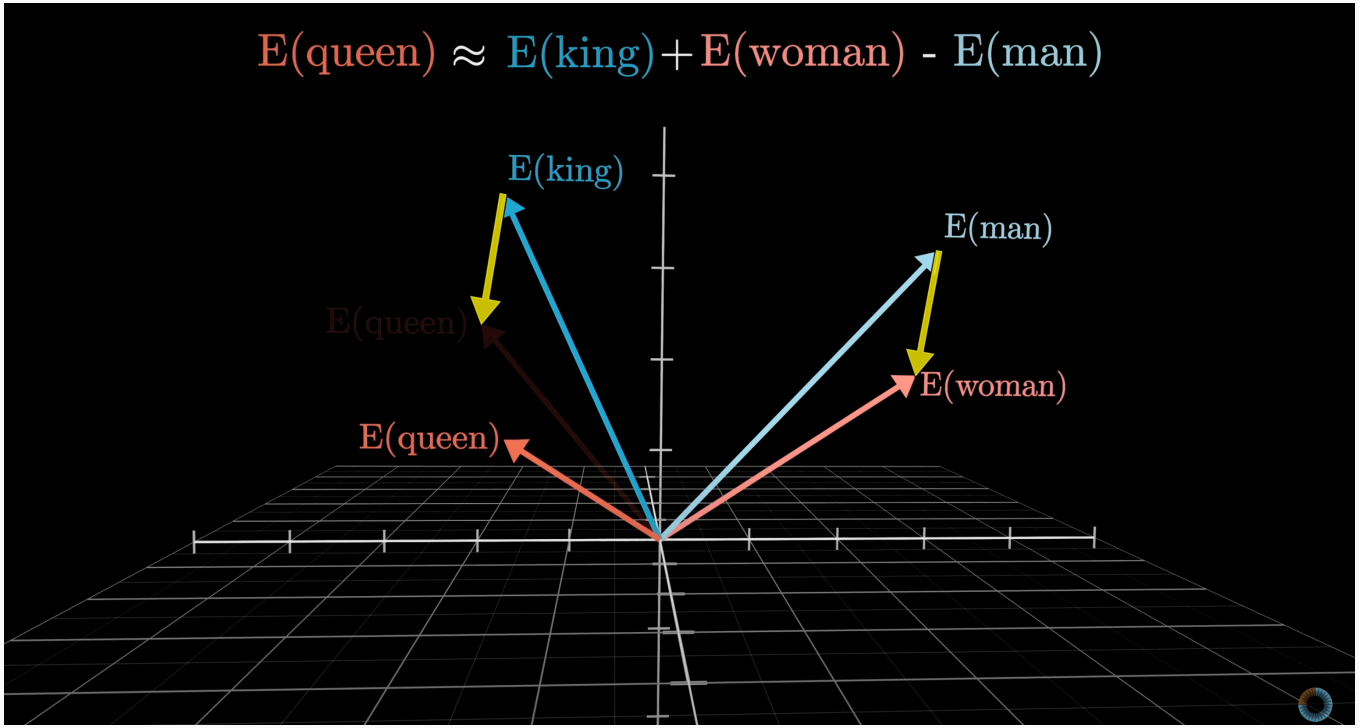
The space of embedding encodes some ”meaning”



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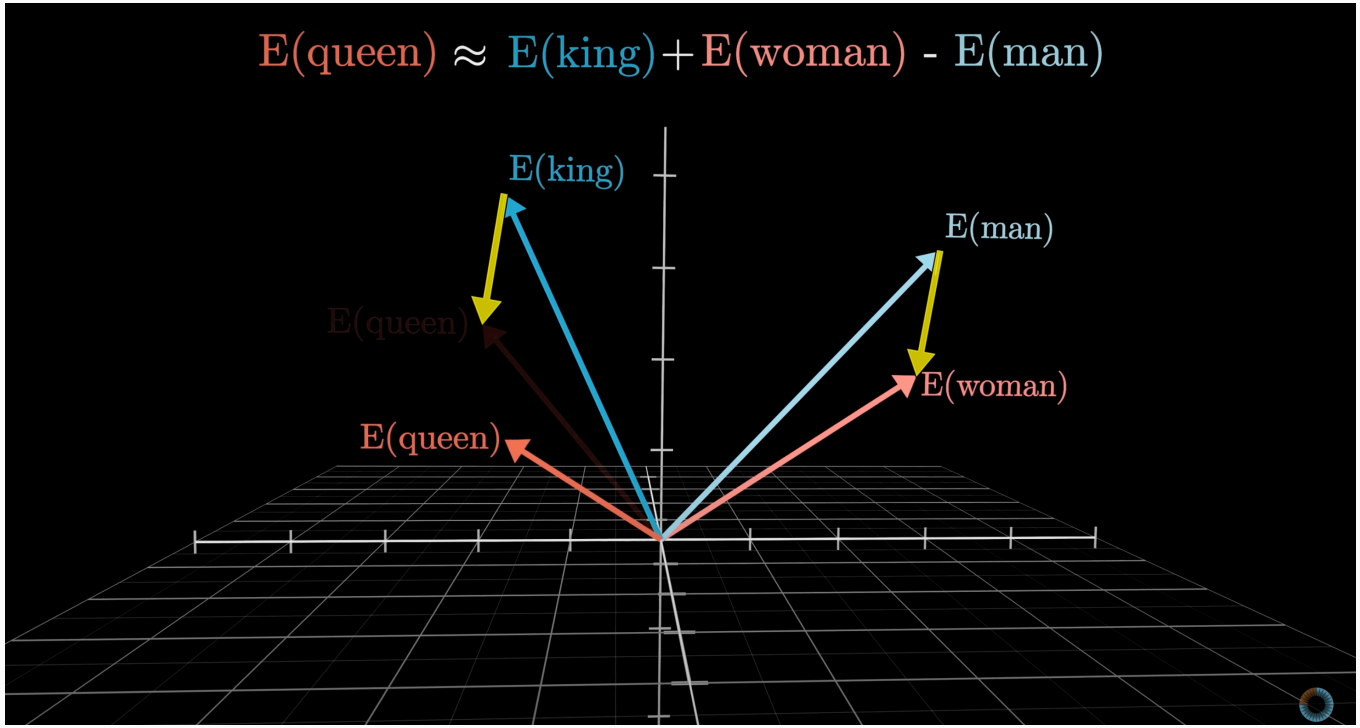
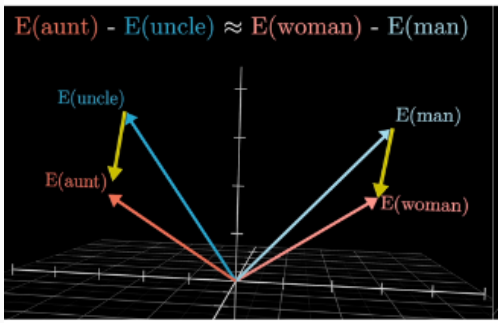
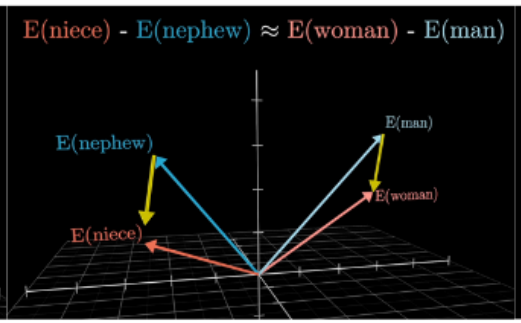
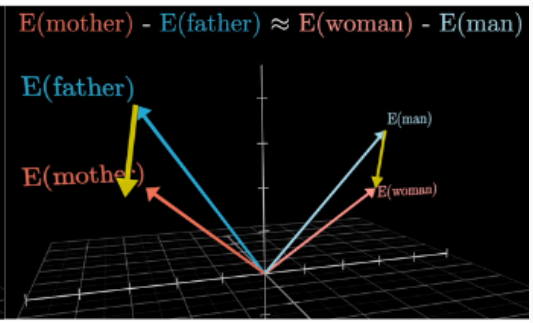


