Machine learning and physical modelling-1

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October 2019

NERSC

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

Overview of the next lectures

1. Lecture 1 (Thursday 14 Oct.): Generalities and principles of Machine Learning
2. Lecture 2 (Tuesday 19 Oct.): Machine learning process, neural networks, deep learning
3. Lecture 3 (Thursday 21 Oct.): How to train a machine learning algorithm?
4. Practical Work (Tuesday 26 Oct.): Emulate a dynamical model using machine learning

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References

Ian Goodfellow, Yoshua Bengio, and Aaron Courville.
Deep Learning.
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.

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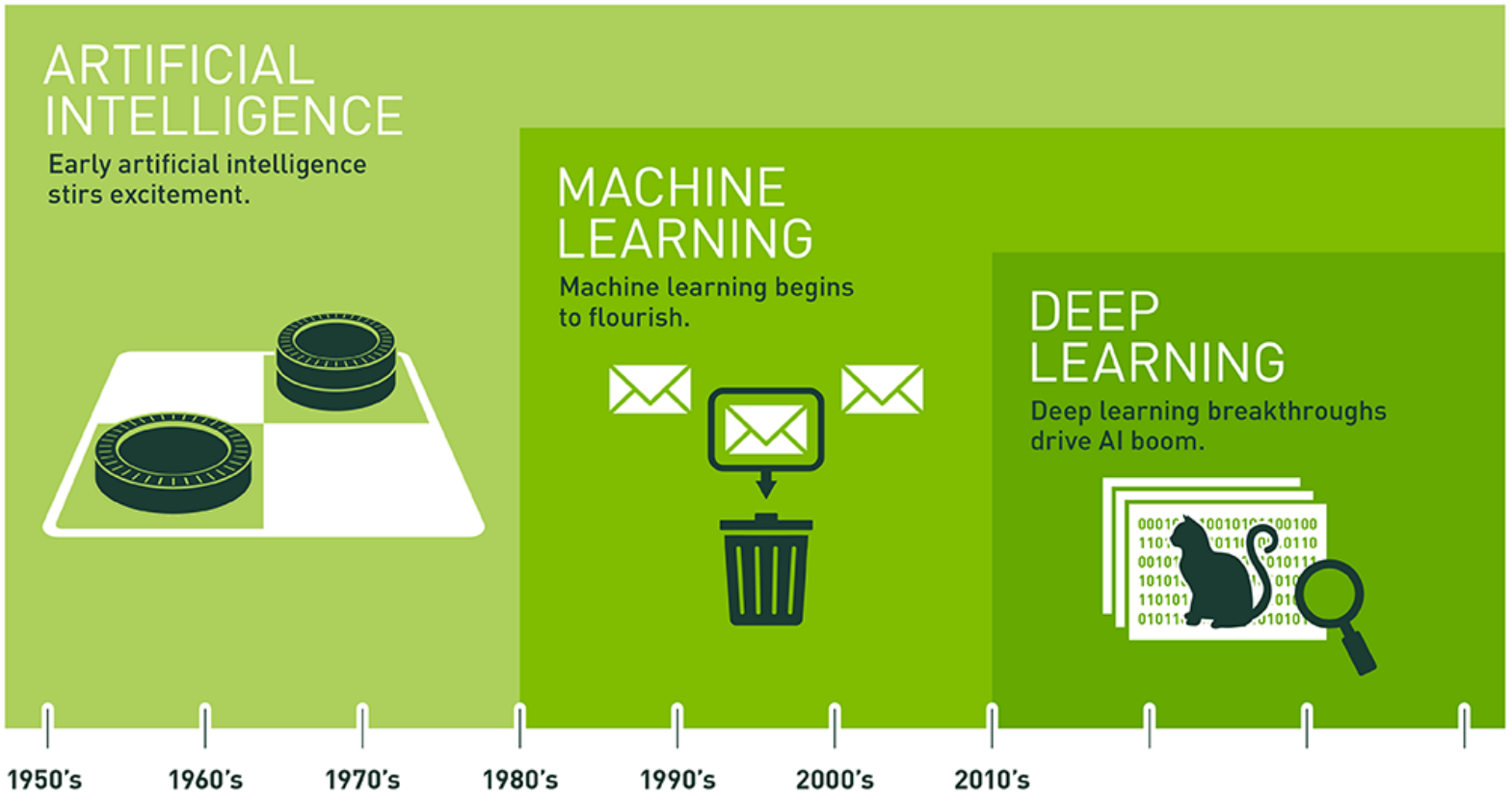
Introduction

