Machine Learning
Lecture 1: intro to ML

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MIPT, 2021

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Outline

1. Introduction to Machine Learning, motivation
2. ML thesaurus and notation
3. Maximum Likelihood Estimation
4. Machine Learning problems overview (selection):
   a. Classification
   b. Regression
   c. Dimensionality reduction
5. Naïve Bayes classifier
6. k Nearest Neighbours (kNN)

Motivation, historical overview and current state of ML and AI

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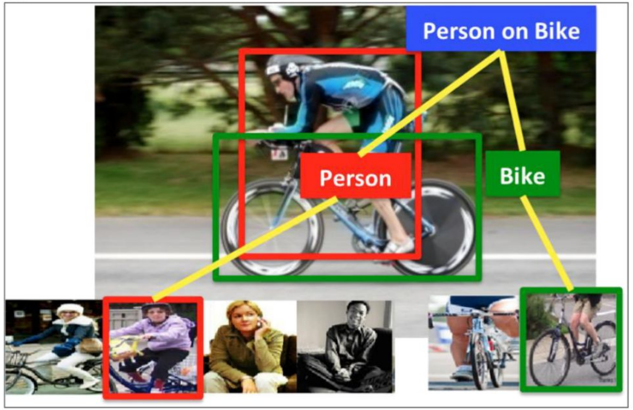
01