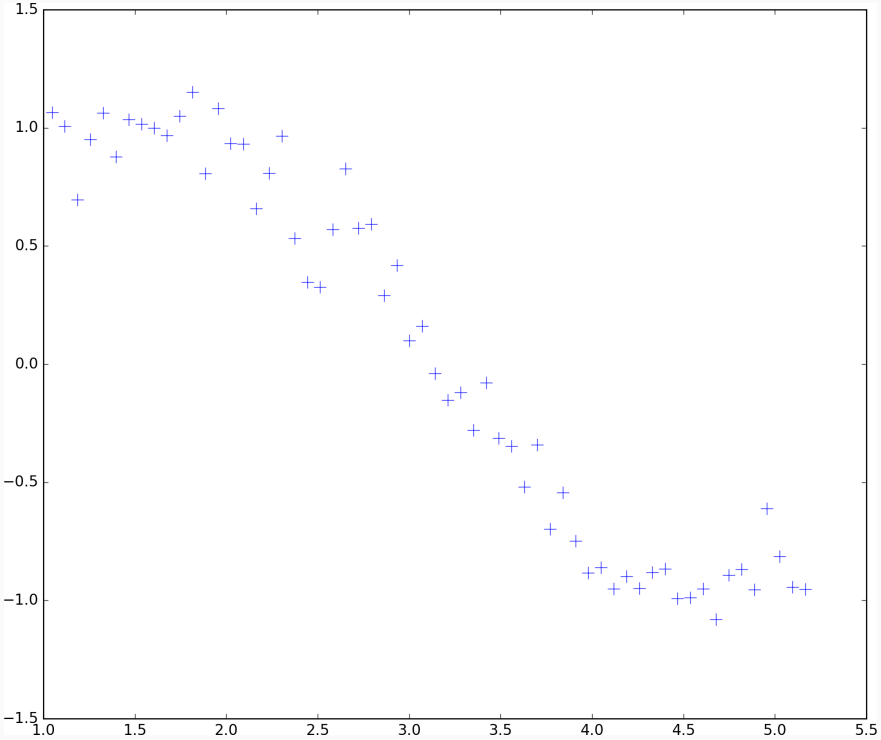






L1/L2 regularization

Example of a non-linear relationship



An idea

We could take a polynomial hypothesis model:

$$h_{\boldsymbol{\theta}}(x) = \theta_0 x^0 + \theta_1 x^1 + \ldots + \theta_p x^p$$

Example

$\{(x_1, y_1), \ldots, (x_n, y_n)\}$ is the learning dataset.

For a given polynomial degree p, parameters $\boldsymbol{\theta}$ are determined minimizing the least-mean square cost function:

$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum (y_i - h_{\boldsymbol{\theta}}(x_i))^2$$

with $h_{\boldsymbol{\theta}}(x) = \theta_0 x^0 + \theta_1 x^1 + \ldots + \theta_p x^p$

- It can be determined using a gradient descent method

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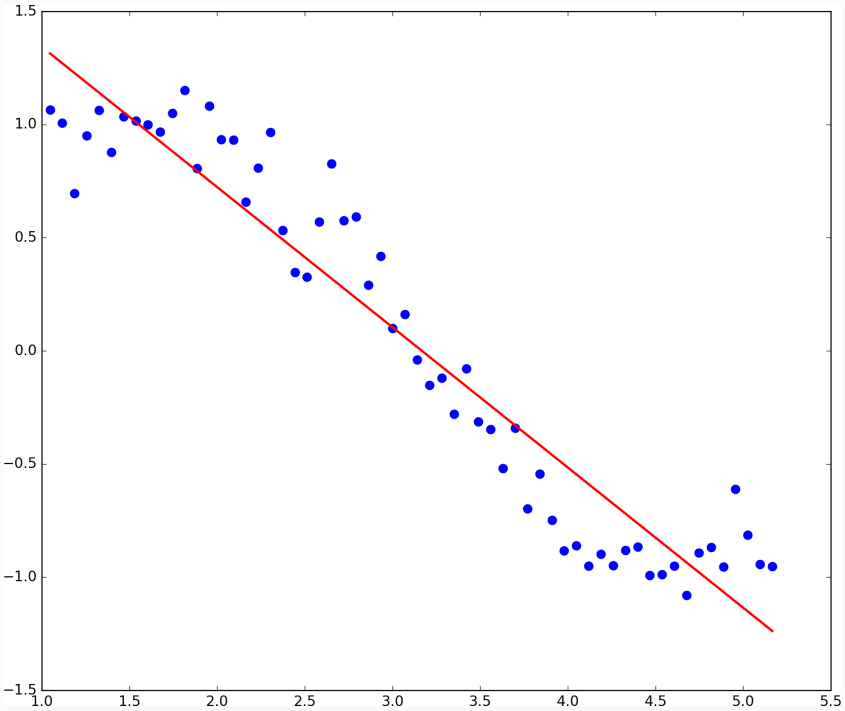
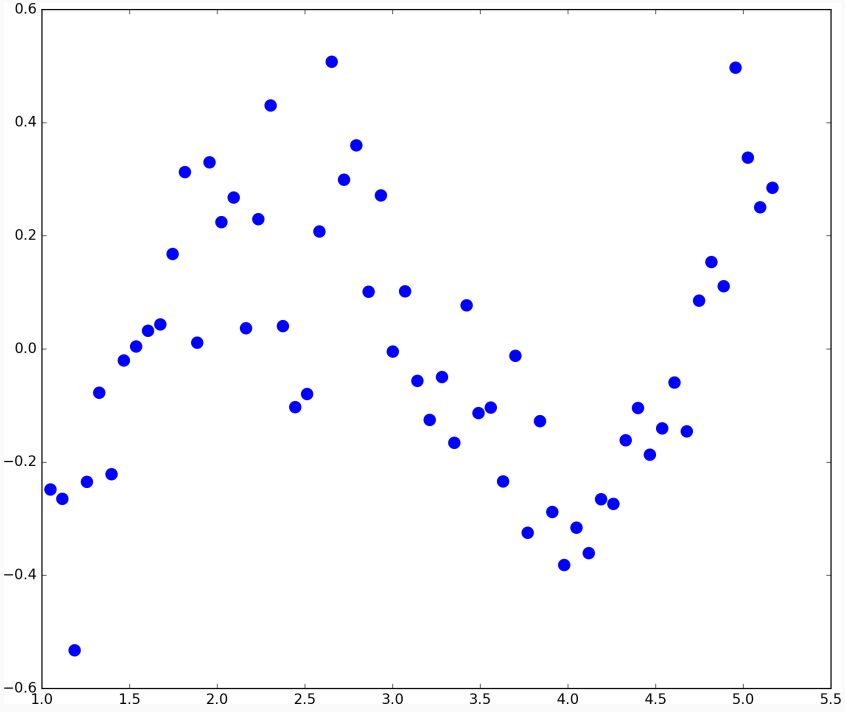
- It can be determined using a gradient descent method
- If the degree of the polynomial $p = 1$, it is a simple linear regression

