Machine learning for graphs and with graphs

Courses 1: introduction

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September 12, 2023

ENS DE LYON

Full course outline

From theory ...

1. Basics of machine learning
2. The graph framework
3. Community detection
4. Spectral embedding of graphs and graph clustering
5. Graph signal processing
6. Kernels for graphs
7. Graph neural networks
8. Optimal transport theory for graphs
9. Learning graphs from (unstructured) data

... to practice

We will use `Python` and various librairies

Some references for machine learning

Shalev-Shwartz and Ben-David 2014

Bach 2022

Hastie, Tibshirani, and Friedman 2001

Others can be found in: `https://tvayer.github.io/courses/coursegraph.html`

Evaluation

- 50 % final exam.
- 50 % project.

Python installations

- The practical sessions of the course will require to run jupyter notebooks.
- We recommend that you install python through the Anaconda distribution (python 3.7, 3.8 or 3.9 is preferrable) available at `https://www.anaconda.com/products/distribution`

You should check that you are able to create and open a jupyter notebook, and inside, run the following imports:

```python
import matplotlib
import numpy
import sklearn
import pytorch
import pandas
import scipy
```

If any of these packages is missing, it can be installed with ‘conda install numpy‘, the command being run in a terminal or in Anaconda prompt for Windows user.

Basics of machine learning

What is machine learning ?

Data in machine learning

From training data to prediction

- Loss functions
- Empirical risk minimization
- Train/validation/test

Model selection and validation

- Split your dataset !

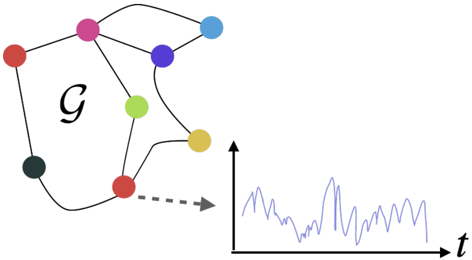
The problems with structured data

- Motivating examples
- A primer on graph theory
- Why “classical ML” struggles with stuctured data

What is machine learning ?

Some applications

1. Energy networks, disease propagation



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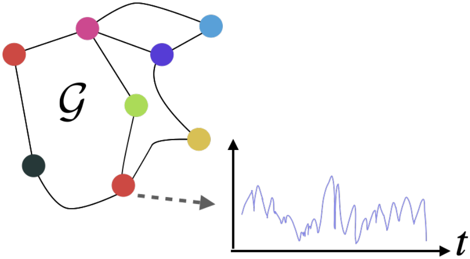
2. Image analysis (medical application, web)



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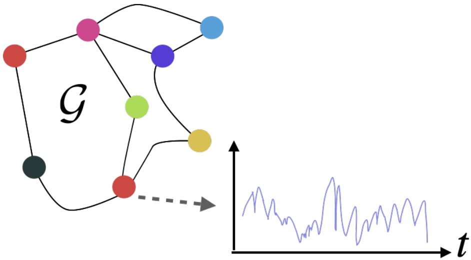

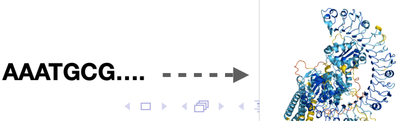

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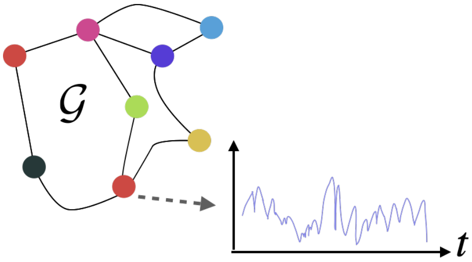

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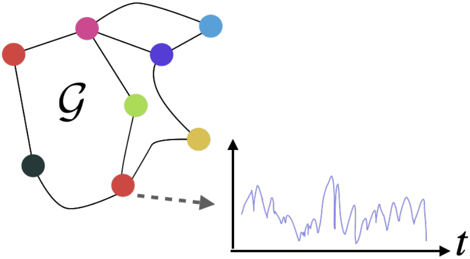