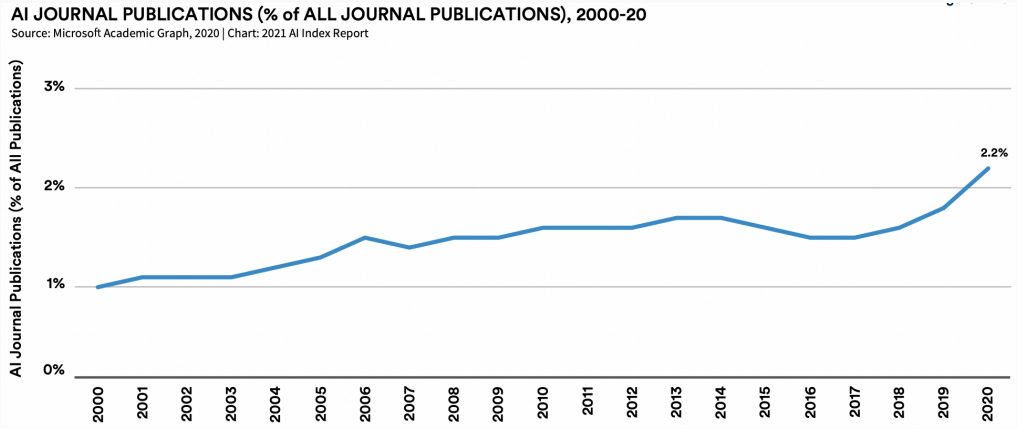
Scope of the lecture: Machine Learning

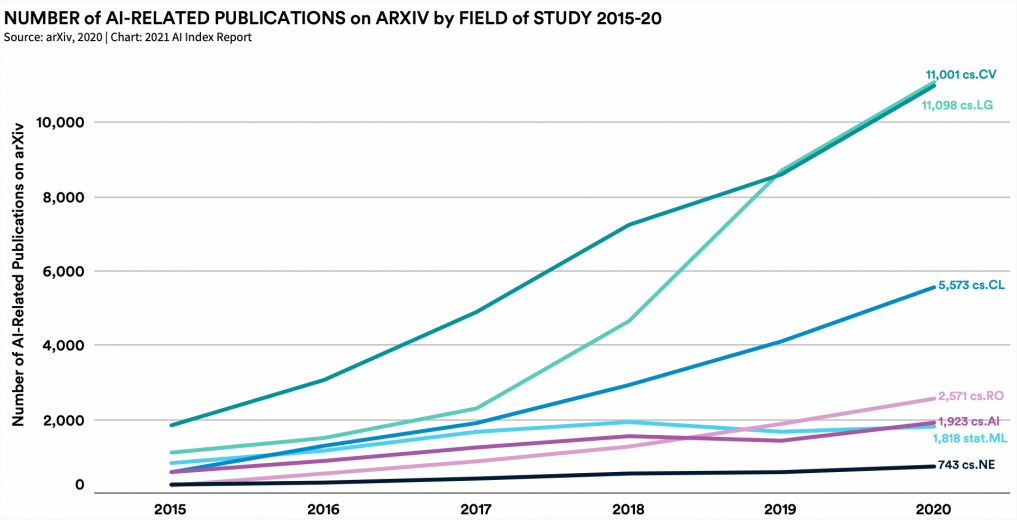


Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

Source: NVidia

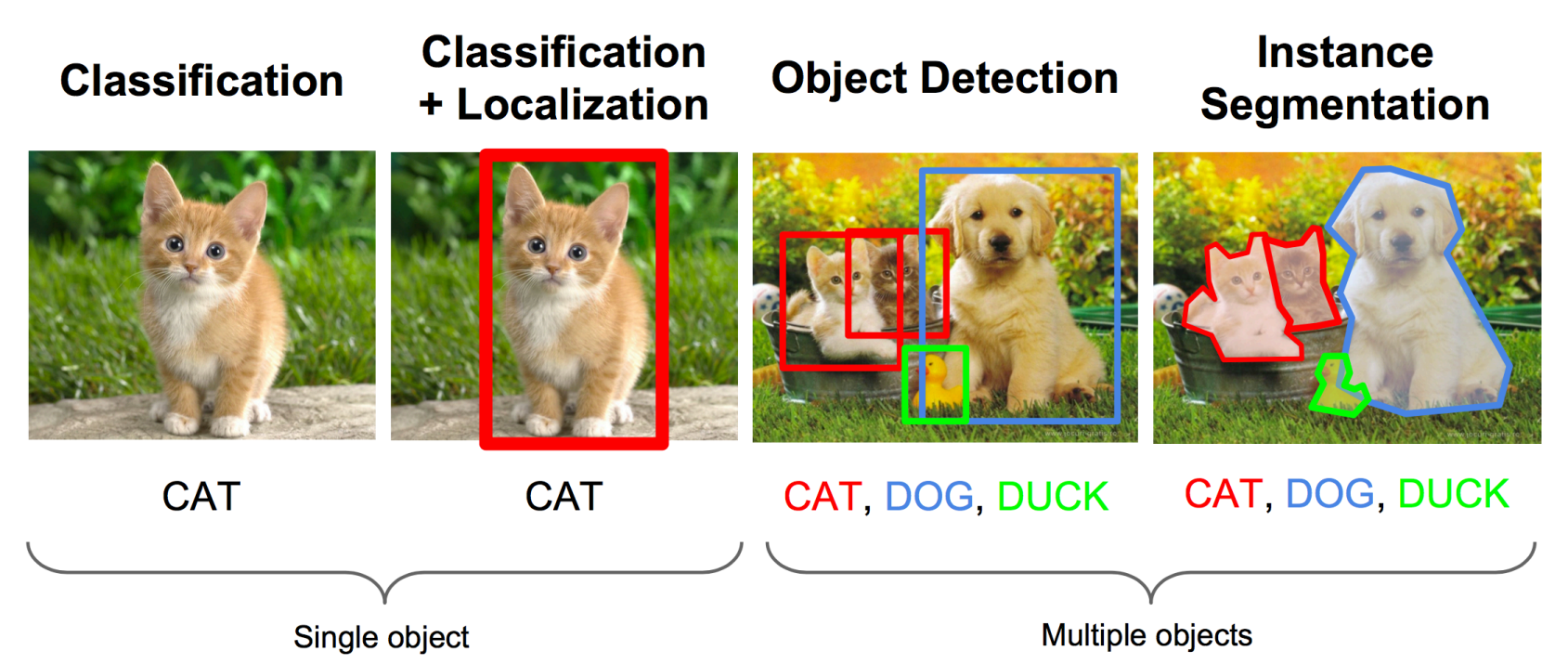
A (very) active field





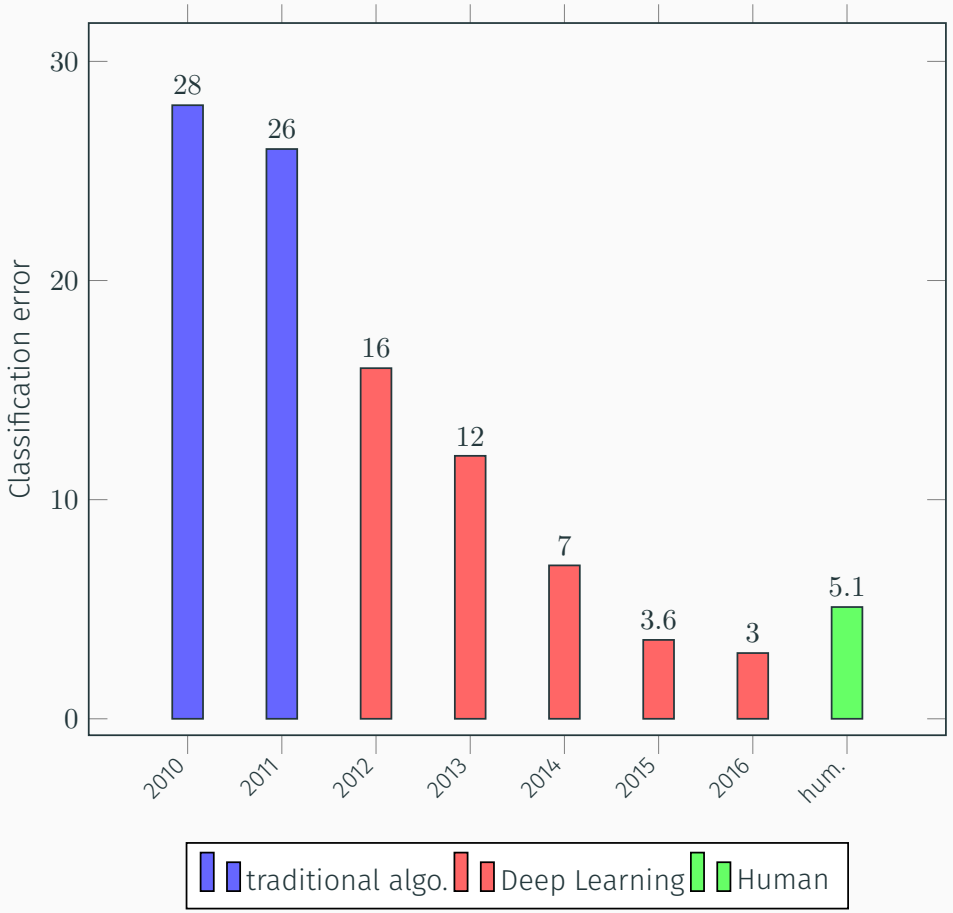
Zhang et al., "The AI Index 2021 Annual Report"

Example 1: Computer Vision



Li, Karpathy and Johnson, 2016, Stanford CS231n course

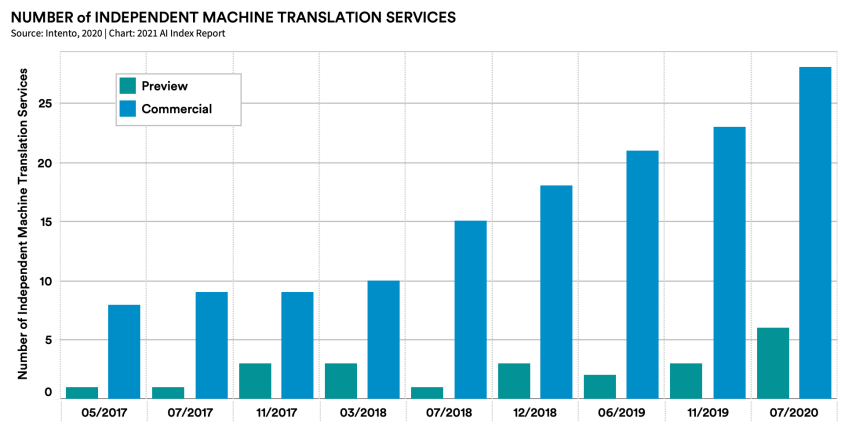
Example 1: Computer Vision



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

Example 2: Machine Translation

Objective : translate a text from a language to another.



Zhang et al., "The AI Index 2021 Annual Report"

- **Oct. 2013**: Pionneering scientic paper (Kalchbrenner, N., and Blunsom, P).
- **2016**: Neural machine translation outperform traditional approaches on public benchmarks
- **2017**: Major systems switch to neural machine translation (using deep recurrent neural networks)

Example 3: 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 4: Protein folding

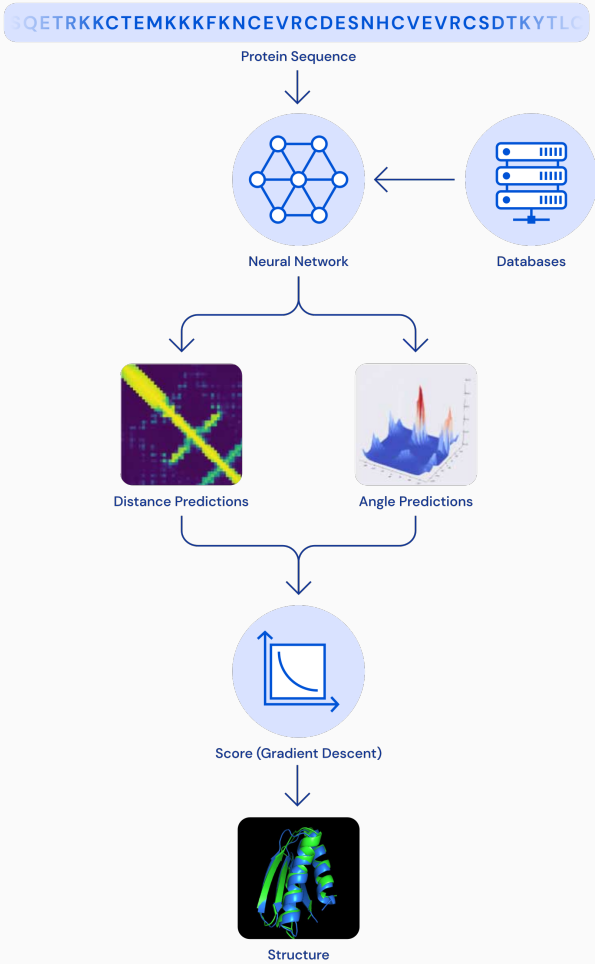


Diagram of Alpha Fold (source: Deepmind)

Senior et al. 2020

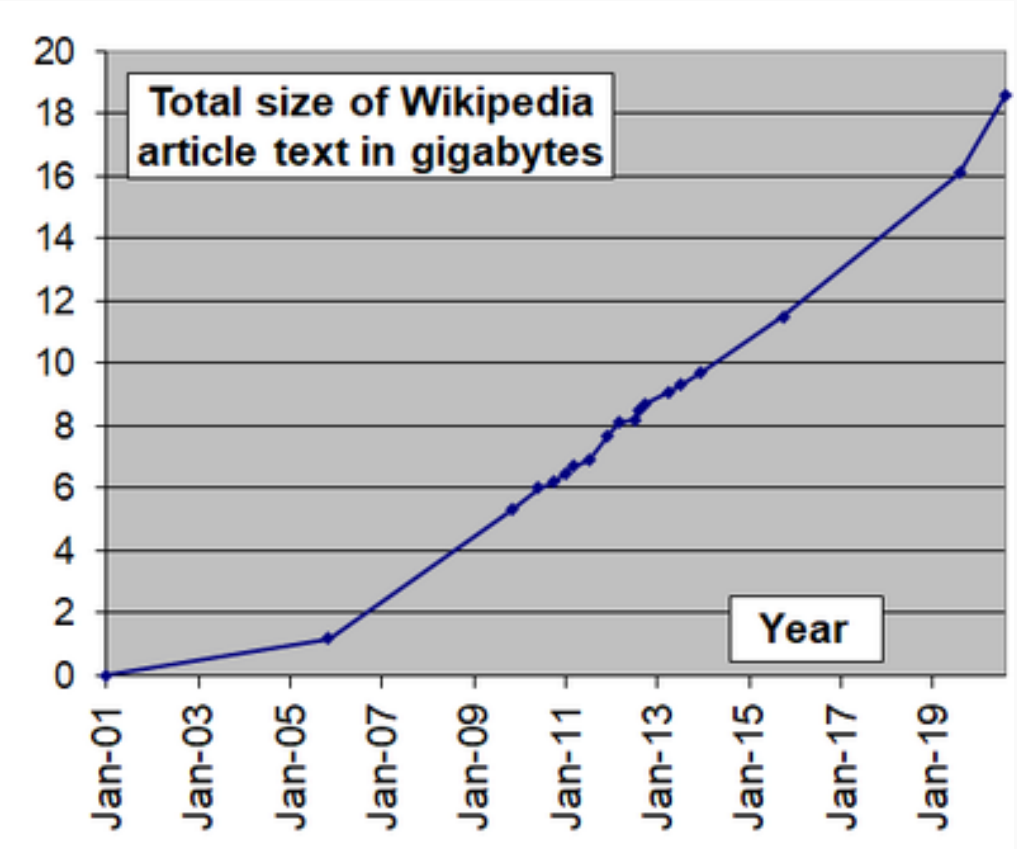
AI Art?

Edmond de Bellamy by Obvious(collective)

Generated using a Generative Adversarial Network.
Selling prince (Oct. 2018): $432,000

Reasons for these recent achievements?