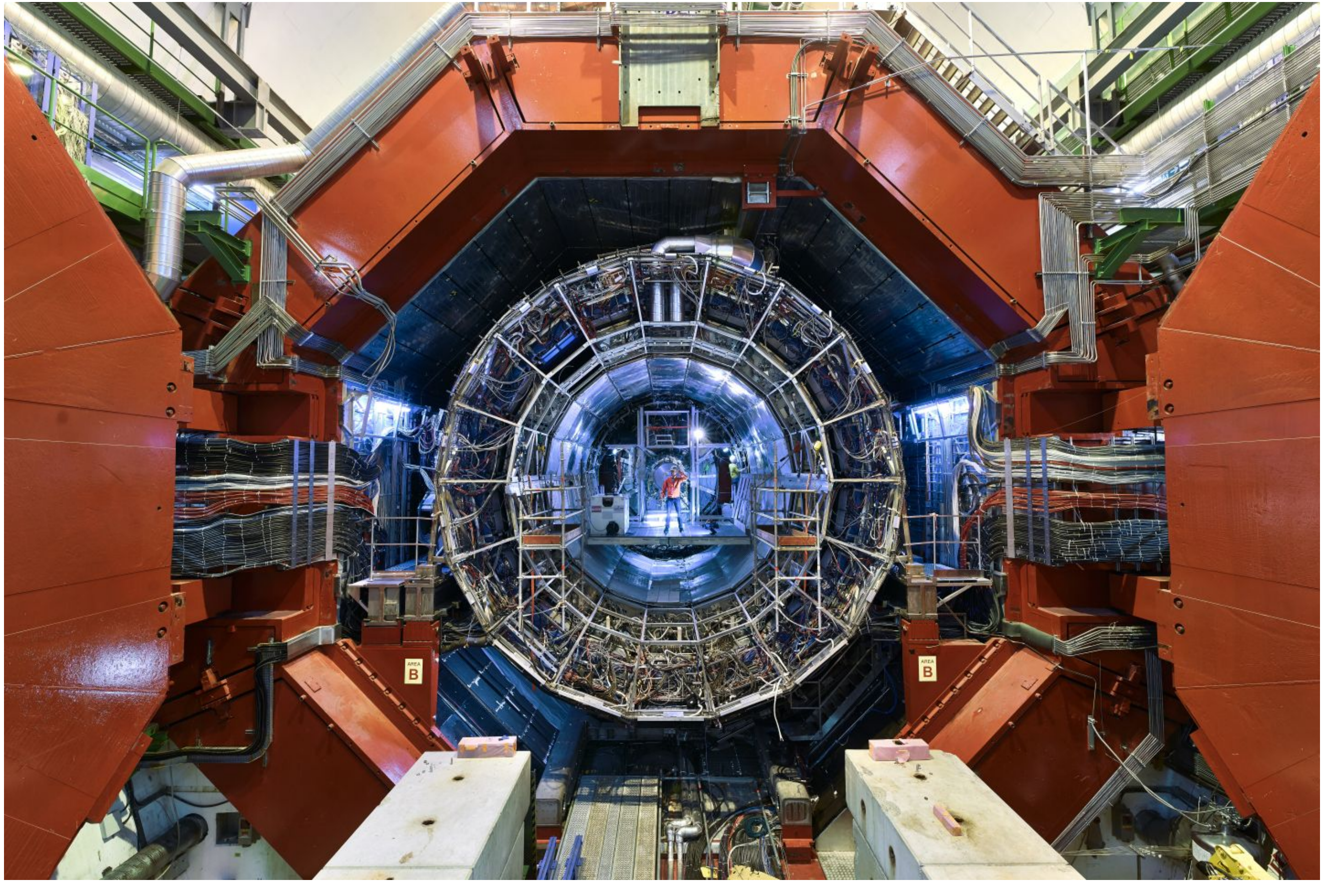
Machine Learning applications

- Object detection
- Action classification
- Image captioning
- …



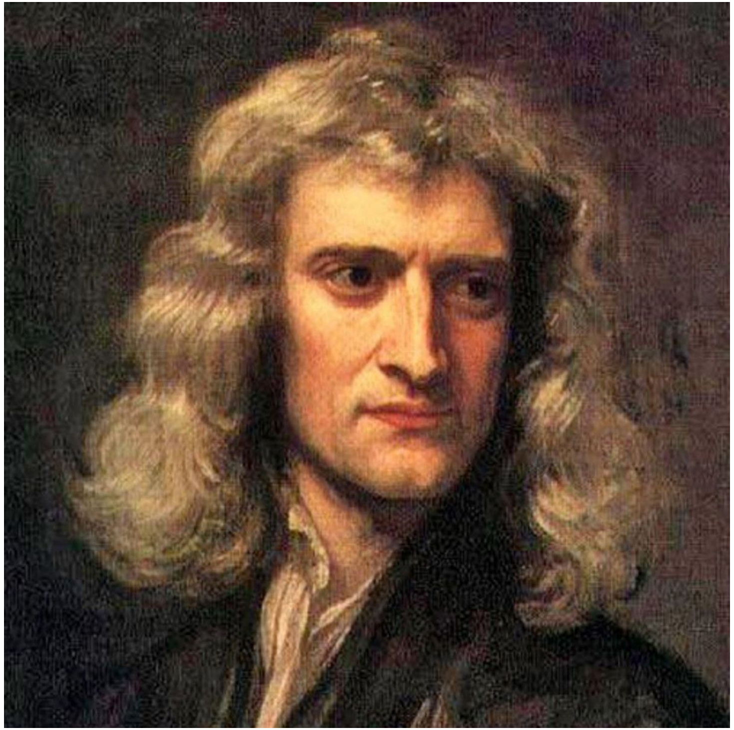
Machine Learning applications

Machine Learning applications



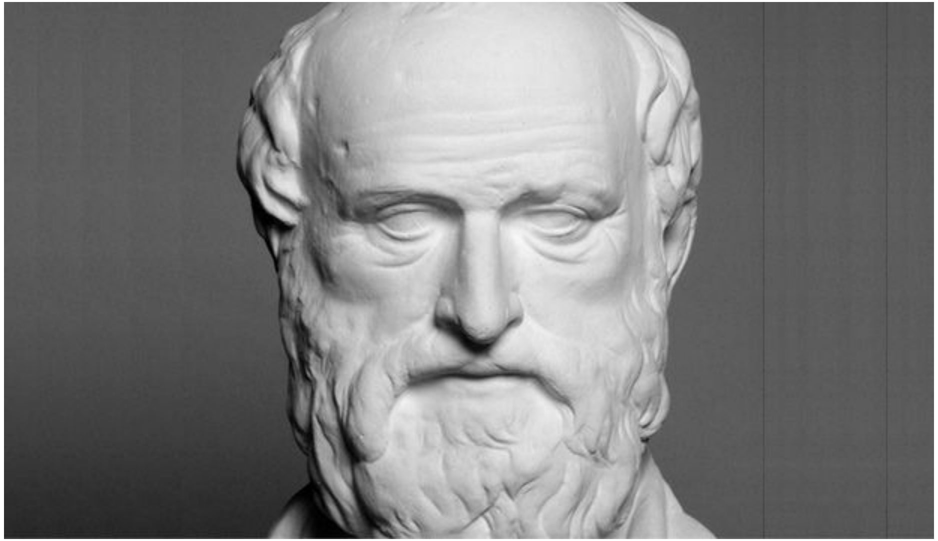
Data → Knowledge

Long before the ML


Isaac Newton


Johannes Kepler

Long before the ML



Eratosthenes

ML thesaurus

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02

ML thesaurus

Denote the ***dataset***.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

ML thesaurus

Observation (or datum, or data point) is one piece of information.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

In many cases the observations are supposed to be ***i.i.d.***

- ***independent***
- ***identically distributed***

ML thesaurus

Feature (or predictor) represents some special property.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

ML thesaurus

These all are features

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
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Some student	23	3	3	NA	Esperanto	2	FALSE

ML thesaurus

These all are features

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
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Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

ML thesaurus

These all are features

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Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
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ML thesaurus

These all are features

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
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Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

ML thesaurus

And even the name is a ***feature***

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

ML thesaurus

The ***design matrix*** contains all the features and observations.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

Features can even be multidimensional, we will discuss it later in this course.

ML thesaurus

Target represents the information we are interested in.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

*Target can be either a **number** (real, integer, etc.) – for **regression** problem*

ML thesaurus

Target represents the information we are interested in.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

*Or a **label** – for **classification** problem*

ML thesaurus

Target represents the information we are interested in.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Target (passed)
John	22	5	4	Brown	English	5	TRUE
Aahna	17	4	5	Brown	Hindi	4	TRUE
Emily	25	5	5	Blue	Chinese	5	TRUE
Michael	27	3	4	Green	French	5	TRUE
Some student	23	3	3	NA	Esperanto	2	FALSE

Mark can be treated as a label too (due to finite number of labels: 1 to 5). We will discuss it later.

ML thesaurus

Further we will work with the numerical target (mark)

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)
John	22	5	4	Brown	English	5
Aahna	17	4	5	Brown	Hindi	4
Emily	25	5	5	Blue	Chinese	5
Michael	27	3	4	Green	French	5
Some student	23	3	3	NA	Esperanto	2

ML thesaurus

The ***prediction*** contains values we predicted using some ***model***.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	4.5
Aahna	17	4	5	Brown	Hindi	4	4.5
Emily	25	5	5	Blue	Chinese	5	5
Michael	27	3	4	Green	French	5	3.5
Some student	23	3	3	NA	Esperanto	2	3

One could notice that prediction just averages of Statistics and Python marks. So our ***model*** can be represented as follows:

$$\hat{\text{mark}}_{ML} = \frac{1}{2}\text{mark}_{Statistics} + \frac{1}{2}\text{mark}_{Python}$$

ML thesaurus

The ***prediction*** contains values we predicted using some ***model***.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	4.5
Aahna	17	4	5	Brown	Hindi	4	4.5
Emily	25	5	5	Blue	Chinese	5	5
Michael	27	3	4	Green	French	5	3.5
Some student	23	3	3	NA	Esperanto	2	3

Different models can provide different predictions:

$$\hat{\text{mark}}_{ML} = \frac{1}{2}\text{mark}_{Statistics} + \frac{1}{2}\text{mark}_{Python}$$

ML thesaurus

The ***prediction*** contains values we predicted using some ***model***.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	1
Aahna	17	4	5	Brown	Hindi	4	5
Emily	25	5	5	Blue	Chinese	5	2
Michael	27	3	4	Green	French	5	4
Some student	23	3	3	NA	Esperanto	2	3

Different models can provide different predictions:

$$\hat{\text{mark}}_{ML} = \text{random}(\text{integer from } [1;\, 5])$$

ML thesaurus

The ***prediction*** contains values we predicted using some ***model***.

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	1
Aahna	17	4	5	Brown	Hindi	4	5
Emily	25	5	5	Blue	Chinese	5	2
Michael	27	3	4	Green	French	5	4
Some student	23	3	3	NA	Esperanto	2	3

Different models can provide different predictions.

*Usually some **hypothesis** lies beneath the model choice.*

ML thesaurus

Loss function measures the error rate of our model.

Square deviation	Target (mark)	Predicted (mark)
16	5	1
1	4	5
9	5	2
1	5	4
1	2	3

- ***Mean Squared Error*** (where **y** is vector of targets):

$$MSE(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N}\|\mathbf{y} - \hat{\mathbf{y}}\|_2^2 = \frac{1}{N}\sum_i (y_i - \hat{y}_i)^2$$

ML thesaurus

Loss function measures the error rate of our model.