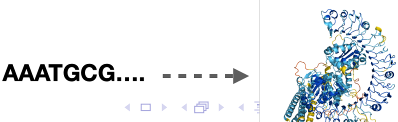

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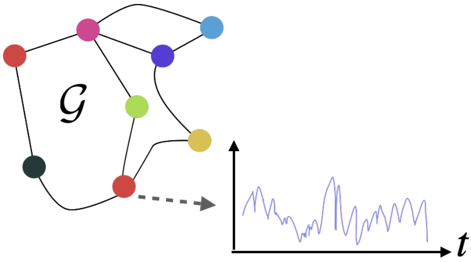
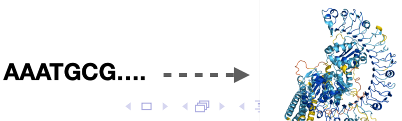
6. For art https://www.youtube.com/watch?v=MwtVkPKx3RA



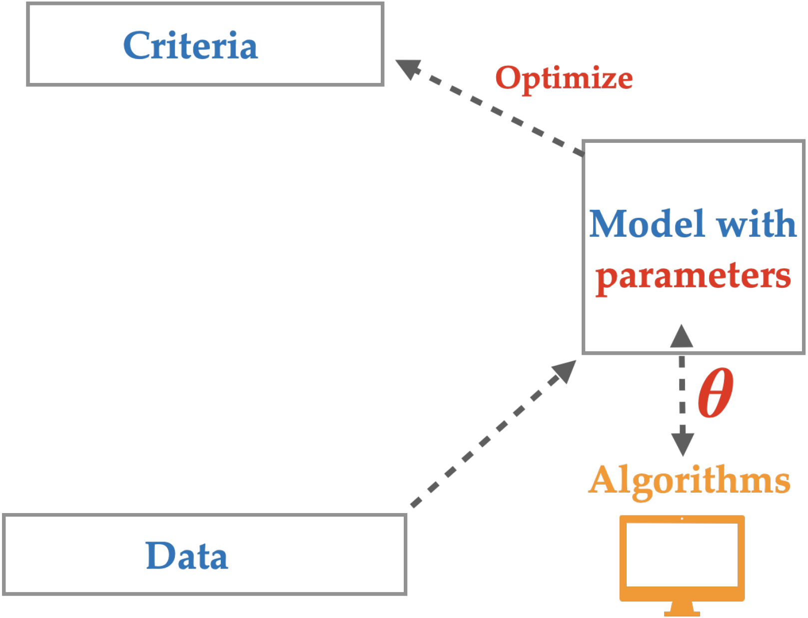


What is machine learning ?

Criteria

Data

What is machine learning ?



What is machine learning ?

The objective of machine learning

Teach a machine to process automatically a some data in order to solve a given problem.

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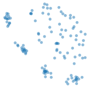
Unsupervised learning: understanding the data

- Clustering & probability density estimation
- Dimensionality reduction



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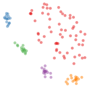

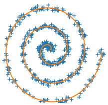

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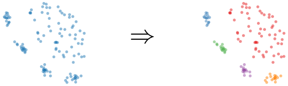
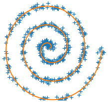
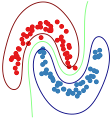
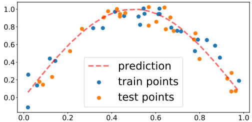




Supervised learning: learning to predict

- Classification: classify points according to some labels
- Regression: predict real (vector) values





Some images and slides have been obtained by the courtesy of Rémi Flamary

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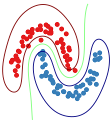

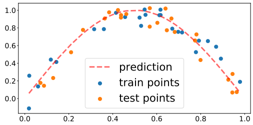

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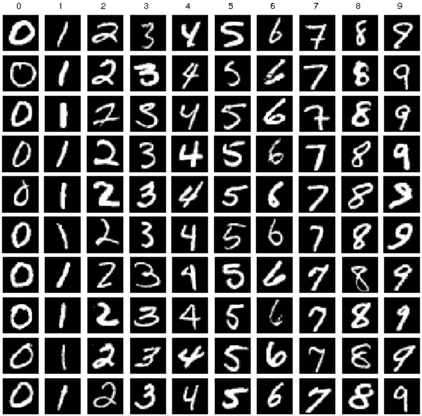
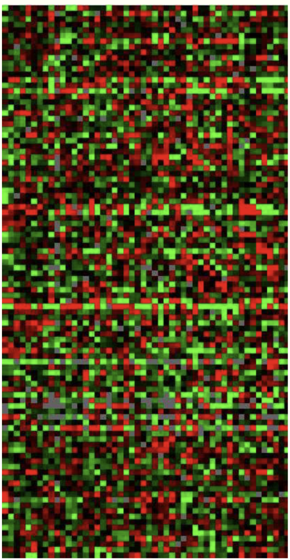


Supervised classification examples

- e.g. to identify the numbers on images from a 16×16 gray level image (image classification)
- SPAM, fraud detection, disease classification ...