A first result

$p = 1$ (linear regression)



residuals

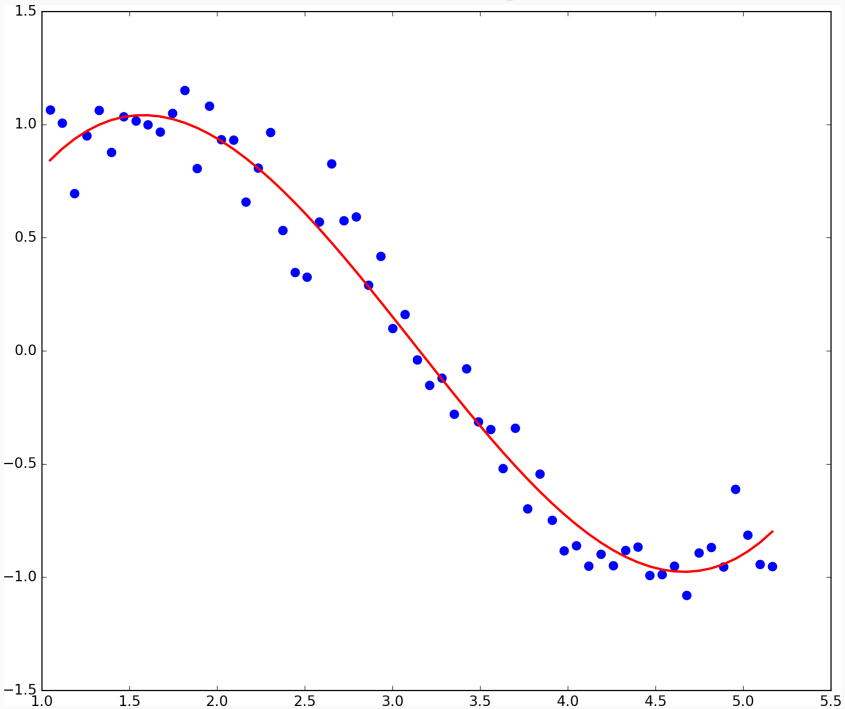


Prediction error

$$\text{err} = \frac{1}{n}\sum \text{res}^2 = 5.46e-2$$

Increasing the polynomial degree ?

$p = 3$ (cubic regression)



Prediction error

$$\text{err} = \frac{1}{n}\sum \text{res}^2 = 1.80e-2$$

Is it different from the linear regression ?

Let's consider :

$$\boldsymbol{x} = \begin{pmatrix} 1 \\ x^1 \\ x^2 \\ \vdots \\ x^p \end{pmatrix}$$

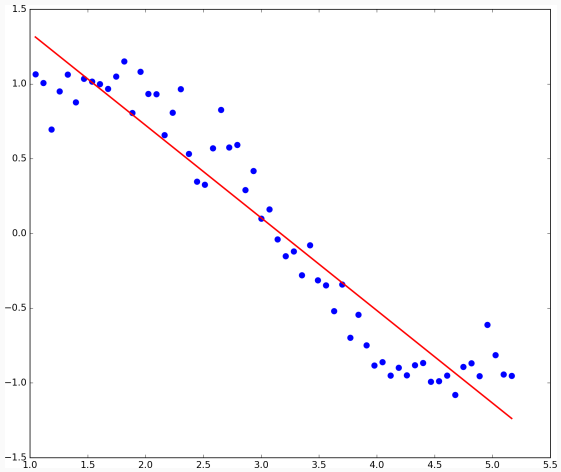
then

$$h_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x^1 + \ldots + \theta_p x^p = \boldsymbol{\theta}^T \boldsymbol{x}$$

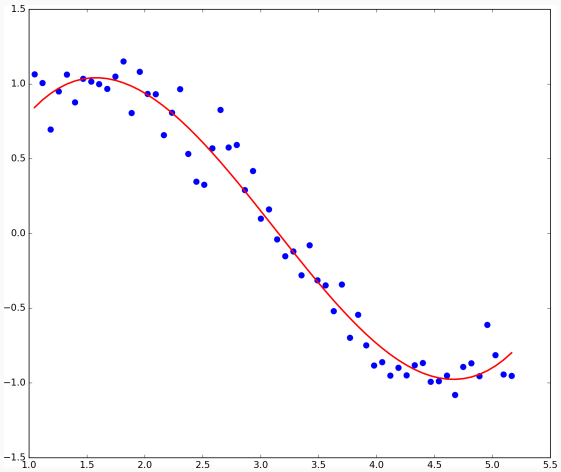
By extending a scalar predictor to a vector, polynomial regression is equivalent to linear regression.

Increasing the degree ?