- Increasing of the datasets in size and quality



source: Wikipedia

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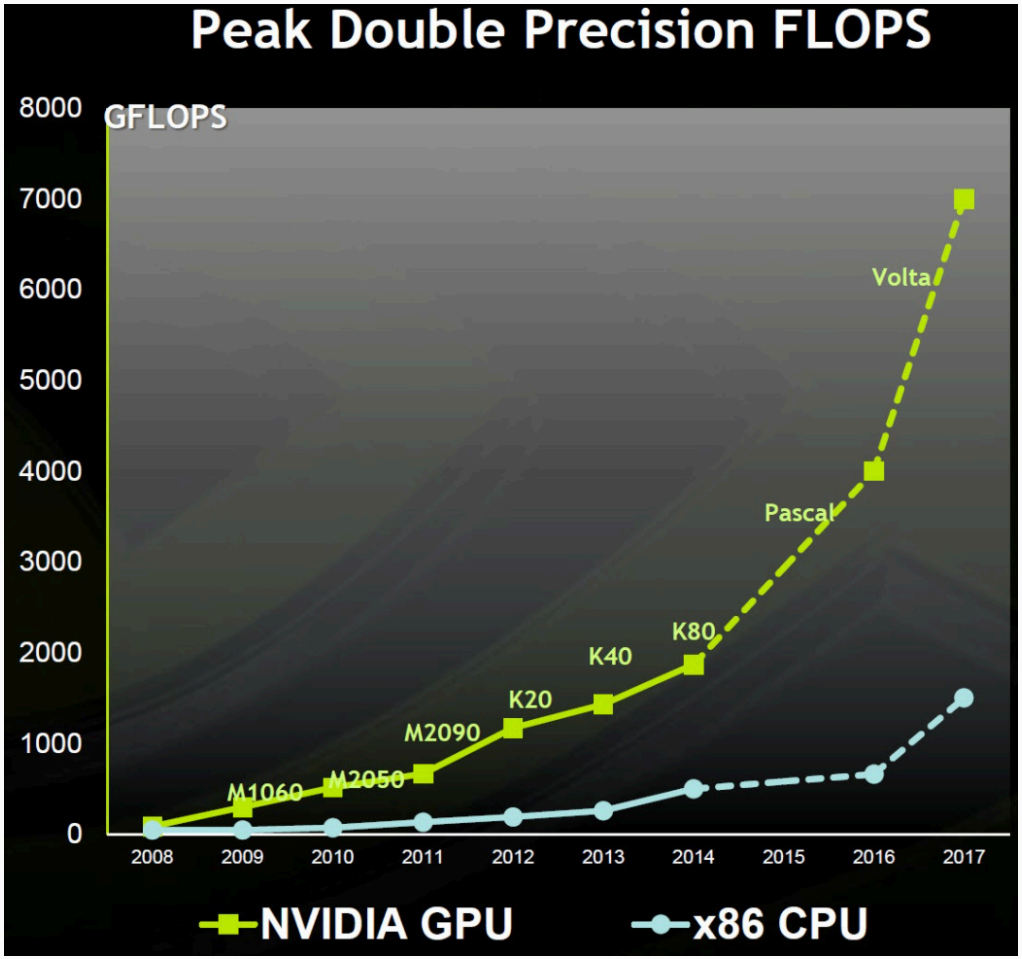

source: NVDIA

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source: Deep Dream Generator

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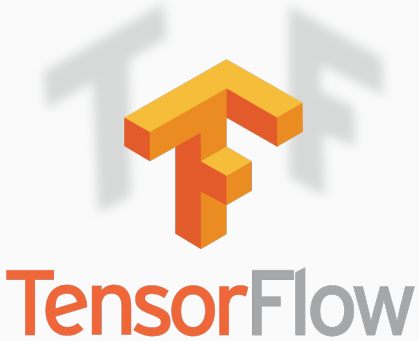
- Very efficient software (GPU, cloud computing, automatic differentiation, ...)



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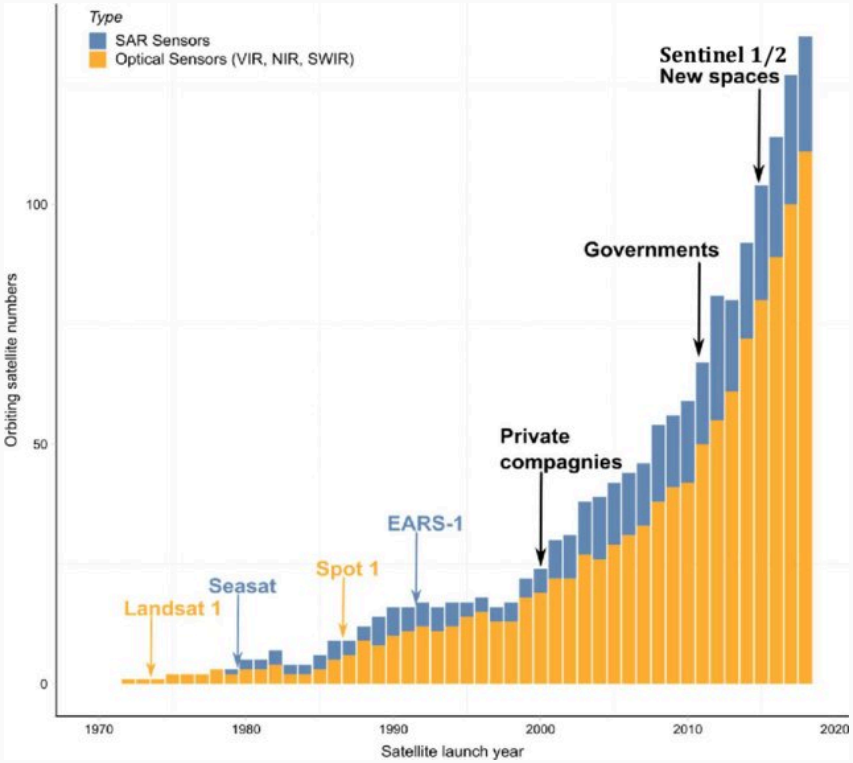
- Very efficient software (GPU, cloud computing, automatic differentiation, ...)
- Free software and open data culture.

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?

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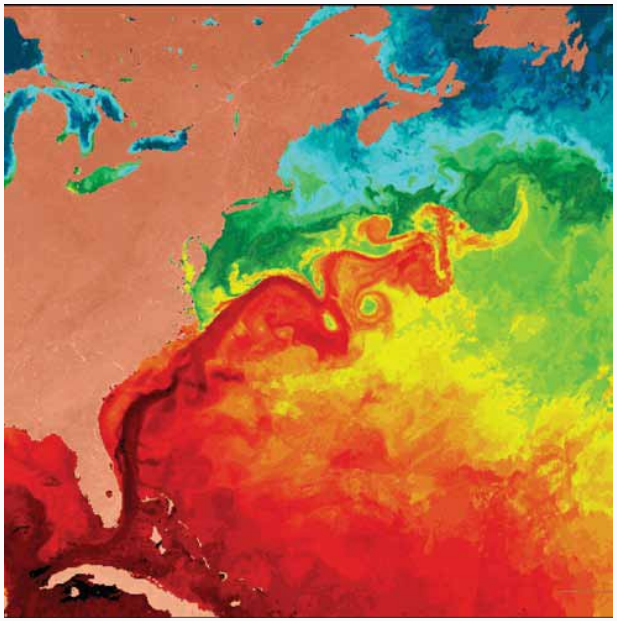
- A increasing number of geophysical data (one spatial mission: 24 TB/day)
- Data with highly significant spatial patterns



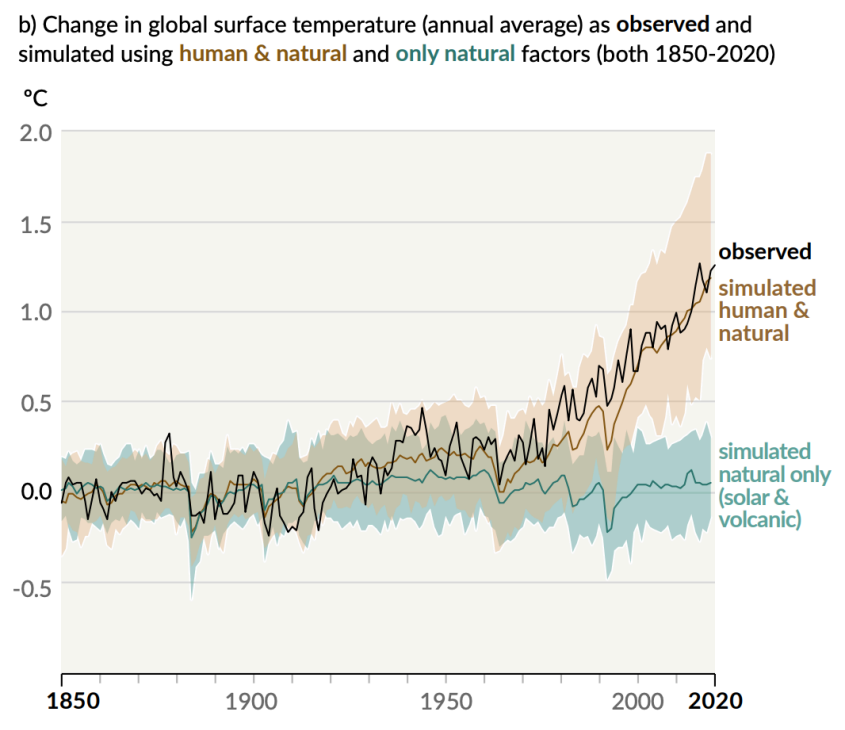
Sea Surface temperature of the gulf stream

source: Talley (2000)

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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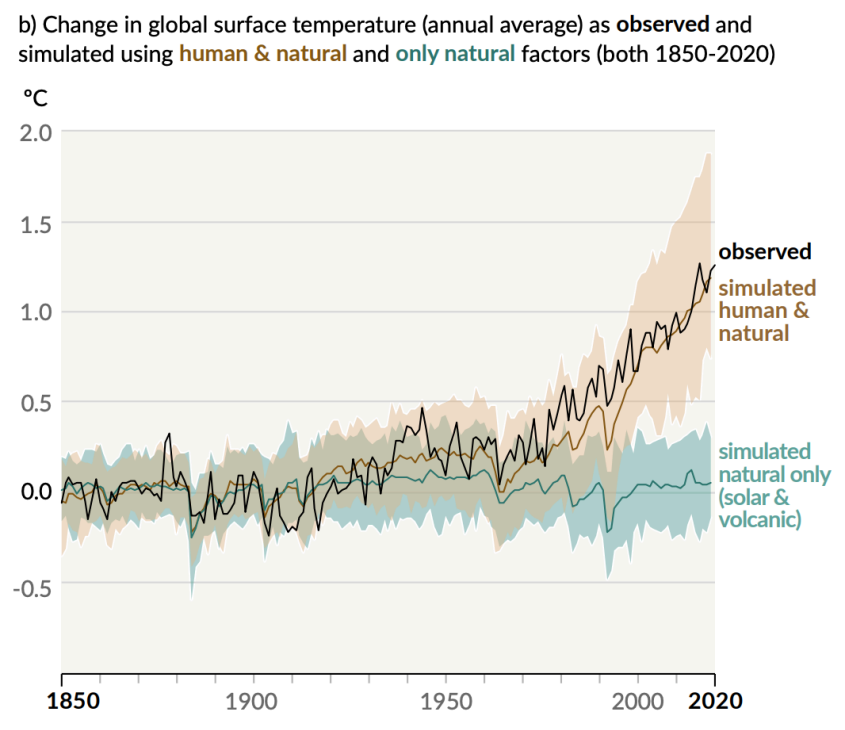

Mostly known dynamical processes (based on physical principles)

What about data assimilation?

Machine learning and data assimilation are closely linked.