What is machine learning ?



Clustering example

- Analyse n sequences (individuals) of d genetical responses
- Groups of similar samples ? Gene with similar expressions ?

Plan

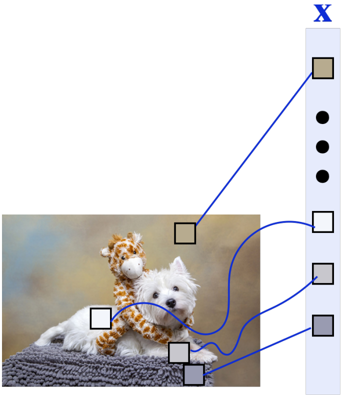
Store a data point

Vectorial representation

One "sample", "data point", "individual":

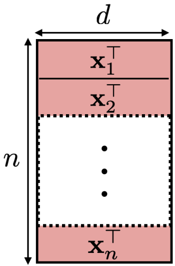
$$\mathbf{x} = (x_1, \cdots, x_d)^\top \in \mathbb{R}^d$$

- d is the dimension, x_i is the ith information i of $\mathbf{x}$
- Can describe information about an individual
- For an image $\mathbf{x}$: each pixel of an image
- Descriptors of a cell, word embedding ...



Unsupervised dataset

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix}$$



Unsupervised learning

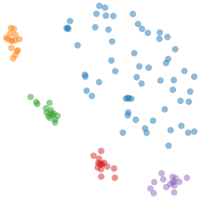
- The dataset contains the samples $(\mathbf{x}_i)_{i=1}^n$ where n is the number of samples of size d.
- d and n define the dimensionality of the learning problem.
- Data stored as a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ that contains the training samples as rows.

Supervised dataset

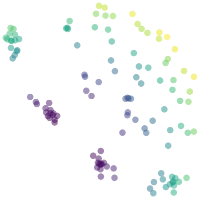
Samples + labels:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Classification



Regression



Supervised learning

- The dataset contains the samples $(\mathbf{x}_i, y_i)_{i=1}^n$ where $\mathbf{x}_i$ is the feature sample and $y_i \in \mathcal{Y}$ its label.
- The values to predict (label) can be concatenated in a vector $\mathbf{y} \in \mathcal{Y}^n$

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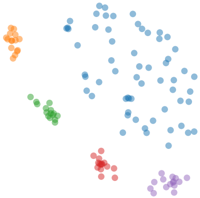

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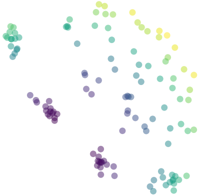

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- Prediction space $\mathcal{Y}$ can be:
  - $\mathcal{Y} = \{-1, 1\}$ or $\mathcal{Y} = \{1, \ldots, K\}$ for classification problems.
  - $\mathcal{Y} = \mathbb{R}$ for regression problems ($\mathbb{R}^p$ for multi-output regression).

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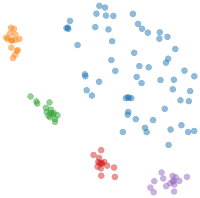

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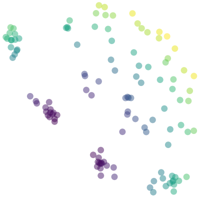

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  - $\mathcal{Y} = \mathbb{R}$ for regression problems ($\mathbb{R}^p$ for multi-output regression).
- Semi-supervised learning: few labeled points are available, but a large number of unlabeled points are given.

Plan

From training data to prediction

Training data

- We have access to n samples $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n) \sim p$
- $p \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$ is the data distribution
- p is unknown ! We only have access to samples.