Absolute deviation	Target (mark)	Predicted (mark)
4	5	1
1	4	5
3	5	2
1	5	4
1	2	3

- ***Mean Absolute Error*** (where **y** is vector of targets):

$$MAE(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{N}\|\mathbf{y} - \hat{\mathbf{y}}\|_1 = \frac{1}{N}\sum_i |y_i - \hat{y}_i|$$

ML thesaurus

To learn something, our ***model*** needs some degrees of freedom:

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	4.5
Aahna	17	4	5	Brown	Hindi	4	4.5
Emily	25	5	5	Blue	Chinese	5	5
Michael	27	3	4	Green	French	5	3.5
Some student	23	3	3	NA	Esperanto	2	3

$$\hat{\text{mark}}_{ML} = w_1 \cdot \text{mark}_{Statistics} + w_2 \cdot \text{mark}_{Python}$$

ML thesaurus

To learn something, our ***model*** needs some degrees of freedom:

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	4.447
Aahna	17	4	5	Brown	Hindi	4	4.734
Emily	25	5	5	Blue	Chinese	5	5.101
Michael	27	3	4	Green	French	5	3.714
Some student	23	3	3	NA	Esperanto	2	3.060

$$\hat{\text{mark}}_{ML} = w_1 \cdot \text{mark}_{Statistics} + w_2 \cdot \text{mark}_{Python}$$

ML thesaurus

To learn something, our ***model*** needs some degrees of freedom:

Name	Age	Statistics (mark)	Python (mark)	Eye color	Native language	Target (mark)	Predicted (mark)
John	22	5	4	Brown	English	5	1
Aahna	17	4	5	Brown	Hindi	4	5
Emily	25	5	5	Blue	Chinese	5	2
Michael	27	3	4	Green	French	5	4
Some student	23	3	3	NA	Esperanto	2	3

$$\hat{\text{mark}}_{ML} = \text{random}(\text{integer from } [1; 5])$$

ML thesaurus

Last term we should learn for now is ***hyperparameter***.

Hyperparameter should be fixed before our model starts to work with the data.

We will discuss it later with kNN as an example.

ML thesaurus

Recap:

- Dataset
- Observation (datum)
- Feature
- Design matrix
- Target
- Prediction
- Model
- Loss function
- Parameter
- Hyperparameter

Maximum Likelihood Estimation

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03

Likelihood

Denote dataset generated by distribution with parameter θ

Likelihood function:

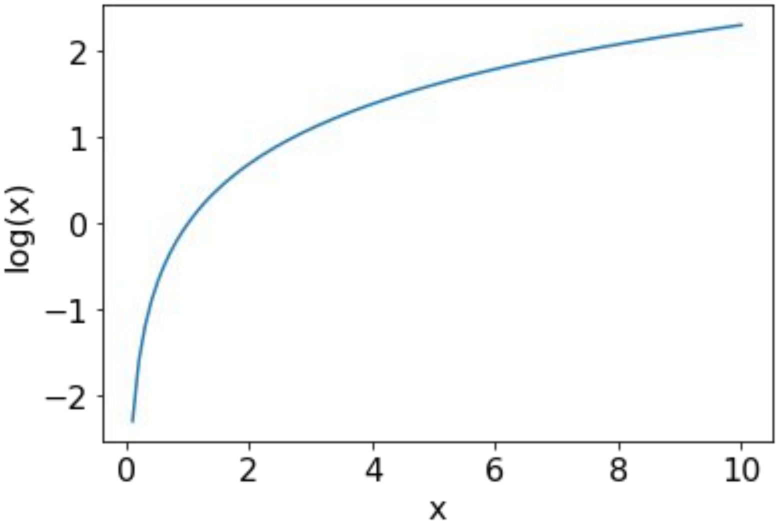
$$L(\theta|X,Y) = P(X,Y|\theta)$$

$$L(\theta|X,Y) \longrightarrow \max_{\theta}$$

samples should be i.i.d.

$$L(\theta|X,Y) = P(X,Y|\theta) = \prod_i P(x_i, y_i|\theta)$$

Maximum Likelihood Estimation



Likelihood

Denote dataset generated by distribution with parameter θ

Likelihood function:

$$L(\theta|X,Y) = P(X,Y|\theta)$$

$$L(\theta|X,Y) \longrightarrow \max_{\theta}$$

samples should be i.i.d.

$$L(\theta|X,Y) = P(X,Y|\theta) = \prod_i P(x_i, y_i|\theta)$$

equivalent to

$$\log L(\theta|X,Y) = \sum_i \log P(x_i, y_i|\theta) \longrightarrow \max_{\theta}$$

Machine Learning problems overview

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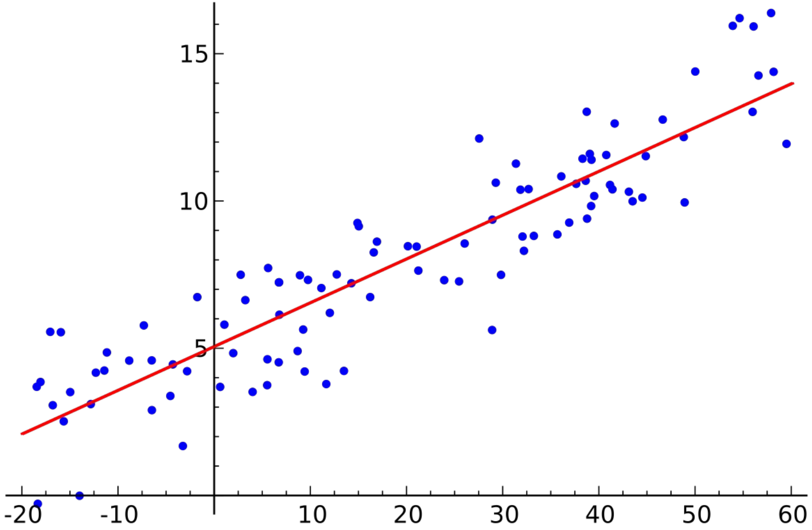
Supervised learning problem statement

Let's denote:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$, where
  - $(\mathbf{x} \in \mathbb{R}^p,\ y \in \mathbb{R}\ )$ for regression
  - $\mathbf{x}_i \in \mathbb{R}^p$, $y_i \in \{+1, -1\}$ for binary classification
- Model $f(\mathbf{x})$ predicts some value for every object
- Loss function $Q(\mathbf{x}, y, f)$ that should be minimized