Some references:

- Geer, A.J., 2021. Learning earth system models from observations: machine learning or data assimilation?. *Philosophical Transactions of the Royal Society A*, 379(2194)
- Brajard et al. 2019. Connections between data assimilation and machine learning to emulate a numerical model. *Proceedings of the 9th International Workshop on Climate informatics*
- Bocquet et al. 2019. Data assimilation as a learning tool to infer ordinary differential equation representations of dynamical models. *Nonlinear processes in geophysics.* 26(3).
- 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

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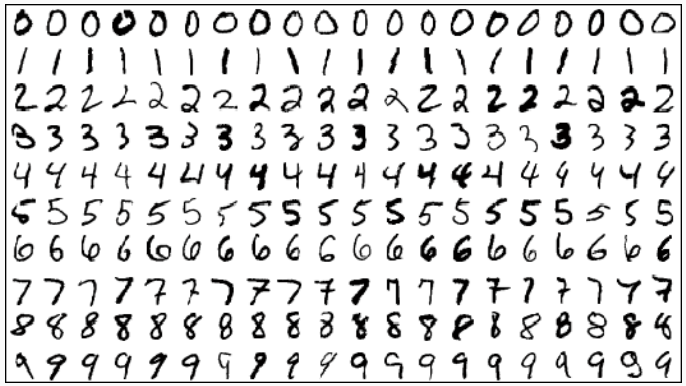

Base of images

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

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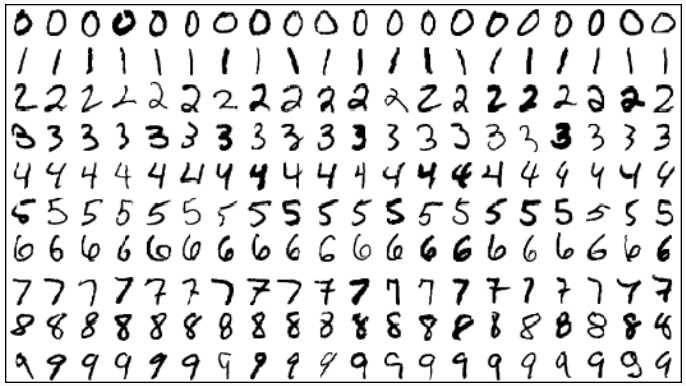

Base of images

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

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

Two classes of Machine 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
    - ...

Two classes of Machine Learning problems

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   - The price of a building from various predictors (Surface, ...)
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   - ...
2. Classification: Determination of a class
   - A digit from a image
   - Identification of the content of an image
   - ...

Two types of objectives

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    - Playing a chess game.

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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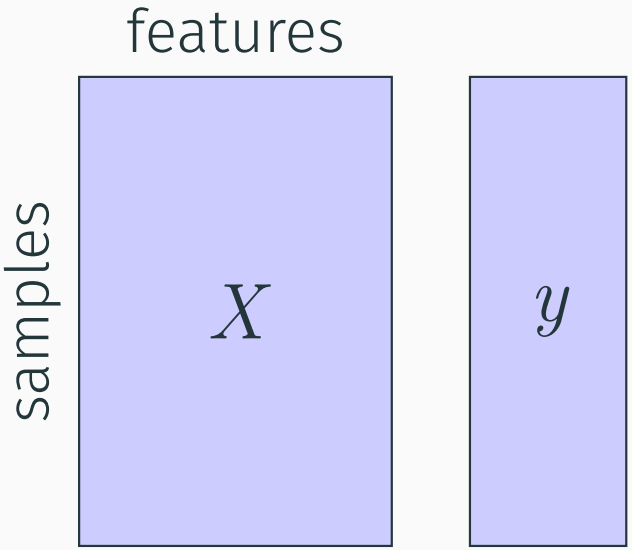
- A learning process
  - Estimation of θ

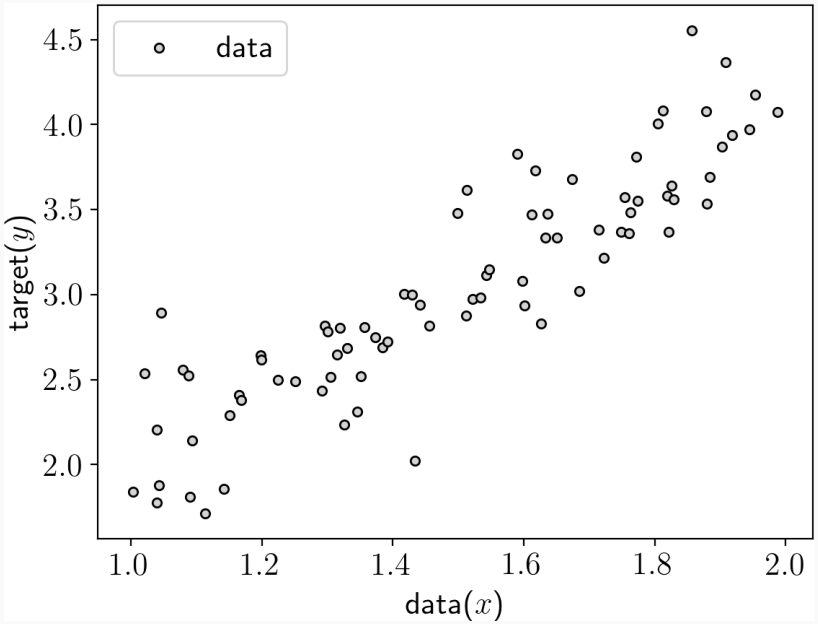
Multidimensional data

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



An illustration

- Some Data



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An illustration

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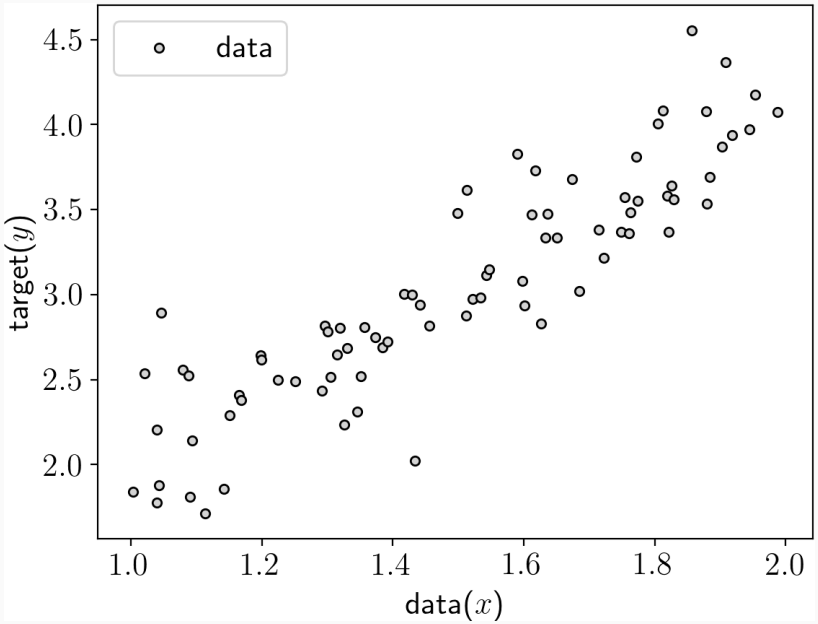

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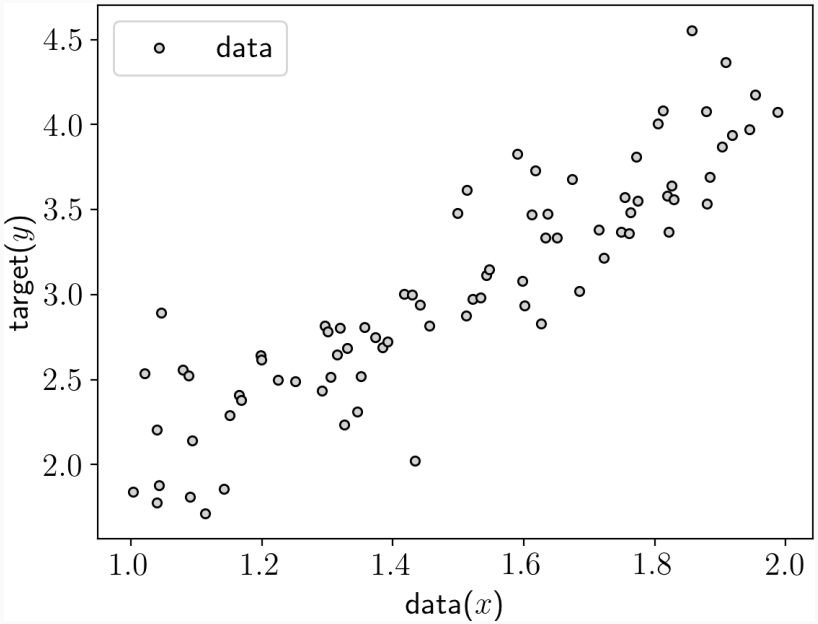

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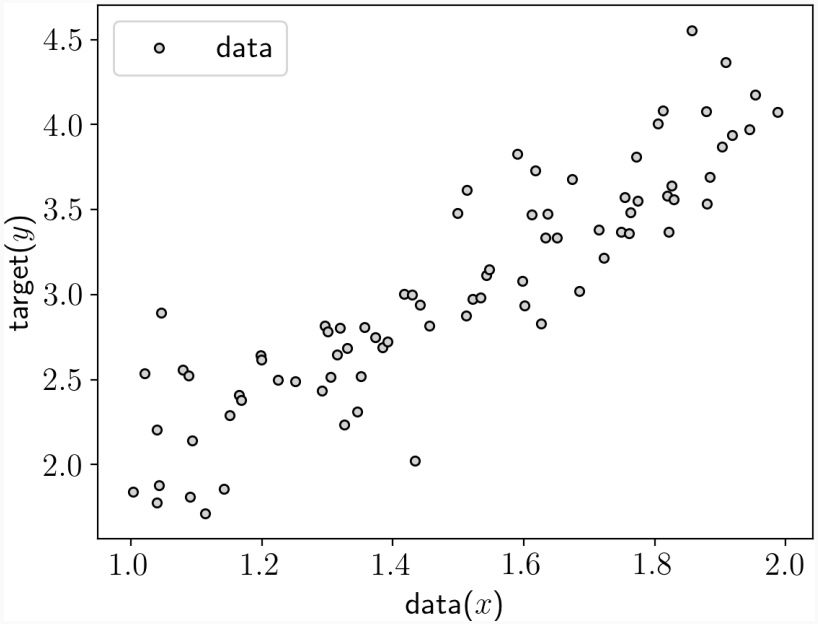