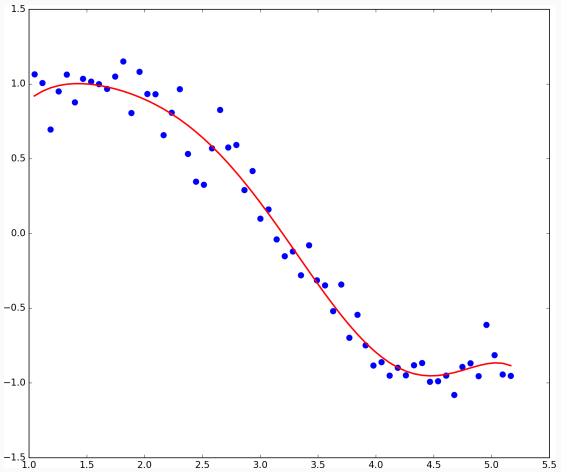
$p = 1$



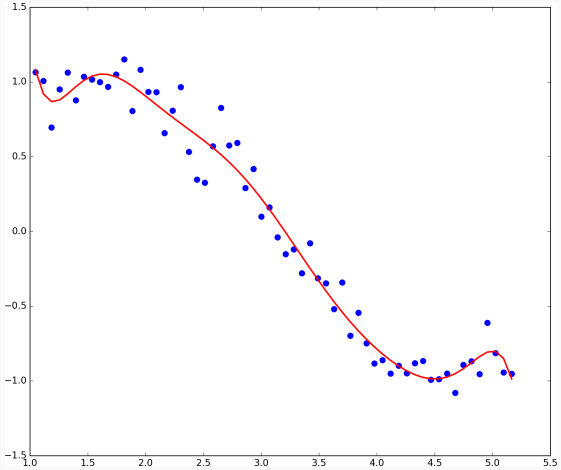
$p = 3$



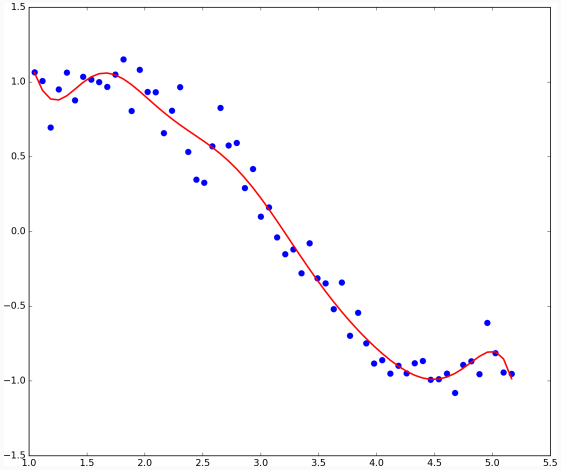
$p = 4$



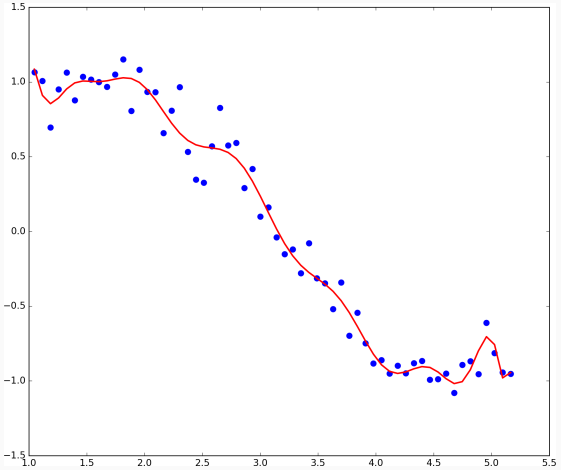
$p = 9$



$p = 12$



$p = 15$



Overfitting

When there are too many parameters to fit, the model can reproduce a random noise, it is called overfitting

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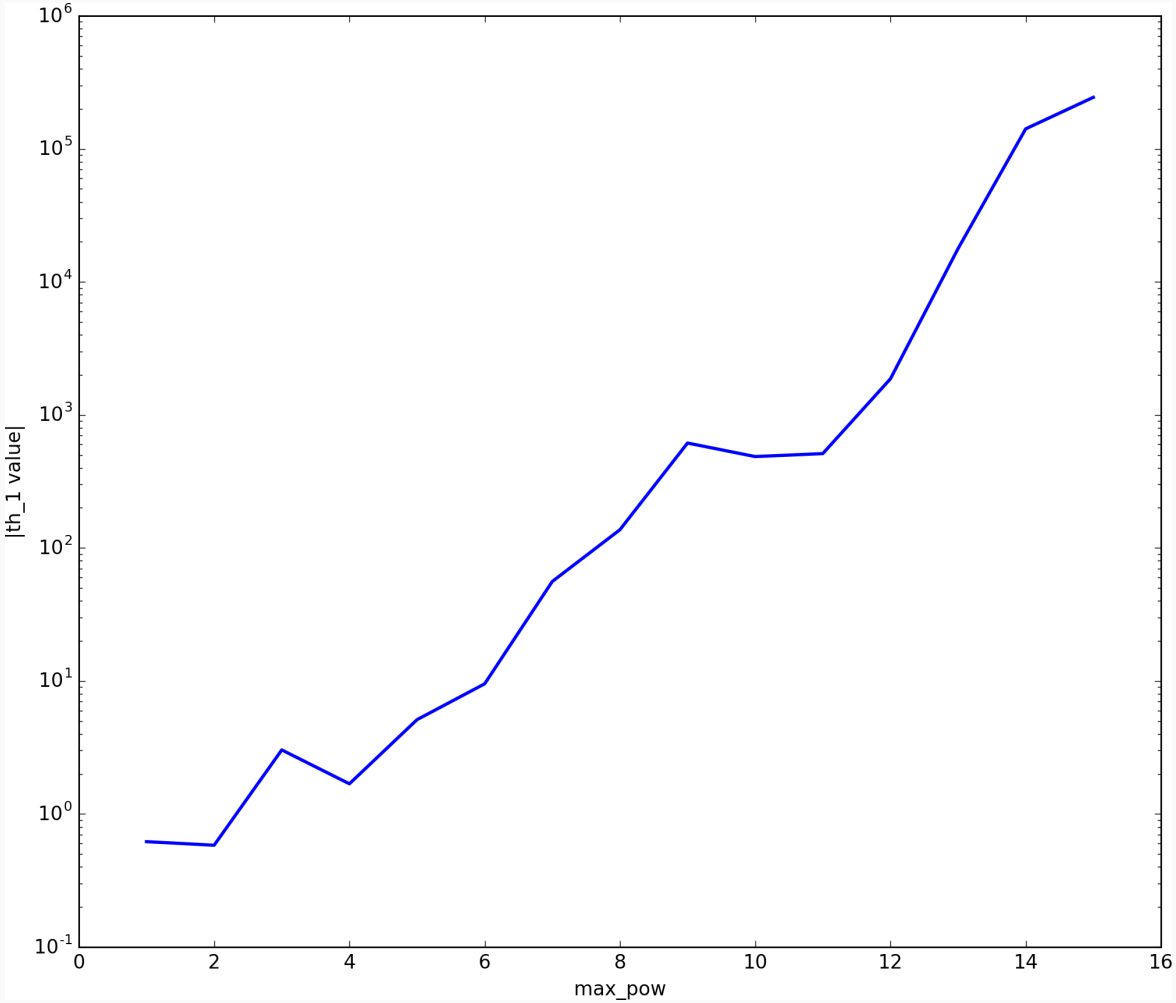
	rmse	th_0	th_1	th_2	th_3	th_4	th_5	th_6	th_7	th_8
max_pow_1	+5.47e-02	+1.96e+00	-6.20e-01	NaN	NaN	NaN	NaN	NaN	NaN	NaN
max_pow_2	+5.46e-02	+1.91e+00	-5.83e-01	-5.96e-03	NaN	NaN	NaN	NaN	NaN	NaN
max_pow_3	+1.84e-02	-1.08e+00	+3.03e+00	-1.29e+00	+1.37e-01	NaN	NaN	NaN	NaN	NaN
max_pow_4	+1.80e-02	-2.66e-01	+1.69e+00	-5.32e-01	-3.57e-02	+1.39e-02	NaN	NaN	NaN	NaN
max_pow_5	+1.70e-02	+2.99e+00	-5.12e+00	+4.72e+00	-1.93e+00	+3.35e-01	-2.07e-02	NaN	NaN	NaN
max_pow_6	+1.65e-02	-2.80e+00	+9.52e+00	-9.71e+00	+5.23e+00	-1.55e+00	+2.33e-01	-1.36e-02	NaN	NaN
max_pow_7	+1.55e-02	+1.93e+01	-5.60e+01	+6.90e+01	-4.46e+01	+1.65e+01	-3.53e+00	+4.05e-01	-1.92e-02	NaN
max_pow_8	+1.53e-02	+4.32e+01	-1.37e+02	+1.84e+02	-1.33e+02	+5.77e+01	-1.53e+01	+2.42e+00	-2.10e-01	+7.68e-03
max_pow_9	+1.46e-02	+1.68e+02	-6.15e+02	+9.63e+02	-8.46e+02	+4.61e+02	-1.62e+02	+3.68e+01	-5.22e+00	+4.22e-01
max_pow_10	+1.46e-02	+1.38e+02	-4.86e+02	+7.26e+02	-5.96e+02	+2.93e+02	-8.75e+01	+1.45e+01	-8.06e-01	-1.38e-01
max_pow_11	+1.45e-02	-7.49e+01	+5.12e+02	-1.33e+03	+1.87e+03	-1.61e+03	+9.14e+02	-3.50e+02	+9.14e+01	-1.61e+01
max_pow_12	+1.45e-02	-3.39e+02	+1.87e+03	-4.42e+03	+6.01e+03	-5.25e+03	+3.12e+03	-1.30e+03	+3.84e+02	-8.03e+01
max_pow_13	+1.43e-02	+3.20e+03	-1.78e+04	+4.46e+04	-6.66e+04	+6.61e+04	-4.61e+04	+2.32e+04	-8.55e+03	+2.30e+03
max_pow_14	+1.31e-02	+2.38e+04	-1.41e+05	+3.79e+05	-6.10e+05	+6.57e+05	-5.03e+05	+2.82e+05	-1.17e+05	+3.66e+04
max_pow_15	+1.17e-02	-3.62e+04	+2.44e+05	-7.46e+05	+1.38e+06	-1.71e+06	+1.53e+06	-1.00e+06	+4.98e+05	-1.88e+05