- Regression problem



Estimated (or predicted) Y value for observation i

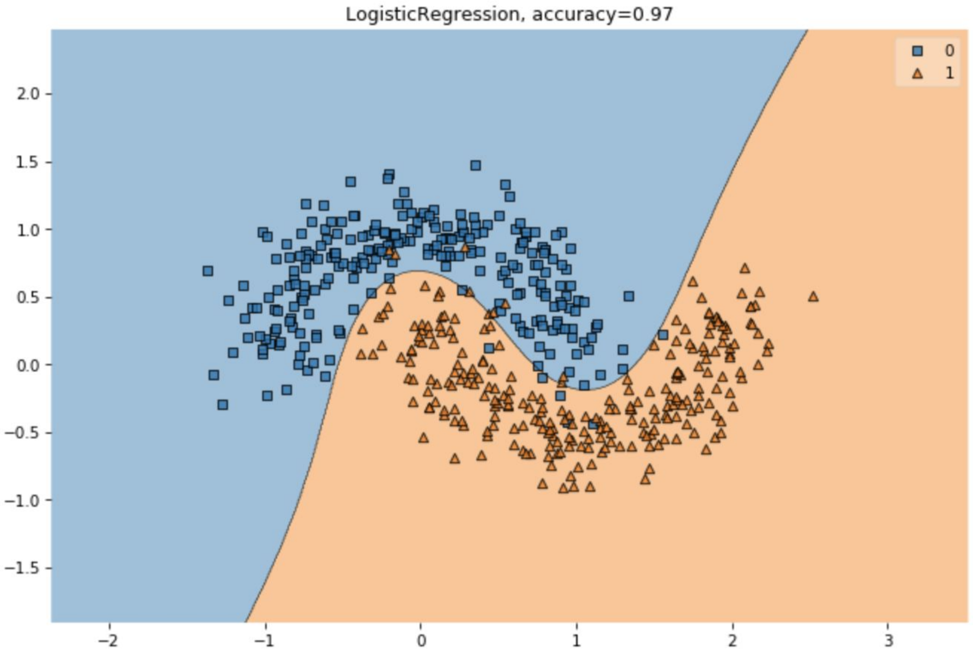
Estimate of the regression intercept

Estimate of the regression slope

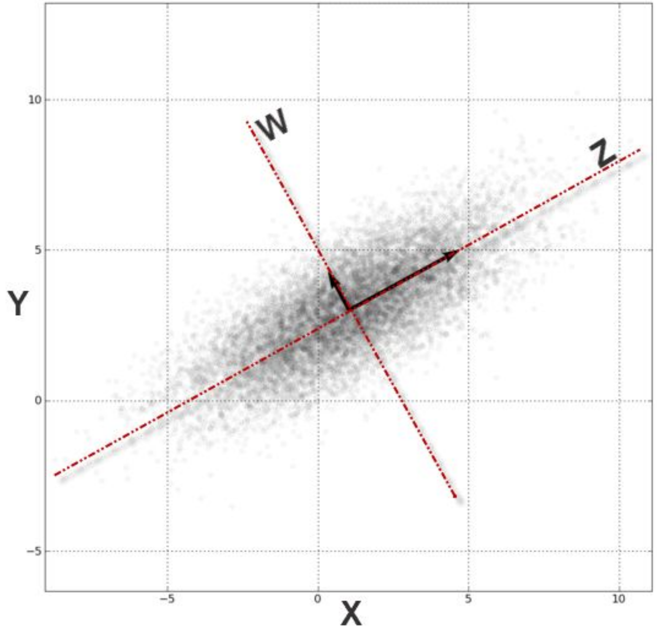
Value of X for observation i

$$\hat{Y}_i = b_0 + b_1 X_i$$

- Regression problem
- Classification problem



- Regression problem
- Classification problem
- Dimensionality reduction



Naïve Bayes classifier

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05

Naïve Bayes classifier

Let's denote:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$, where
  - $\mathbf{x}_i \in \mathbb{R}^p$, $y_i \in \{C_1, \ldots, C_k\}$ for k-class classification

Bayes' theorem

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

or, in our case

$$P(y_i = C_k|\mathbf{x}_i) = \frac{P(\mathbf{x}_i|y_i = C_k)P(y_i = C_k)}{P(\mathbf{x}_i)}$$

Naïve Bayes classifier

Let's denote:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$, where
  - $\mathbf{x}_i \in \mathbb{R}^p$, $y_i \in \{C_1, \ldots, C_K\}$ for K-class classification

$$P(y_i = C_k|\mathbf{x}_i) = \frac{P(\mathbf{x}_i|y_i = C_k)P(y_i = C_k)}{P(\mathbf{x}_i)}$$

Naïve assumption: features are ***independent***

Naïve Bayes classifier

$$P(y_i = C_k|\mathbf{x}_i) = \frac{P(\mathbf{x}_i|y_i = C_k)P(y_i = C_k)}{P(\mathbf{x}_i)}$$

Naïve assumption: features are ***independent:***

$$P(\mathbf{x}_i|y_i = C_k) = \prod_{l=1}^{p} P(x_i^l|y_i = C_k)$$

Naïve Bayes classifier

$$P(y_i = C_k|\mathbf{x}_i) = \frac{P(\mathbf{x}_i|y_i = C_k)P(y_i = C_k)}{\cancel{P(\mathbf{x}_i)}}$$

Optimal class label:

$$C^* = \arg\max_k P(y_i = C_k|\mathbf{x_i})$$

To find maximum we even do not need the denominator

But we need it to get probabilities

kNN – k Nearest Neighbors

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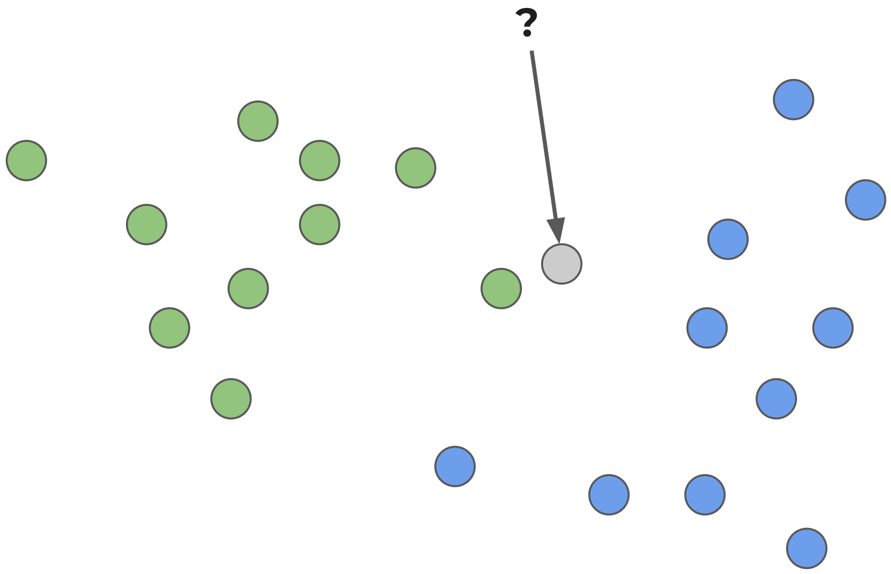
kNN - k Nearest Neighbours