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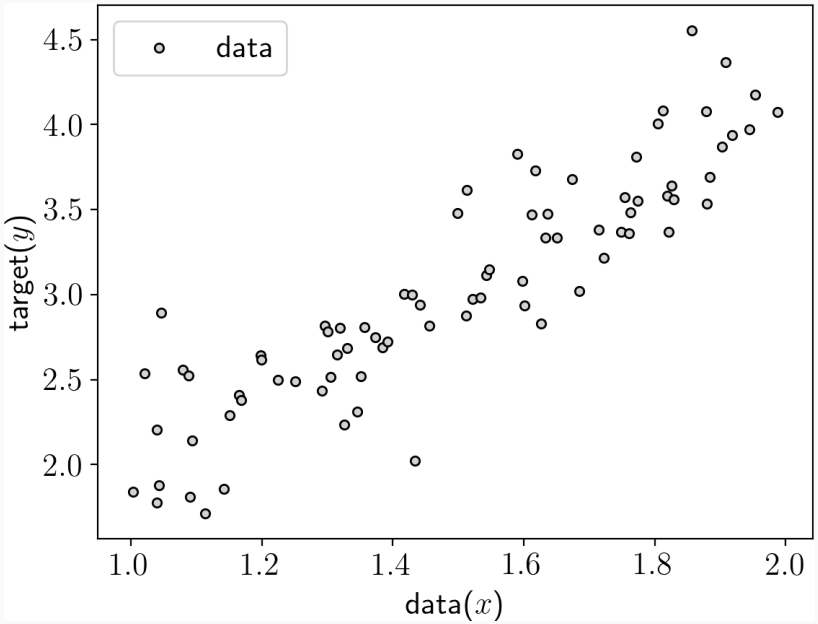

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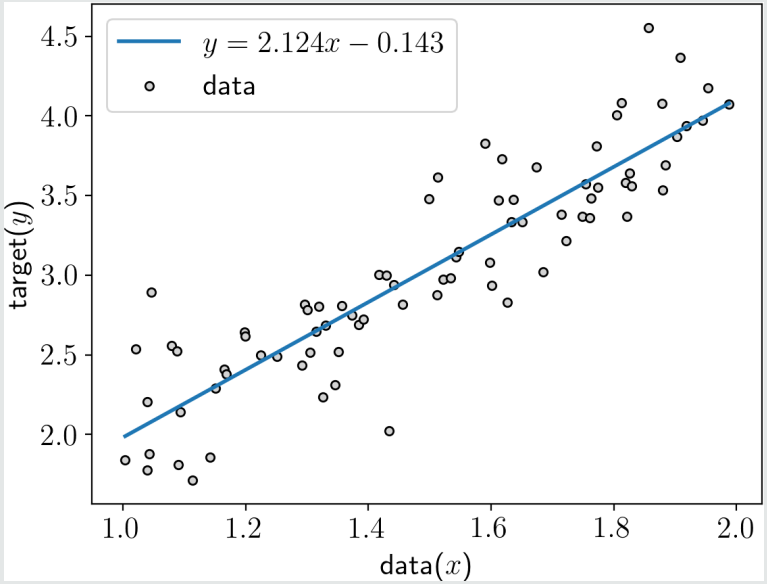
Result



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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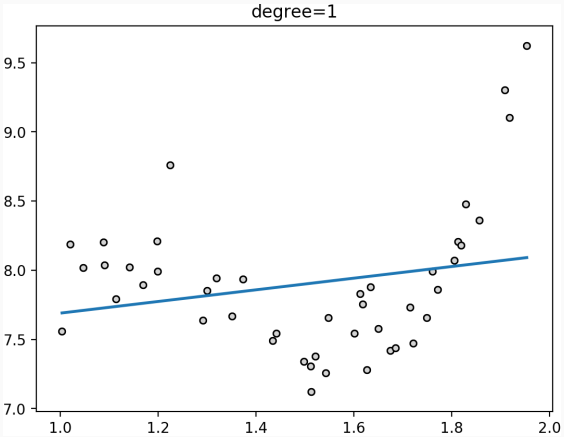

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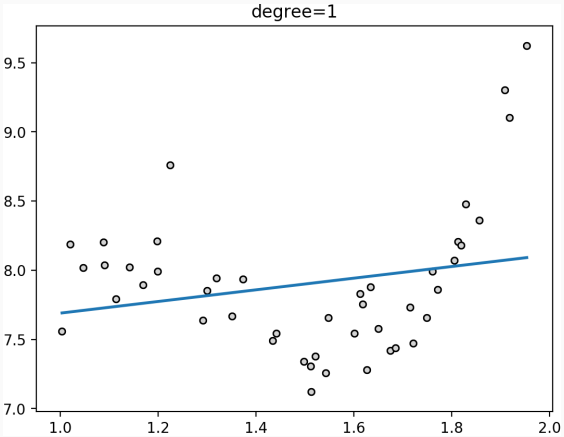
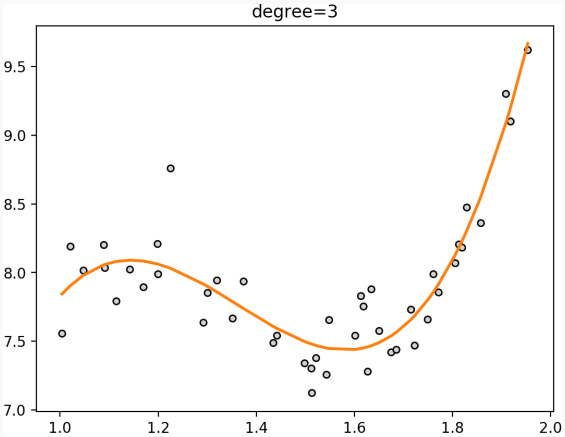


degree = 3



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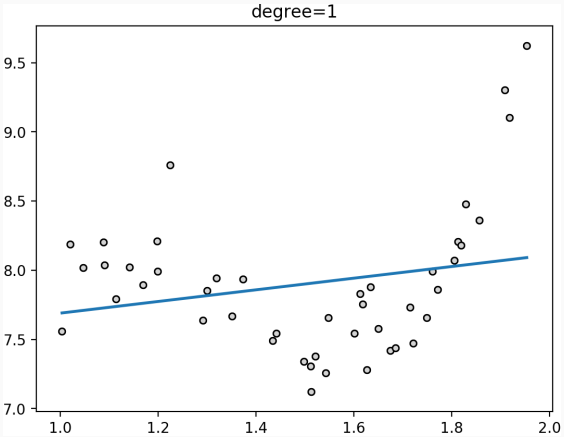

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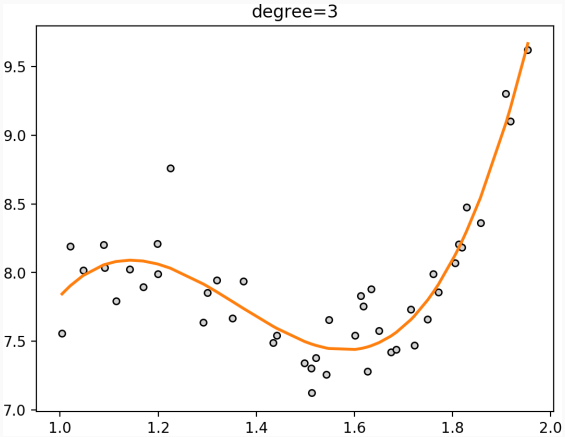
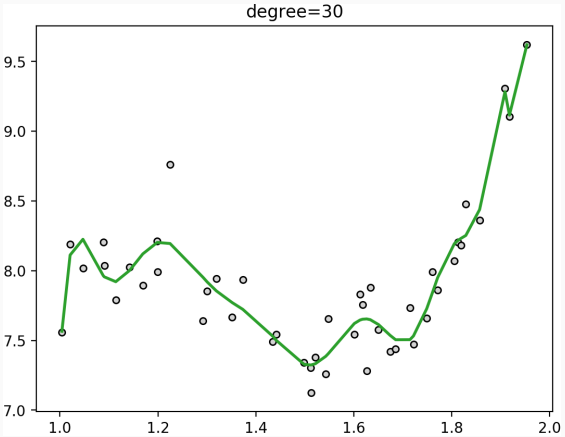


degree = 30



What is the best model?

Train/Validation split

The idea

Evaluate a score on a independent dataset

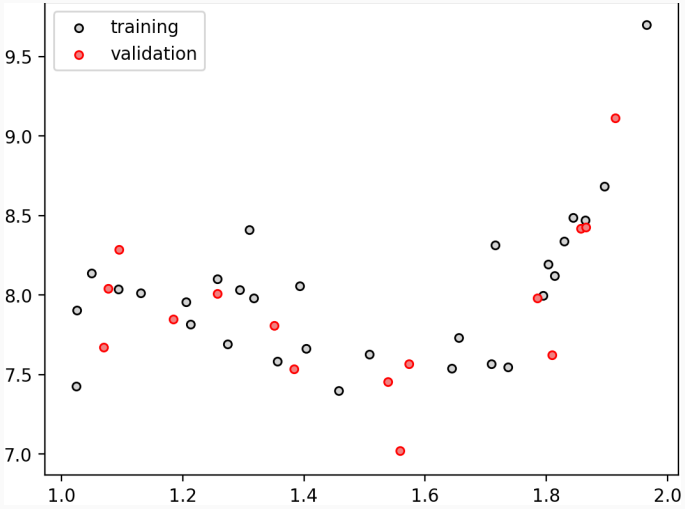
Train/Validation split

The idea

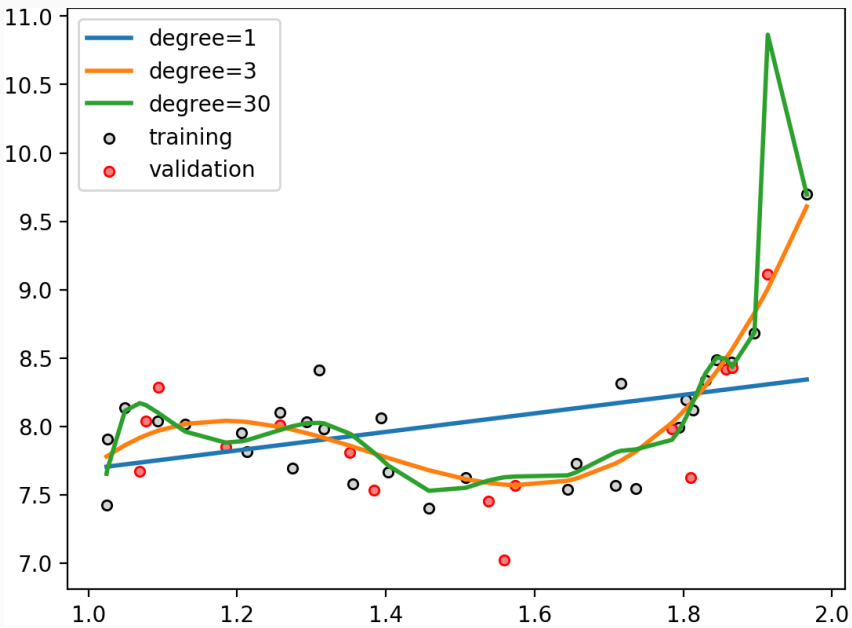
Evaluate a score on a independent dataset

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)