High parameters values

Value of the parameters $|\theta_1|$ with respect with the degree of the polynomial regression



Regularization

The idea

The idea of regularization is to perform a regression minimizing a cost function that includes a term to penalize "big" values for the parameters:

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum(y_i - h_{\boldsymbol{\theta}}(x_i))^2 + \alpha P(\boldsymbol{\theta})$$

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- Lasso Regularization (L1): $P(\boldsymbol{\theta}) = \sum_{i=0}^{p} |\theta_i|$
- Elastic Net combines both regularizations

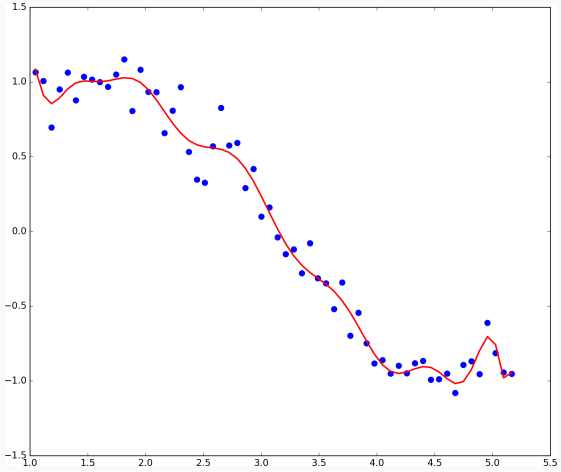
Ridge regression (L2)

Ridge regression is a linear regression with a Ridge regularization:

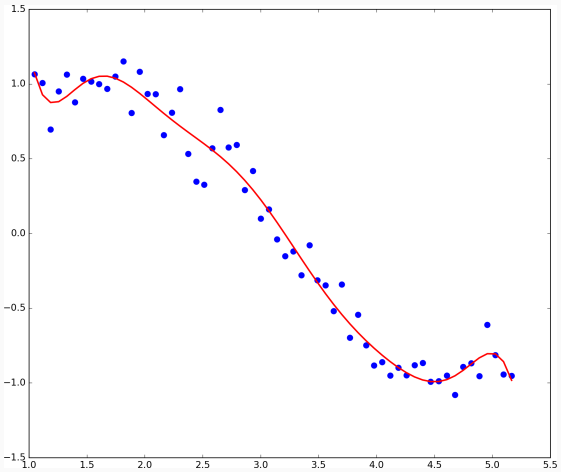
$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum(y_i - h_{\boldsymbol{\theta}}(x_i))^2 + \alpha\sum_{i=0}^{p}\theta_i^2$$