kNN - k Nearest Neighbours



k Nearest Neighbors Method

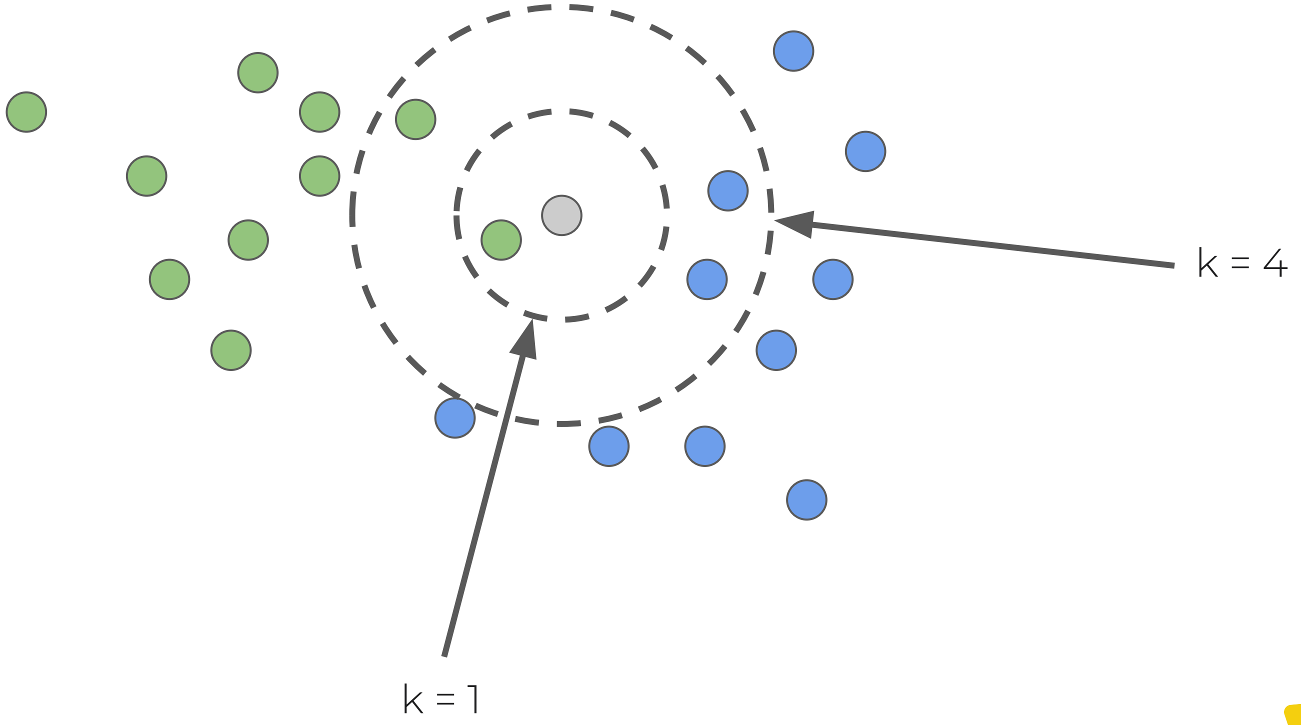
Given a new observation:

1. Calculate the distance to each of the samples in the dataset.
2. Select samples from the dataset with the minimal distance to them.
3. The label of the new observation will be the most frequent label among those nearest neighbors.

How to make it better?

- The number of neighbors k (it is a **hyperparameter**)

kNN - k Nearest Neighbours

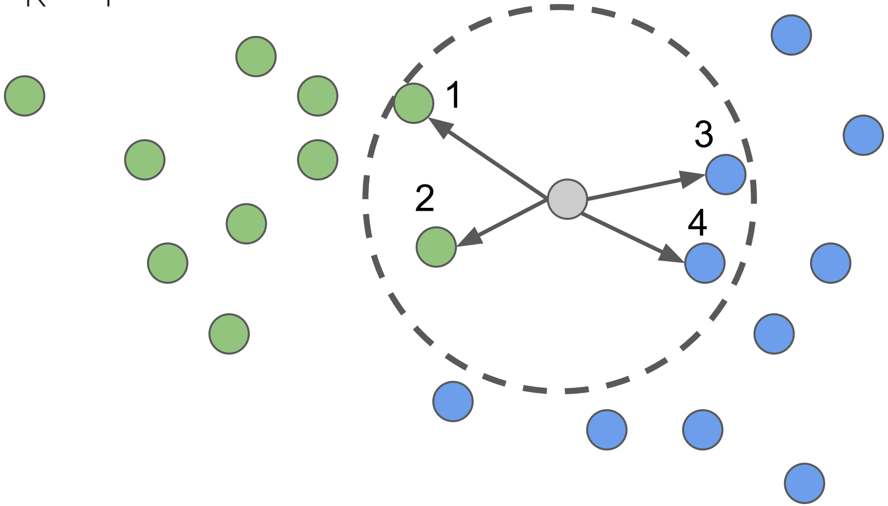


How to make it better?

- The number of neighbors k (it is a ***hyperparameter***)
- The distance measure between samples
    a. Hamming
    b. Euclidean
    c. cosine
    d. Minkowski distances
    e. etc.
- Weighted neighbours