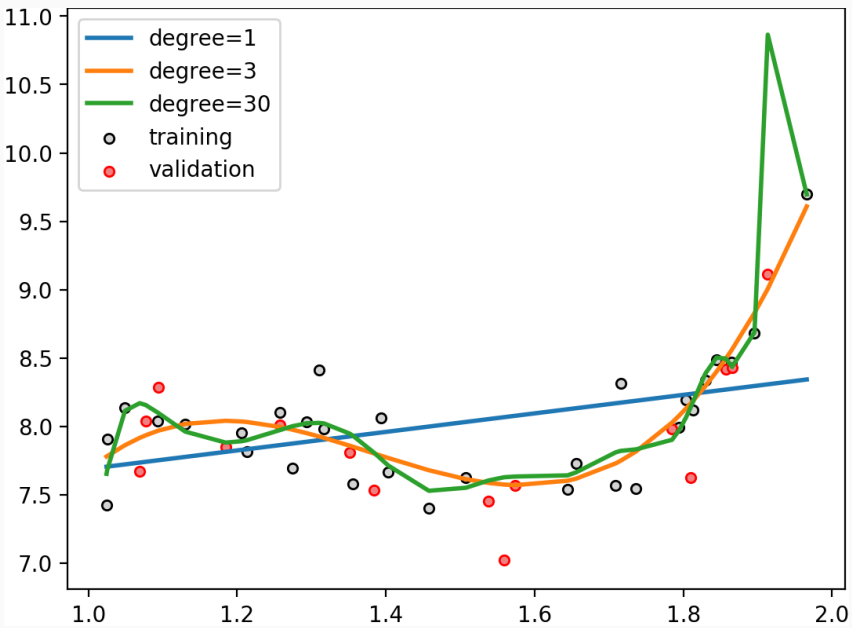
Choice of the model



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

Choice of the model



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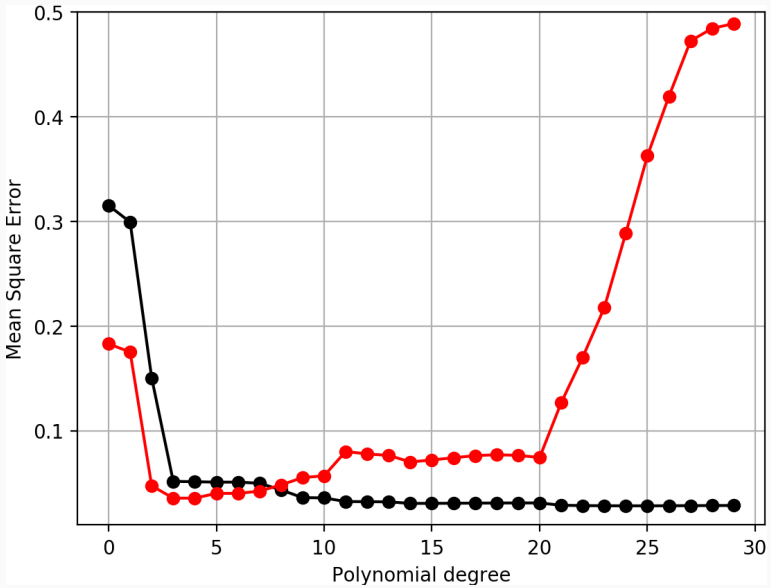
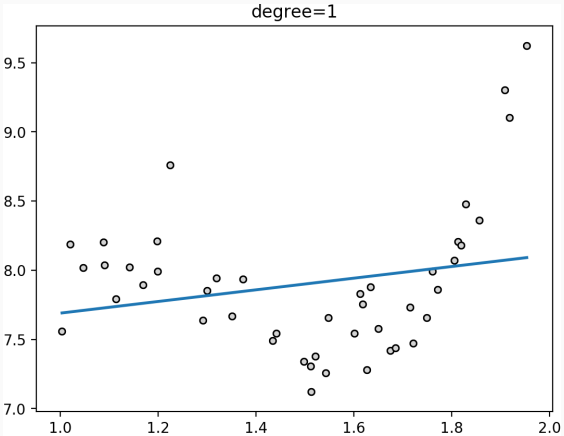


Choice of the model

Polynomial regression

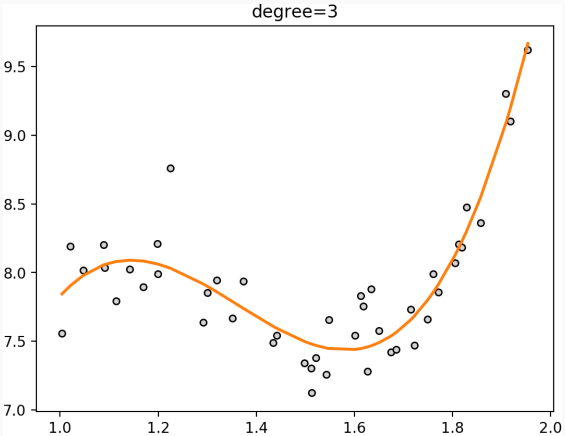
$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d = \sum_{i=0}^{d} \theta_i X^i$$

degree = 1 (linear)



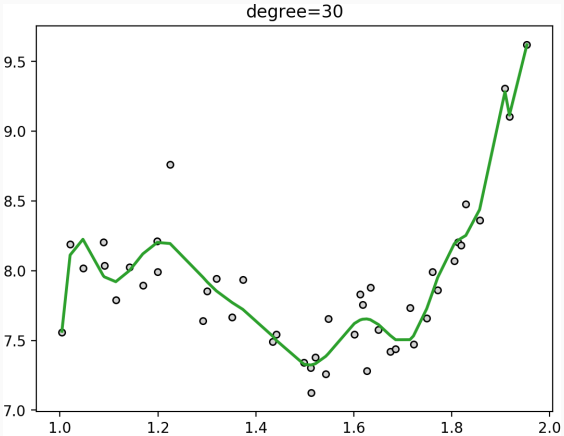
underfitting

degree = 3



good fit

degree = 30



overfitting

Train/Validation split

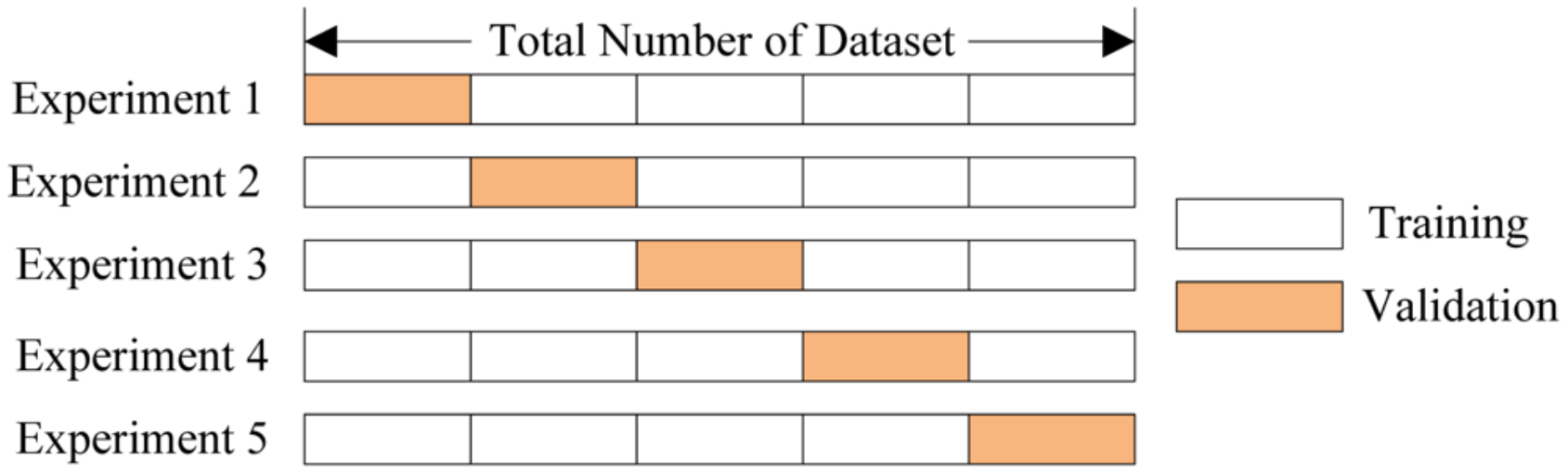
Drawbacks

- drastically reduce the number of samples which 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