Results for $p = 15$ and varying α

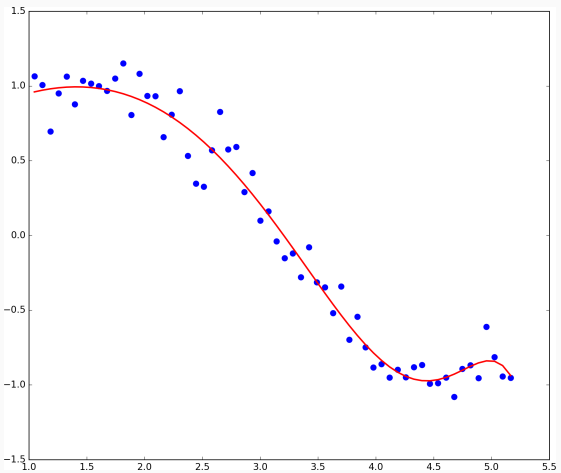
$\alpha = 0$



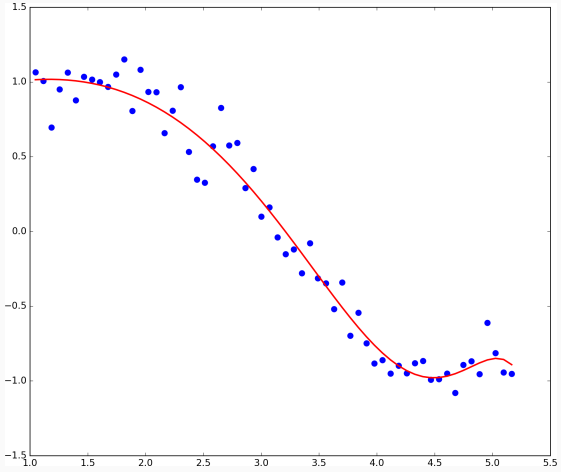
$\alpha = 1e-15$



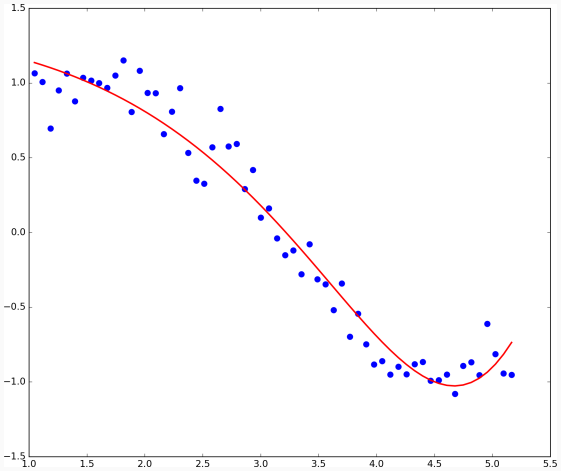
$\alpha = 1e-4$



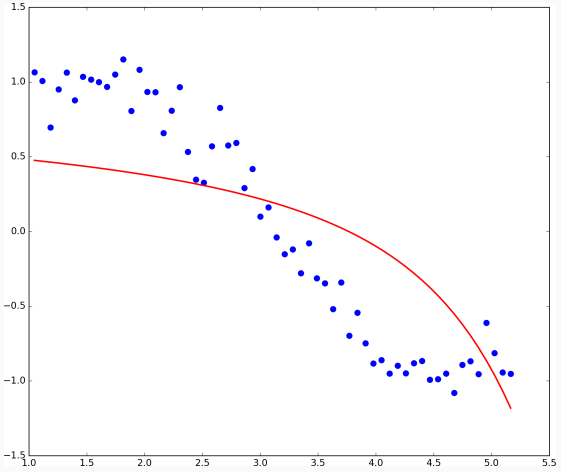
$\alpha = 1e-3$



$\alpha = 1e-2$

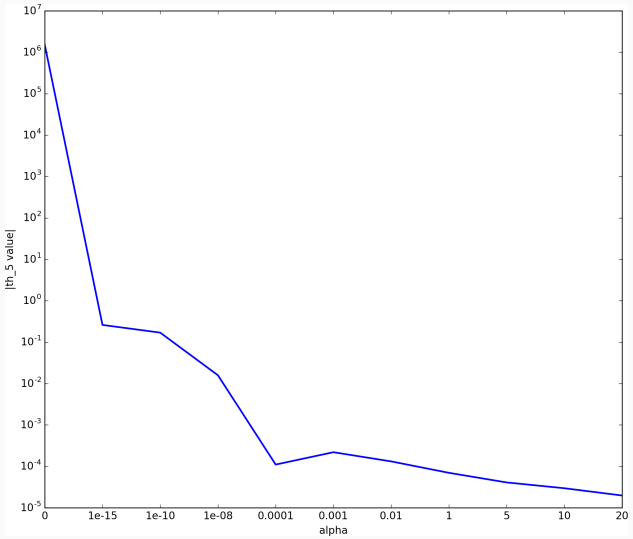


$\alpha = 5$



Values of coefficients

	rmse	th_0	th_1	th_2	th_3	th_4	th_5	th_6	th_7	th_8
alpha_0	+1.17e-02	-3.62e+04	+2.44e+05	-7.46e+05	+1.38e+06	-1.71e+06	+1.53e+06	-1.00e+06	+4.98e+05	-1.88e+05
alpha_1e-15	+1.46e-02	+9.43e+01	-2.98e+02	+3.79e+02	-2.37e+02	+6.72e+01	-2.60e-01	-4.35e+00	+5.62e-01	+1.42e-01
alpha_1e-10	+1.54e-02	+1.12e+01	-2.90e+01	+3.11e+01	-1.52e+01	+2.89e+00	+1.69e-01	-9.10e-02	-1.08e-02	+1.98e-03
alpha_1e-08	+1.58e-02	+1.34e+00	-1.53e+00	+1.75e+00	-6.80e-01	+3.88e-02	+1.58e-02	+1.59e-04	-3.60e-04	-5.37e-05
alpha_0.0001	+1.60e-02	+5.61e-01	+5.47e-01	-1.28e-01	-2.57e-02	-2.82e-03	-1.10e-04	+4.06e-05	+1.52e-05	+3.65e-06
alpha_0.001	+1.67e-02	+8.18e-01	+3.05e-01	-8.67e-02	-2.05e-02	-2.84e-03	-2.19e-04	+1.81e-05	+1.24e-05	+3.43e-06
alpha_0.01	+2.39e-02	+1.30e+00	-8.84e-02	-5.15e-02	-1.01e-02	-1.41e-03	-1.32e-04	+7.23e-07	+4.14e-06	+1.30e-06
alpha_1	+9.41e-02	+9.69e-01	-1.39e-01	-1.93e-02	-3.00e-03	-4.66e-04	-6.97e-05	-9.90e-06	-1.29e-06	-1.43e-07
alpha_5	+2.31e-01	+5.48e-01	-5.89e-02	-8.52e-03	-1.42e-03	-2.41e-04	-4.08e-05	-6.87e-06	-1.15e-06	-1.91e-07
alpha_10	+3.00e-01	+4.00e-01	-3.72e-02	-5.53e-03	-9.50e-04	-1.67e-04	-2.96e-05	-5.23e-06	-9.25e-07	-1.63e-07
alpha_20	+3.79e-01	+2.77e-01	-2.25e-02	-3.40e-03	-5.99e-04	-1.08e-04	-1.97e-05	-3.60e-06	-6.58e-07	-1.20e-07



Value of θ_5

Determination of the parameters in the ridge regression

Considering the cost function J:

$$J(\boldsymbol{\theta}) = J_{lms}(\boldsymbol{\theta}) + \alpha \sum_{i=0}^{p} \theta_i^2$$

In a gradient algorithm, update of the parameters:

$\theta_i^{k+1} = \theta_i^k - \nu.(\frac{\partial J_{lms}}{D\theta_i} - 2\alpha\theta_i^k)$

So the update rule is:

$$\theta_i^{k+1} = \theta_i^k(1 - 2\nu\alpha) - \Delta_{lms}$$

where Δ_{lms} is the update in case of non-regularized regression

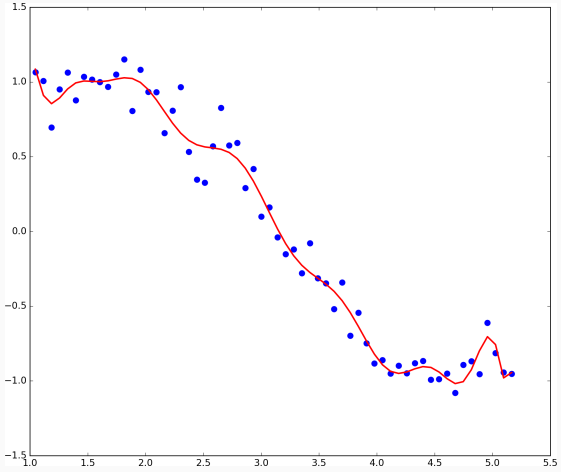
Lasso regression (L1)

Lasso regression is a linear regression with a Lasso regularization:

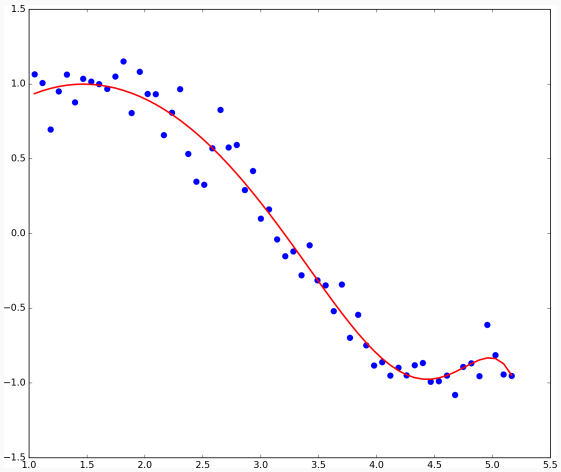
$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum(y_i - h_{\boldsymbol{\theta}}(x_i))^2 + \alpha\sum_{i=0}^{p}|\theta_i|$$

Results for $p = 15$ and varying α

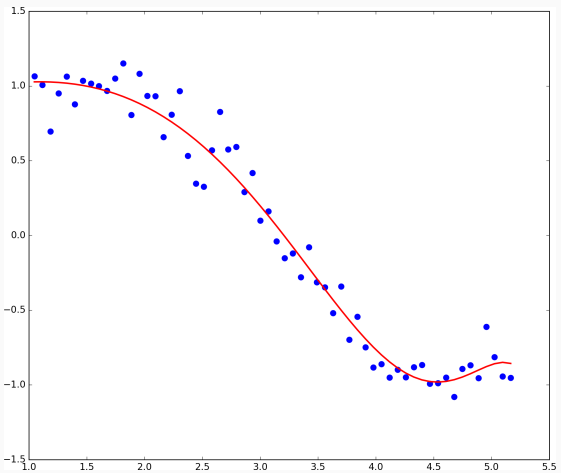
$\alpha = 0$



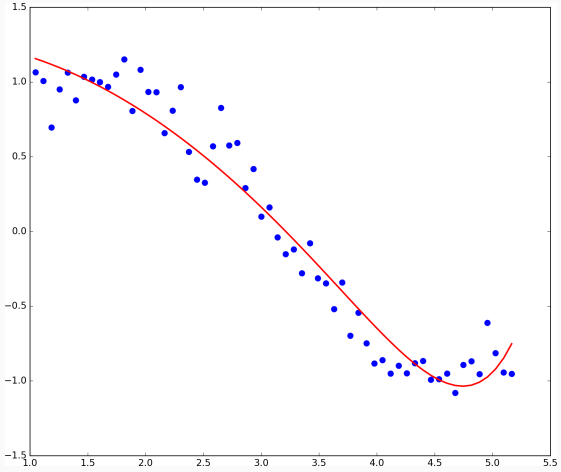
$\alpha = 1e-15$



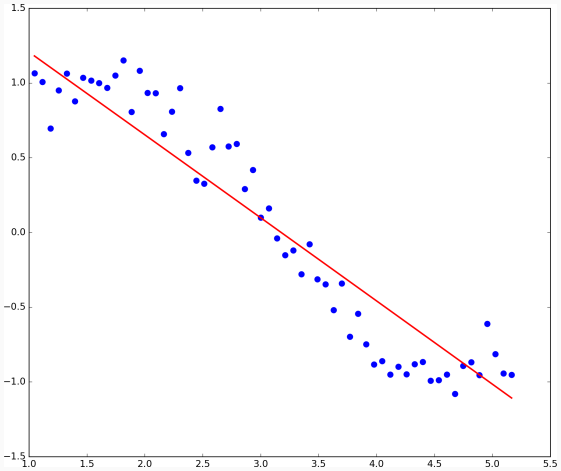
$\alpha = 1e-4$



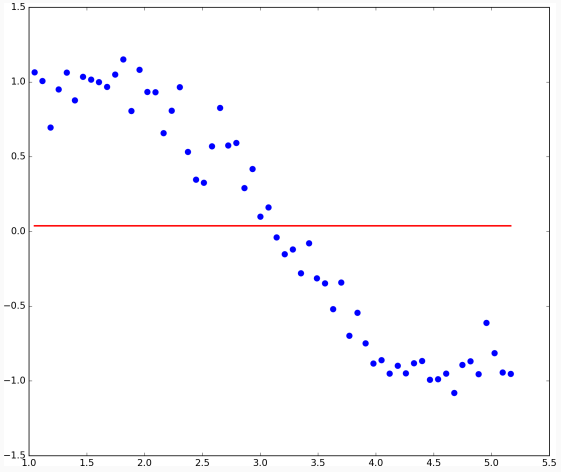
$\alpha = 1e-3$



$\alpha = 1e-2$

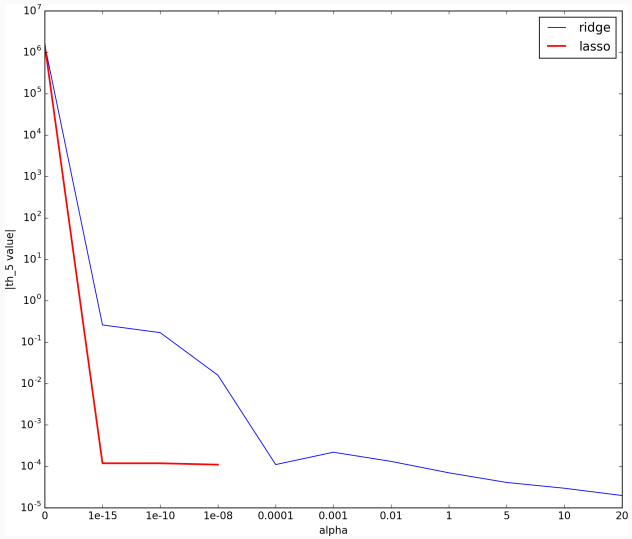


$\alpha = 5$



Values of coefficients

	rmse	th_0	th_1	th_2	th_3	th_4	th_5	th_6	th_7	th_8
alpha_0	+1.17e-02	-3.62e+04	+2.44e+05	-7.46e+05	+1.38e+06	-1.71e+06	+1.53e+06	-1.00e+06	+4.98e+05	-1.88e+05
alpha_1e-15	+1.59e-02	+2.22e-01	+1.06e+00	-3.69e-01	+8.85e-04	+1.63e-03	-1.19e-04	-6.44e-05	-6.28e-06	+1.45e-06
alpha_1e-10	+1.59e-02	+2.22e-01	+1.06e+00	-3.69e-01	+8.84e-04	+1.63e-03	-1.18e-04	-6.44e-05	-6.28e-06	+1.45e-06
alpha_1e-08	+1.59e-02	+2.22e-01	+1.06e+00	-3.69e-01	+7.69e-04	+1.62e-03	-1.10e-04	-6.45e-05	-6.32e-06	+1.43e-06
alpha_0.0001	+1.72e-02	+9.03e-01	+1.71e-01	-0.00e+00	-4.78e-02	-0.00e+00	-0.00e+00	+0.00e+00	+0.00e+00	+9.47e-06
alpha_0.001	+2.80e-02	+1.29e+00	-0.00e+00	-1.26e-01	-0.00e+00	-0.00e+00	-0.00e+00	+0.00e+00	+0.00e+00	+0.00e+00
alpha_0.01	+6.07e-02	+1.76e+00	-5.52e-01	-5.62e-04	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_1	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_5	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_10	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00
alpha_20	+6.16e-01	+3.80e-02	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00	-0.00e+00