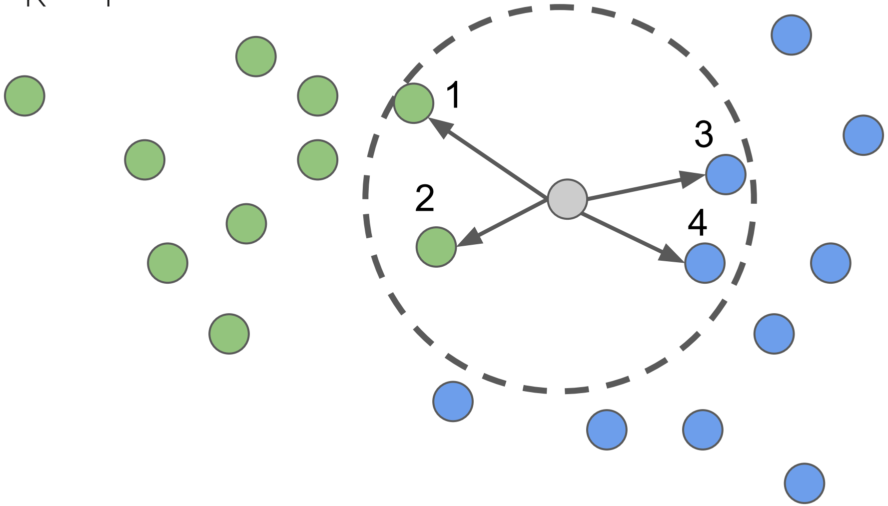
Weighted kNN

k = 4



Weighted kNN

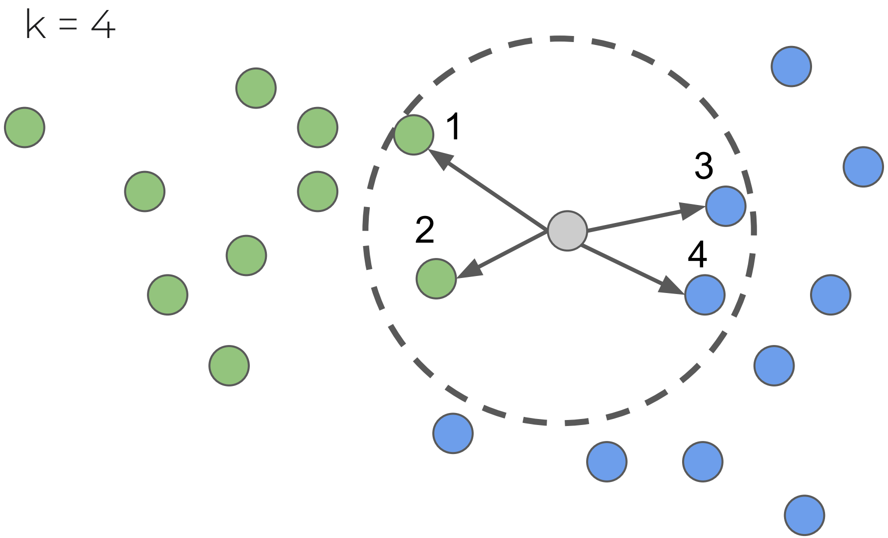
k = 4



- Weights can be adjusted according to the neighbors order,

$$w\left(\mathbf{x}_{(i)}\right) = w_i$$

Weighted kNN



- Weights can be adjusted according to the neighbors order,

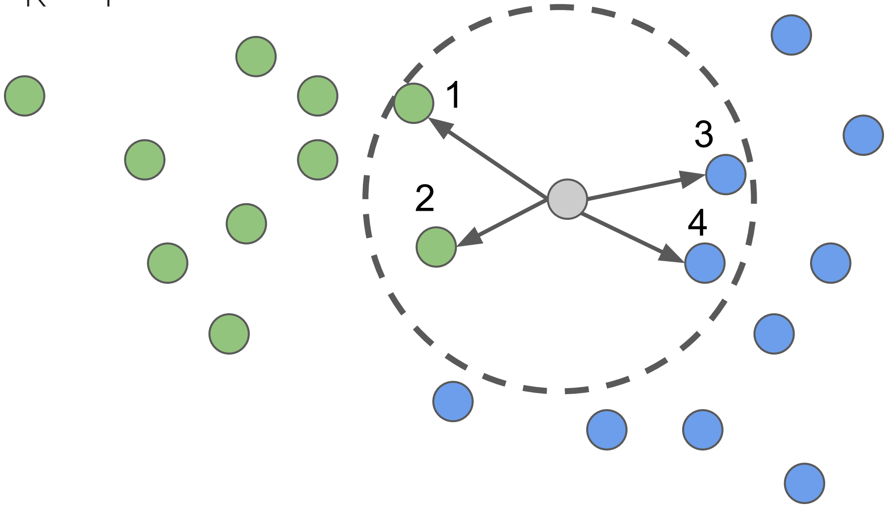
$$w(\mathbf{x}_{(i)}) = w_i$$

- or on the distance itself

$$w(\mathbf{x}_{(i)}) = w(d(\mathbf{x}, \mathbf{x}_{(i)}))$$

Weighted kNN

k = 4



- Weights can be adjusted according to the neighbors order,

$$w(\mathbf{x}_{(i)}) = w_i$$

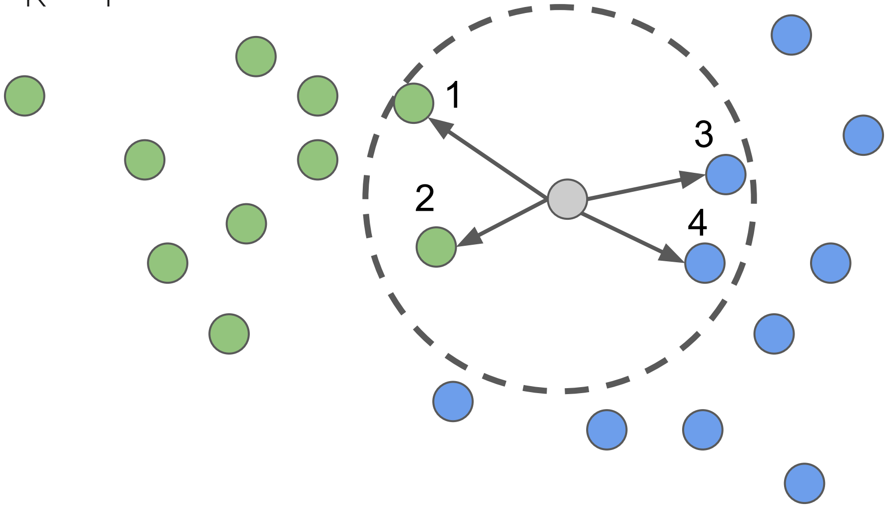
- or on the distance itself

$$w(\mathbf{x}_{(i)}) = w(d(\mathbf{x}, \mathbf{x}_{(i)}))$$

$$p_{\text{green}} = \frac{\boxed{w(\mathbf{x}_1) + w(\mathbf{x}_2)}}{w(\mathbf{x}_1) + w(\mathbf{x}_2) + w(\mathbf{x}_3) + w(\mathbf{x}_4)}$$

Weighted kNN

k = 4



- Weights can be adjusted according to the neighbors order,

$$w\left(\mathbf{x}_{(i)}\right) = w_i$$

- or on the distance itself

$$w\left(\mathbf{x}_{(i)}\right) = w\left(d\left(\mathbf{x}, \mathbf{x}_{(i)}\right)\right)$$

$$p_{\text{blue}} = \frac{\boxed{w\left(\mathbf{x}_3\right) + w\left(\mathbf{x}_4\right)}}{w\left(\mathbf{x}_1\right) + w\left(\mathbf{x}_2\right) + w\left(\mathbf{x}_3\right) + w\left(\mathbf{x}_4\right)}$$

Outro

- Remember the i.i.d. property
- Usually the first dimension corresponds to the batch size, the second (and so on) to the features/time/...
- Even the naïve assumptions may be suitable in some cases
- Simple models provide great baselines

Revise

1. Introduction to Machine Learning, motivation
2. ML thesaurus and notation
3. Maximum Likelihood Estimation
4. Machine Learning problems overview (selection):
   a. Classification
   b. Regression
   c. Dimensionality reduction
5. Naïve Bayes classifier
6. k Nearest Neighbours (kNN)

Q&A

Thanks for attention!