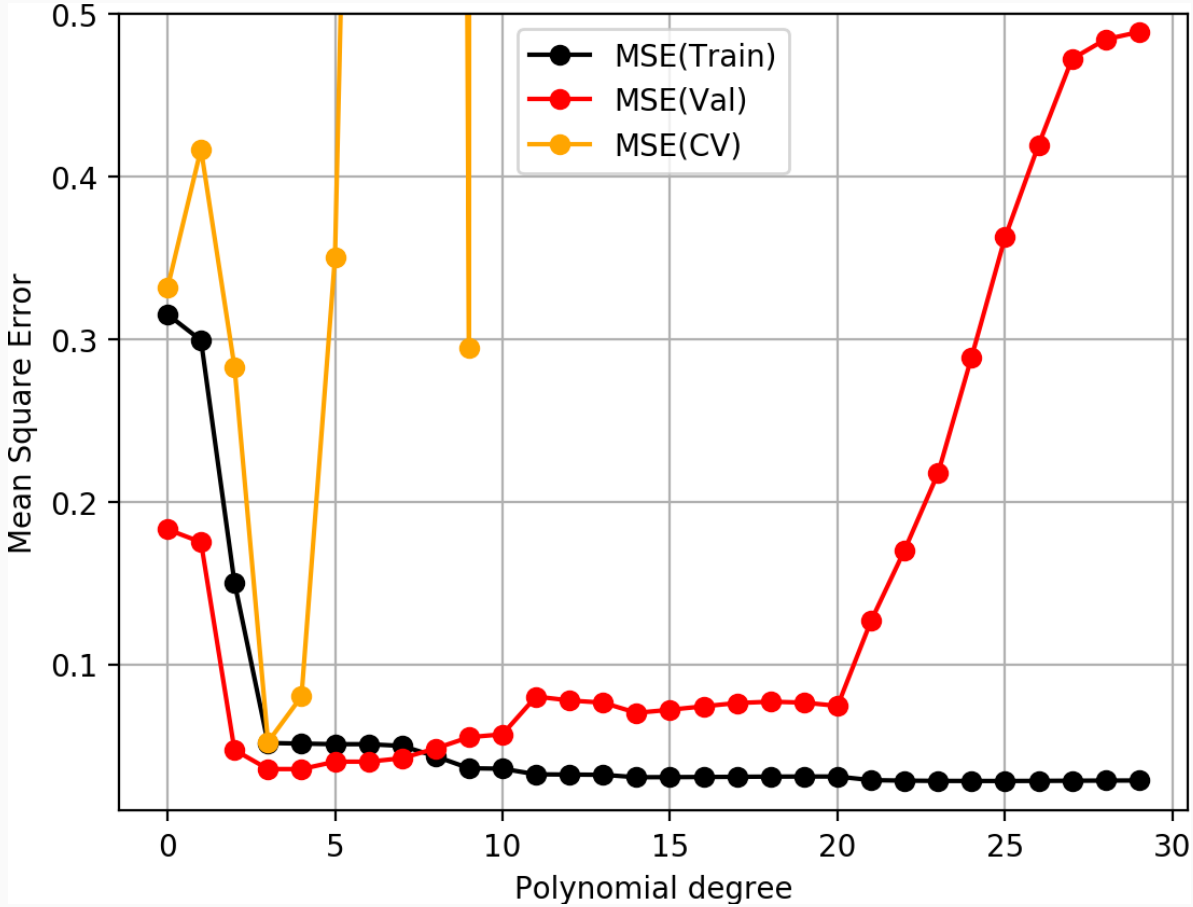
The idea

- 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

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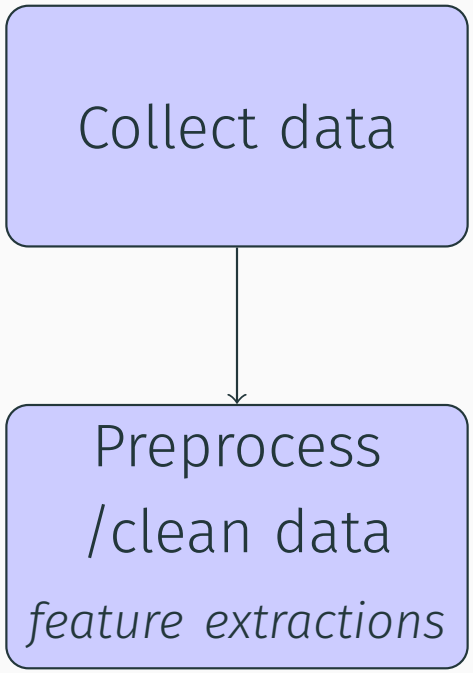
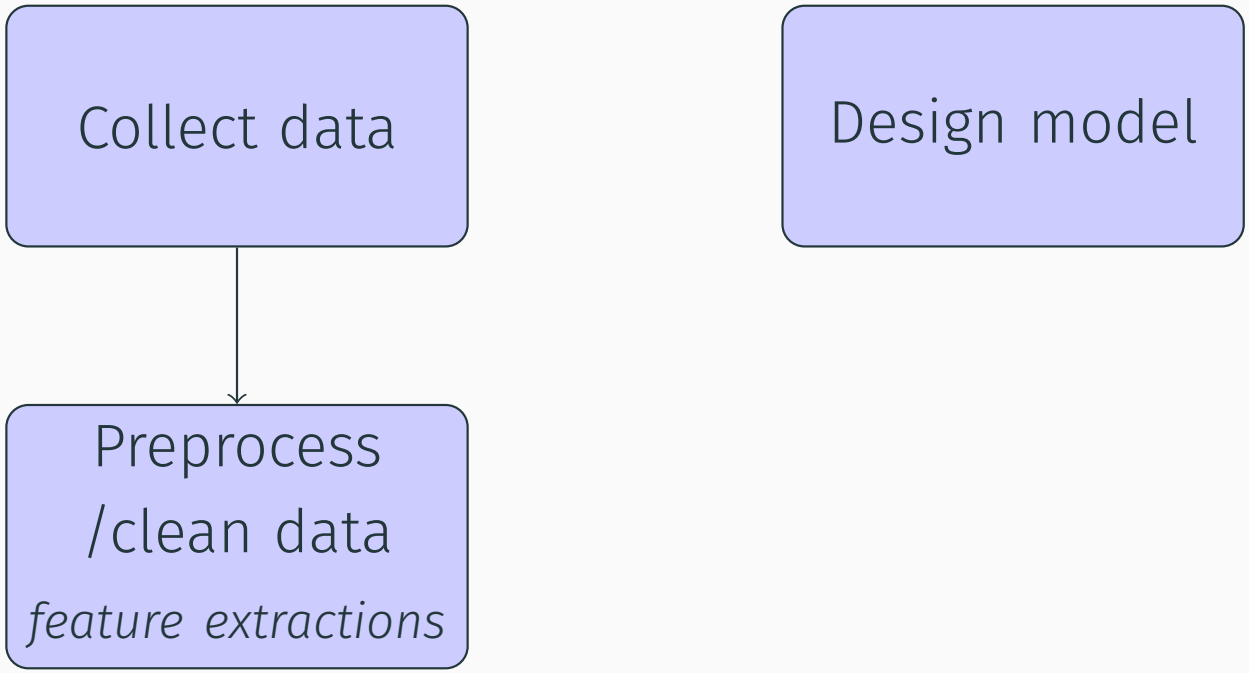
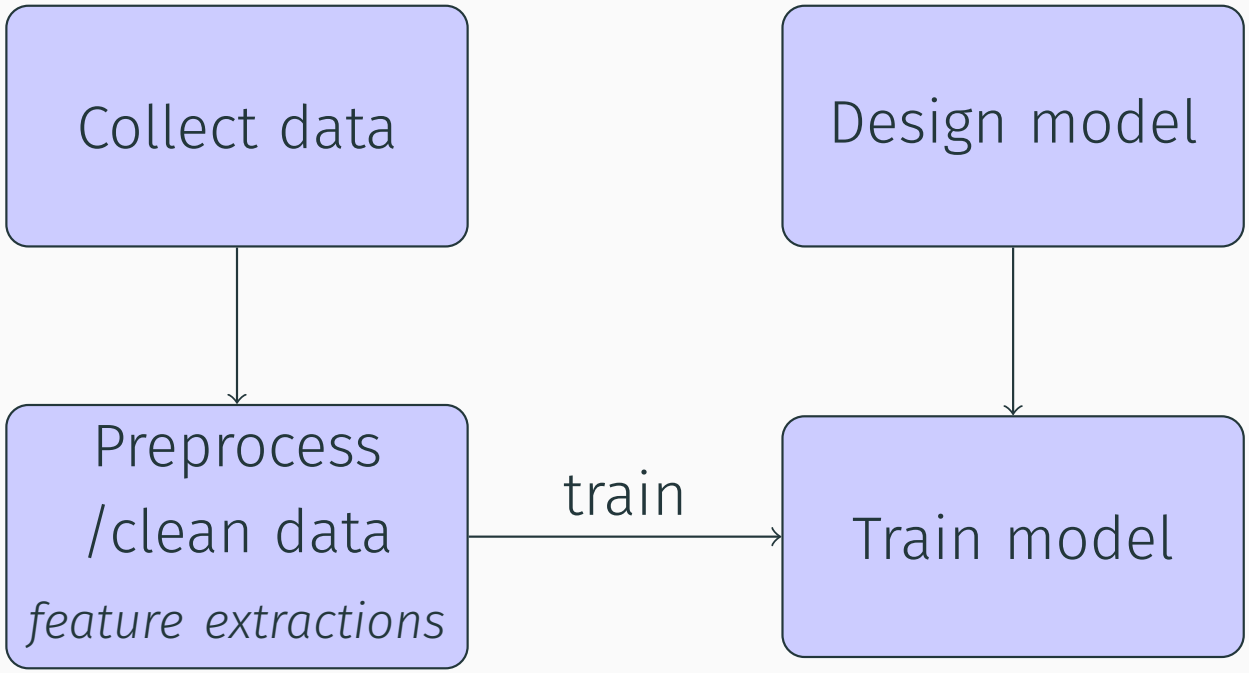