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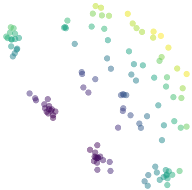
Objective

- We have a task to solve: classification, regression, clustering ...
- Most ML problems formulate as **finding some function f that "best" solves our task**
- f is called **an hypothesis** and is **implemented by a computer**
- Most of the time f depends on some parameter $\boldsymbol{\theta} \in \Theta$

Regression



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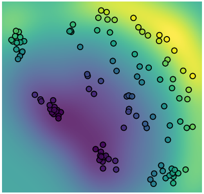

Objective

$$(\mathbf{x}_i, y_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \rightarrow \mathbb{R}$$

- Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting a continuous value ($\mathcal{Y} = \mathbb{R}$).
- Can be extended to multi-value prediction ($\mathcal{Y} = \mathbb{R}^p$).

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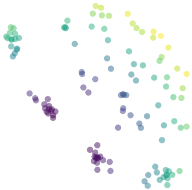

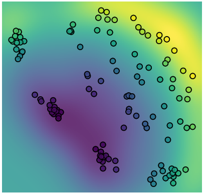

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Hyperparameters

- Type of function (linear, kernel, neural network).
- Performance measure.
- Regularization.

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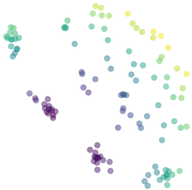

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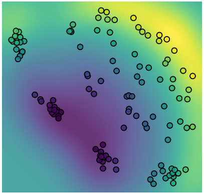

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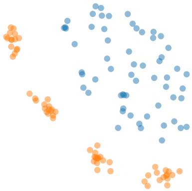
Methods

- Least Square (LS).
- Ridge regression, Lasso.
- Kernel regression.
- Deep learning.

Binary classification



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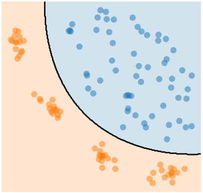

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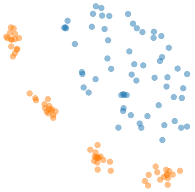
- Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting a binary value ($\mathcal{Y} = \{-1, 1\}$).
- $f(\mathbf{x}) = 0$ defines the boundary on the partition of the feature space.

Binary classification



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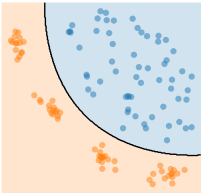

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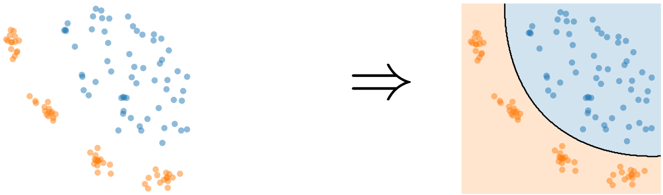

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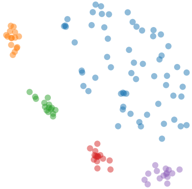
Methods

- Bayesian classifier (LDA, QDA)
- Linear and kernel discrimination
- Decision trees, random forests.
- Deep learning.

Multiclass classification



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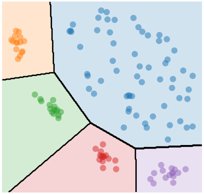


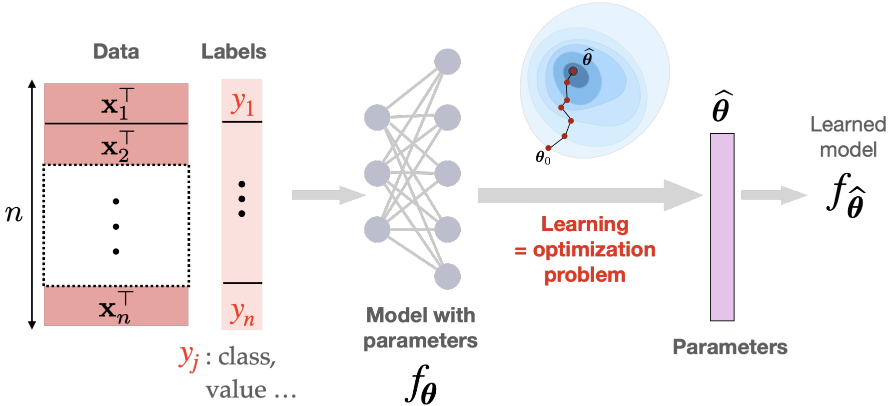
Objective

$$(\mathbf{x}_i, y_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \rightarrow \{1, \ldots, K\}$$

- Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting an integer value ($\mathcal{Y} = \{1, \ldots, K\}$).
- In practice K continuous score functions f_k are estimated and the prediction is
$$f(\mathbf{x}) = \arg\max_k f_k(\mathbf{x})$$
- Softmax can be used instead of argmax to get probability estimates.