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Model validation and evaluation

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Supervised learning problem statement

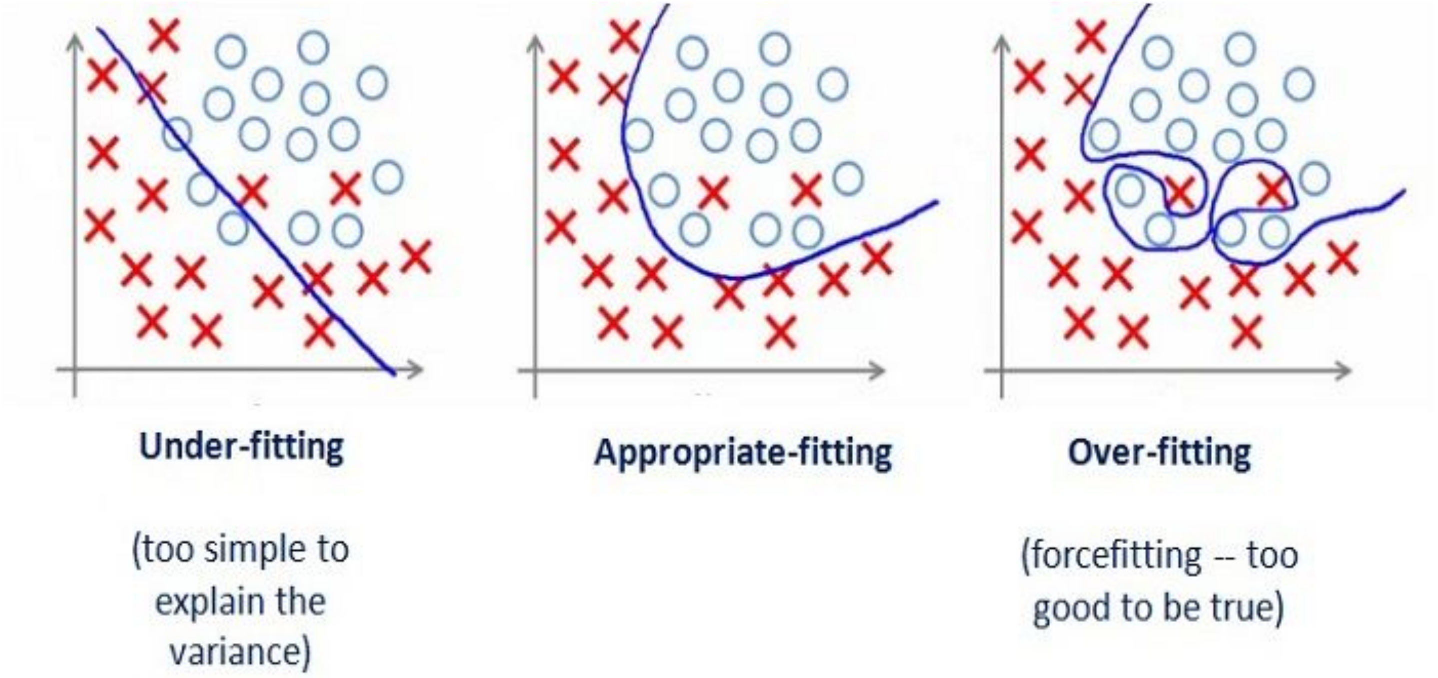
Let's denote:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$, where
  - $(\mathbf{x} \in \mathbb{R}^p,\ y \in \mathbb{R})$ for regression
  - $\mathbf{x}_i \in \mathbb{R}^p$, $y_i \in \{+1, -1\}$ for binary classification

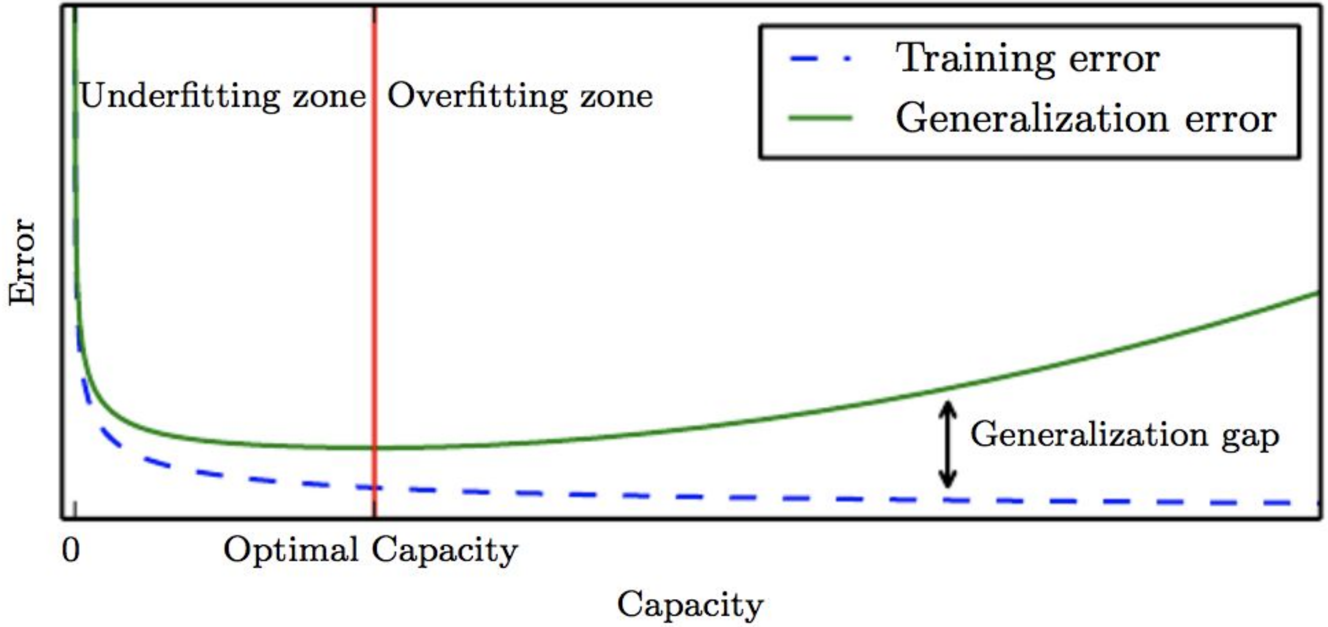
Model $f(\mathbf{x})$ predicts some value for every object