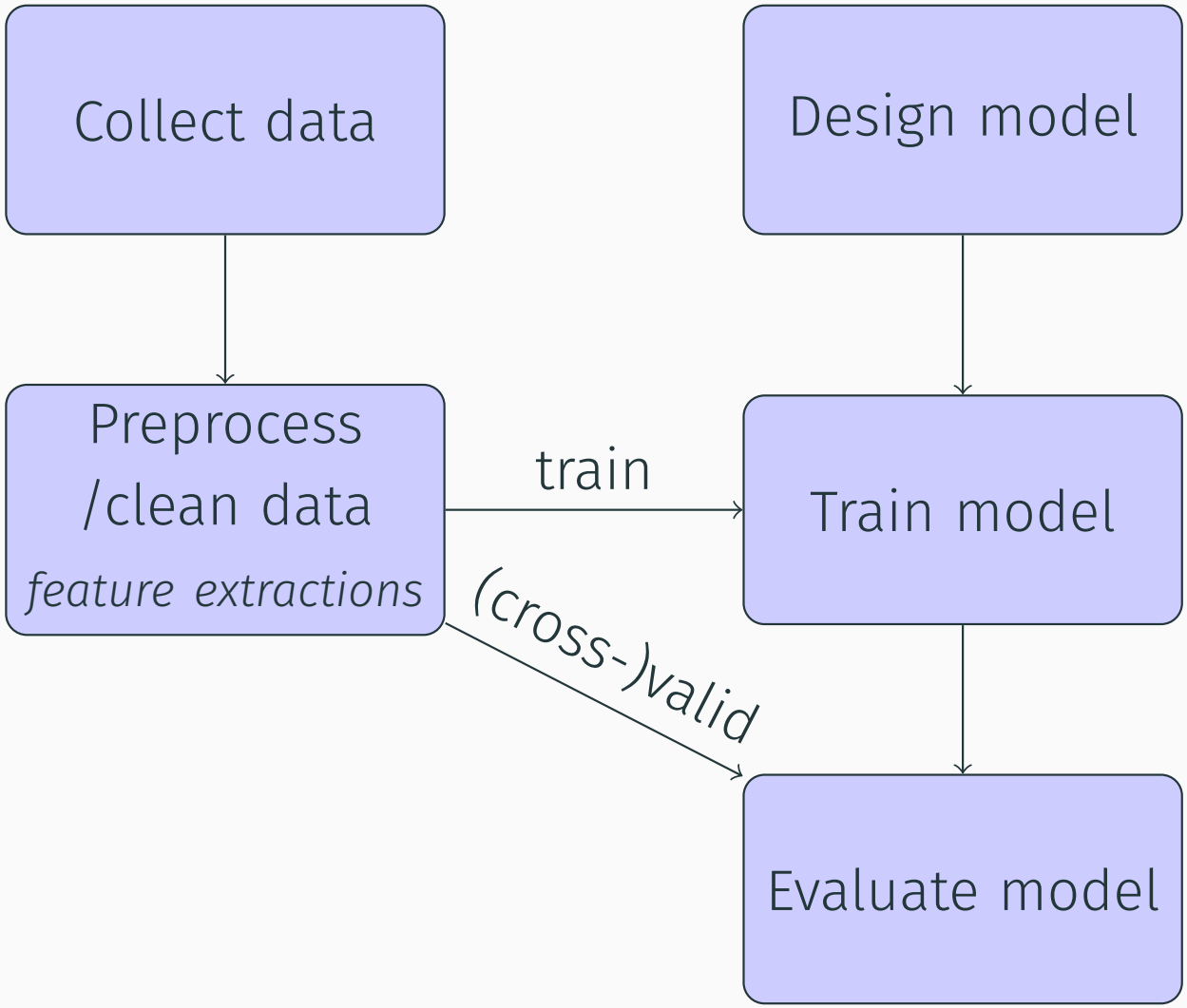
Steps


Collect data
Preprocess
/clean data
feature extractions
Design model

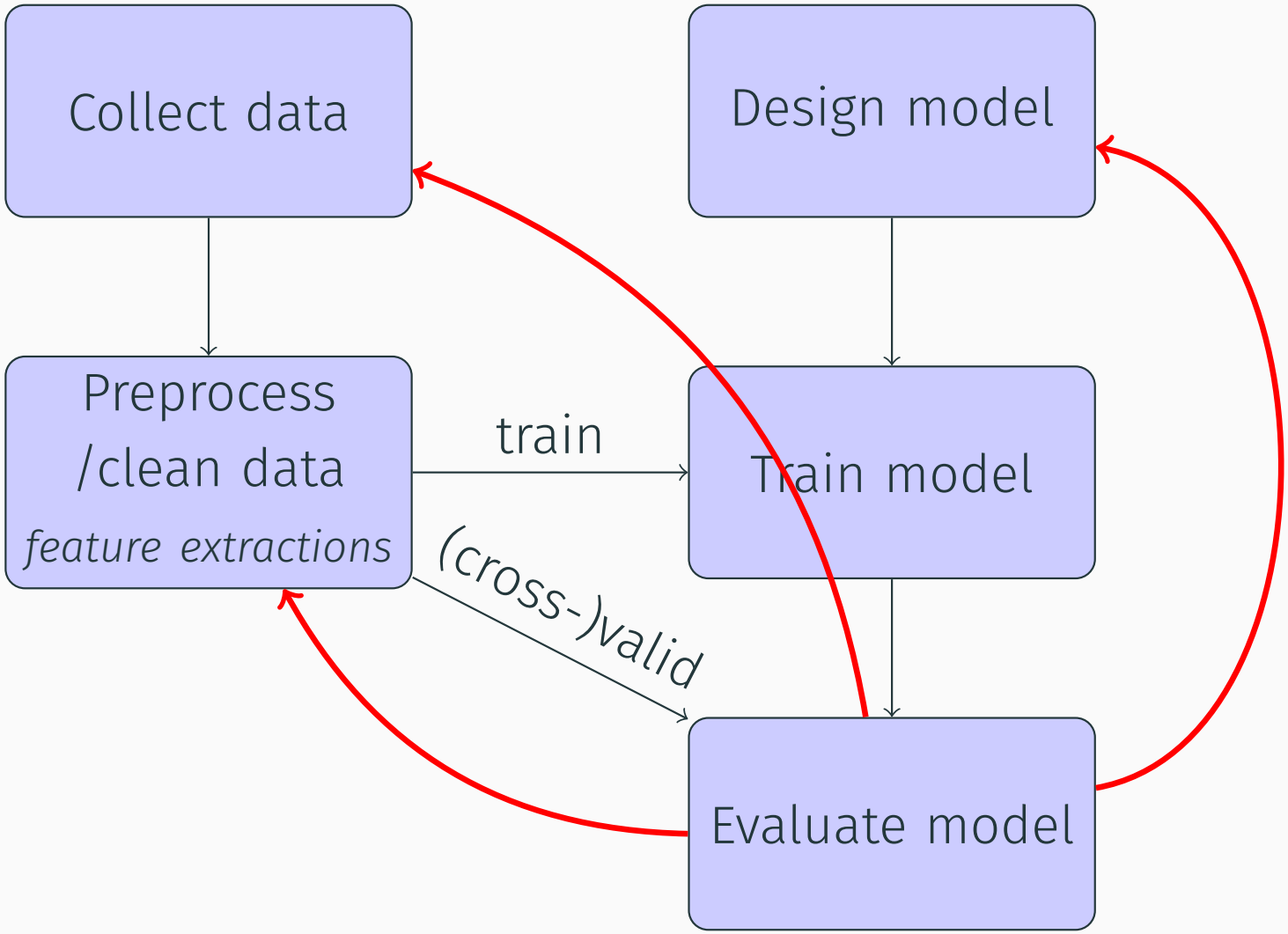
Steps


Collect data
Design model
Preprocess
/clean data
feature extractions
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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Train model
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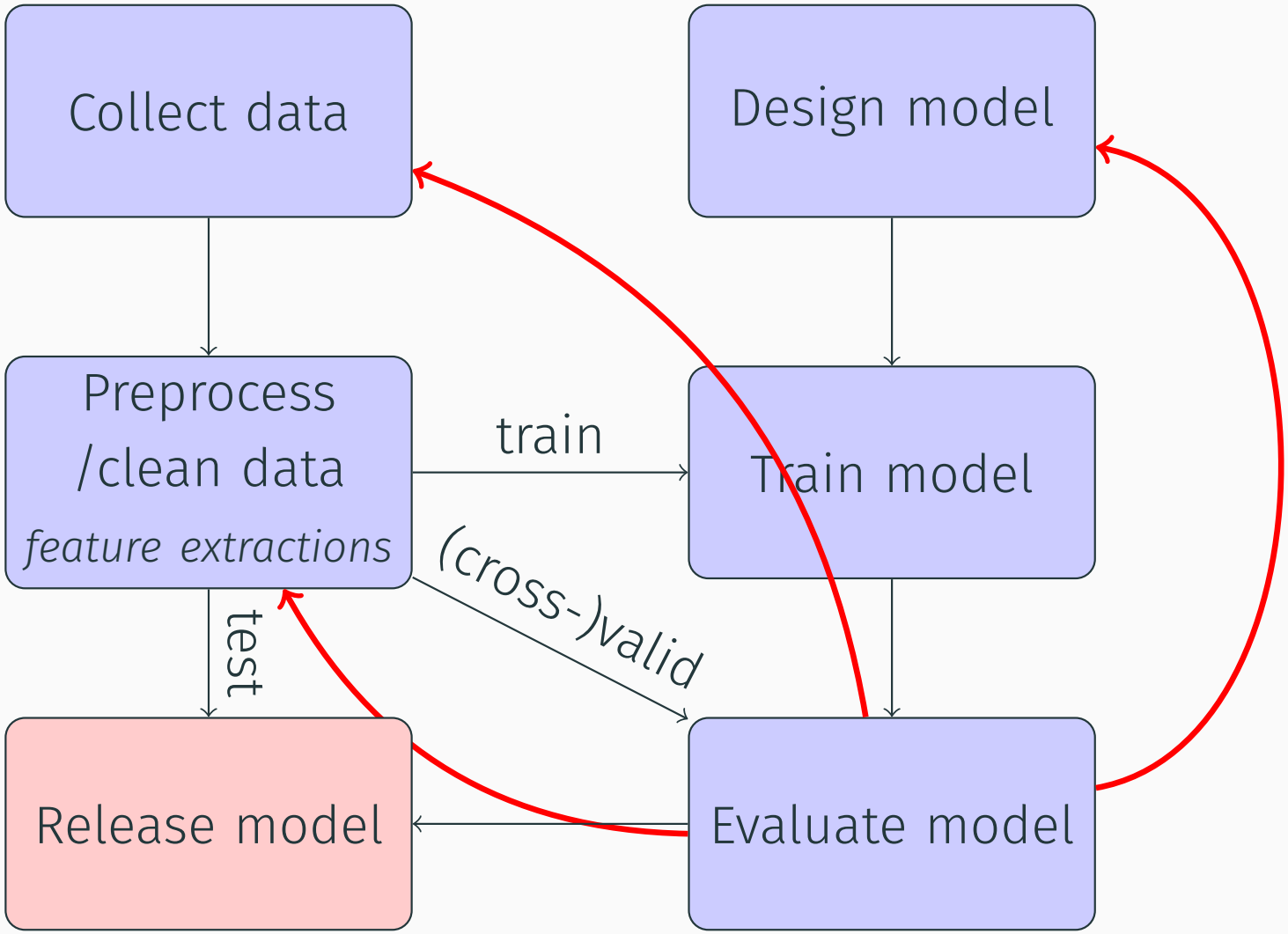
Evaluate model

Steps


Collect data
Design model
Preprocess
/clean data
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.

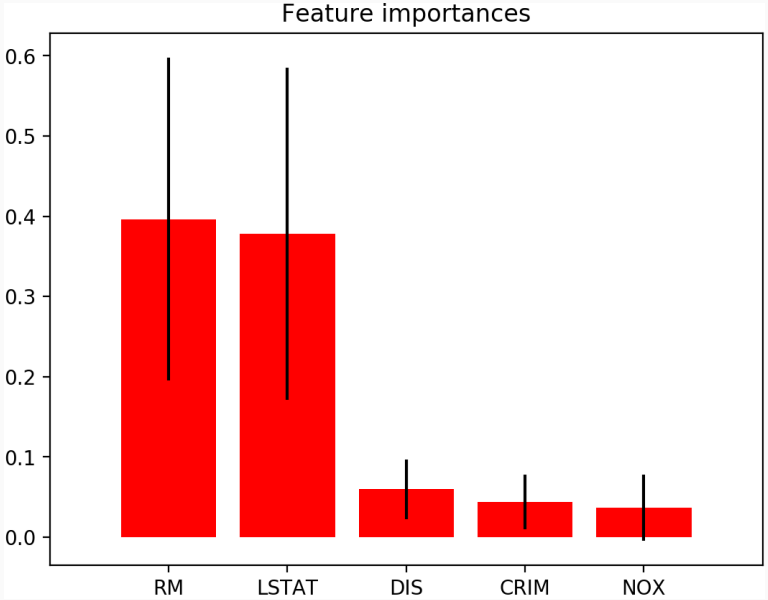
- A test dataset (independent from the two other) to estimate the final performance of the model.

Feature processing

Feature importance

```
rf = RandomForestRegressor(n_estimators=1000,
    max_features=10,random_state=10)
rf.fit(X,y)
importances = rf.feature_importances_
```

Indicates the impact of a feature in predicting the target.



CRIM	per capita crime rate by town
NOX	nitric oxides concentration
RM	average number of rooms per dwelling
DIS	distance to employment centres
LSTAT	lower status of the population

Type of features

- quantitative/continuous features (e.g. distance to employment centres, 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 produce 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)

one example: word cloud

On the introduction of the *Goodfellow et al.* book.

$\mathbf{v}$ is 3-dimensional (x,y,size)

https://www.wordclouds.com

An example using scikit-learn

Boston House Prices

Questions addressed in this lecture

- What are the more common area of application of machine learning? [GBC16, 1]
- What are the different class of ML problems? [Van16, 5.1]
- What are the different types of learning (supervised, ...)? [Van16, 5.1]
- How to validate/select a model? [Van16, 5.3]
- What is the cross-validation? [Van16, 5.3]
- How to encode qualitative features? [Van16, 5.4]

Refs

[Van16, n]: Jake VanderPlas, *Python Data Science Handbook*, section n
[GBC16, n]: Goodfellow etal., Deep Learning, chapter n