Value of θ_5

Determination of the parameters in the lasso regression

Considering the cost function J:

$$J(\boldsymbol{\theta}) = J_{lms}(\boldsymbol{\theta}) + \alpha \sum_{i=0}^{p} |\theta_i|$$

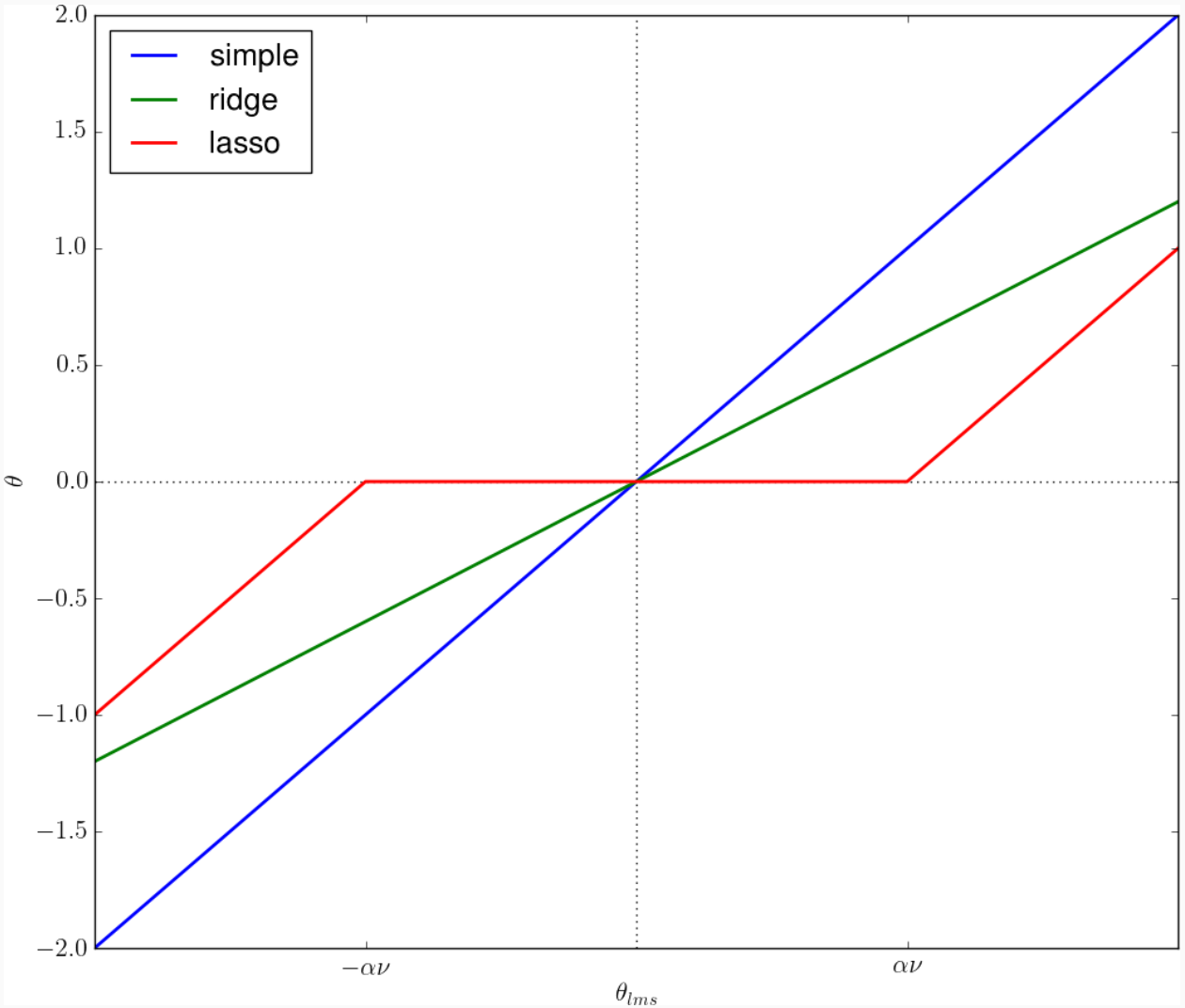
In a gradient algorithm, update of the parameters would be:

J is not differentiable. If we consider $\theta_{lms} = \theta_i^k - \nu . \frac{\partial J_{lms}}{D\theta_i}$

The update rule is:

- $\theta_i^{k+1} = \theta_{lms} + \alpha\nu$ if $\theta_{lms} < -\alpha\nu$
- $\theta_i^k = 0$ if $-\alpha\nu < \theta_{lms} < \alpha\nu$
- $\theta_i^{k+1} = \theta_{lms} - \alpha\nu$ if $\theta_{lms} > \alpha\nu$

Summary of parameters updates



Comparison Ridge/Lasso

Ridge (L2)

- Prevents the overfitting
- includes all the features (dimensions) of the predictor, so it can be useless for high-dimensional predictors

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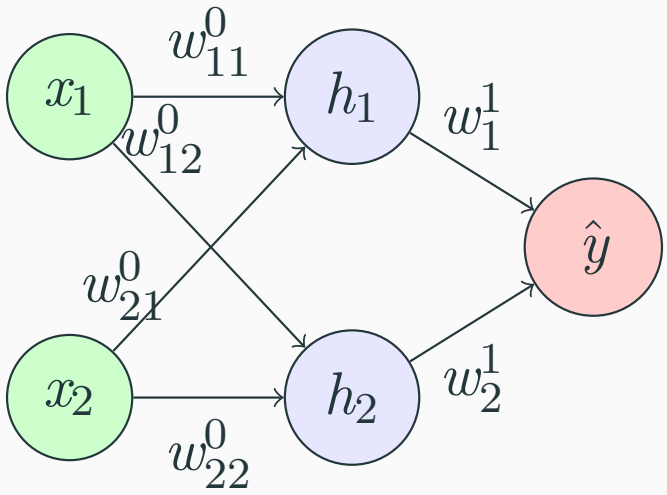
Lasso (L1)

- Provides sparse solutions and reduces the dimension of the predictor
- If some features in the predictor are correlated, arbitrarily select one from the others.

In a neural network

L2 (Ridge) and L1 (Lasso) regularization are widely used in Neural Network architectures.



- Non-regularized loss function: $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2$.
- L2-regularized loss function:
  $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2 + \alpha \sum_{i=0}^{p} |w_i|$.
- L1-regularized loss function:
  $L(\mathbf{w}) = ||\hat{y}(\mathbf{w}) - y||^2 + \alpha \sum_{i=0}^{p} w_i^2$.

Wrapping-up

Advantage

L1/L2 regularization prevents overfitting even for large architecture (a big weight vector to optimize)

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Advantage

L1/L2 regularization prevents overfitting even for large architecture (a big weight vector to optimize)

But...

It comes with an extra hyperparameter to tune (using, e.g., cross-validation): α

An example using scikit-learn

California House Pricing