Loss function $Q(\mathbf{x}, y, f)$ that should be minimized

Overfitting vs. underfitting



Overfitting vs. underfitting



Overfitting vs. underfitting

- We can control overfitting / underfitting by altering model's capacity (ability to fit a wide variety of functions):
- select appropriate hypothesis space
- learning algorithm's effective capacity may be less than the representational capacity of the model family

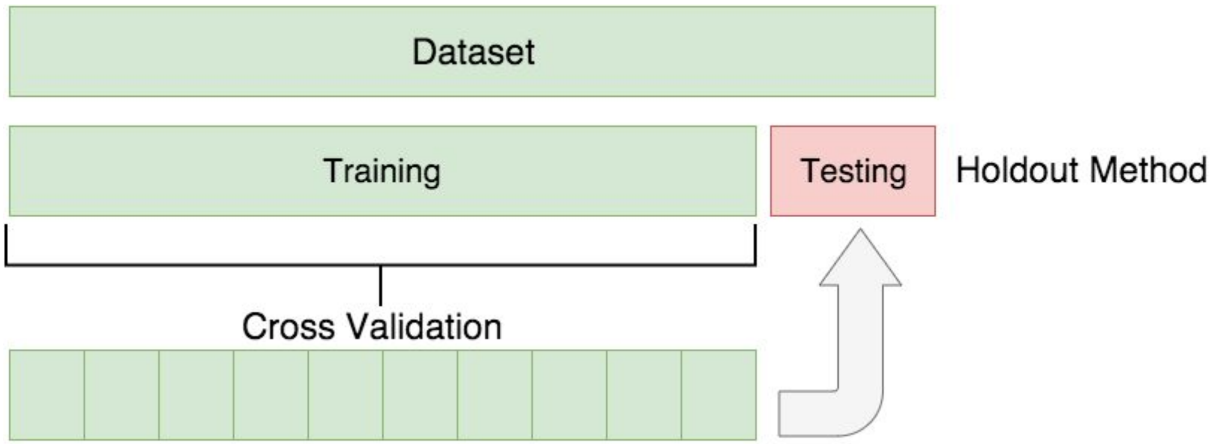
Evaluating the quality

Evaluating the quality

Is it good enough?

Image credit: Joseph Nelson [@josephofiowa](https://twitter.com/josephofiowa)

Evaluating the quality



Evaluating the quality

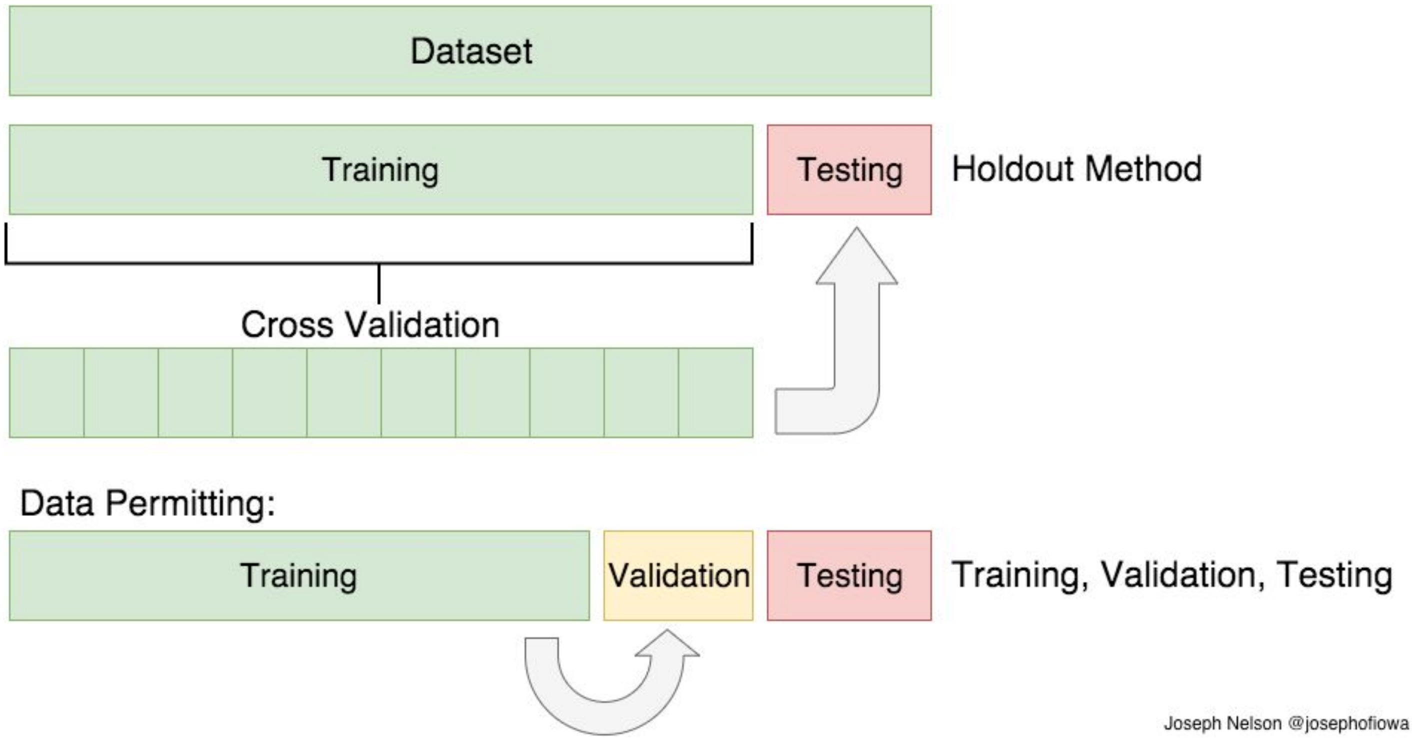


Image credit: Joseph Nelson [@josephofiowa]

Cross-validation