The big picture of (parametrized) ML

But how to find this function ?



The goal in the **learning step** will be to find the parameters $\widehat{\boldsymbol{\theta}}$ (hence the function) that **minimizes a measure of error on the data**

Loss functions

Supervised case

A loss function is $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ so that:

$$\ell\,(\text{true value}\ ,\text{predicted value}) = \ \text{how good is my prediction}$$

Regression problems

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- E.g. $y_i \in \mathbb{R}$ $\ell(y_i, f(\mathbf{x}_i)) = (y_i - f(\mathbf{x}_i))^2$ (square loss)

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- E.g. $\mathbf{y}_i \in \mathbb{R}^p$ $\ell(y_i, f(\mathbf{x}_i)) = \|\mathbf{y}_i - f(\mathbf{x}_i)\|_q^q$ (ℓ_q loss)

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- E.g. $\mathbf{y}_i \in \mathbb{R}^p$ $\ell(y_i, f(\mathbf{x}_i)) = \|\mathbf{y}_i - f(\mathbf{x}_i)\|_q^q$ (ℓ_q loss)

Classification problems

- E.g. $y_i \in \{-1, 1\}$ $\ell(y_i, f(\mathbf{x}_i)) = \mathbf{1}_{y_i \neq f(\mathbf{x}_i)}$ (0/1 loss)

Empirical risk minimization

Train by minimizing the train error

To find f the idea is to **minimize the averaged error** on the training samples:

$$\min_f \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) \tag{ERM}$$

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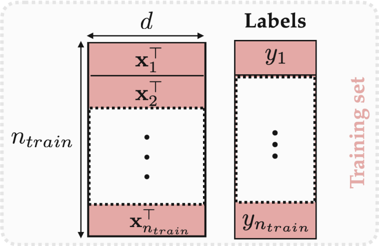
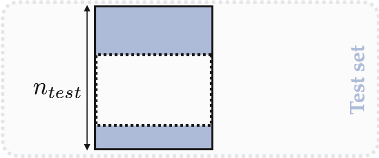
Once solved how do I know if my model is good ?

Train/validation/test

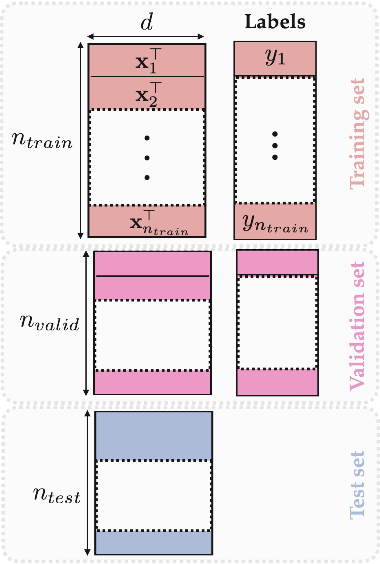




Train, validation and test data

- Data are divided in two sets: a train and a test set
- Learning a ML model = on the train set where you know the output of the model
- The test set is **never available**, used only to deploy the model

Train/validation/test



Train, validation and test data

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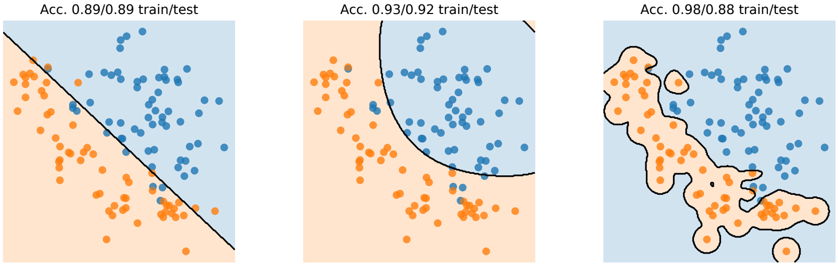
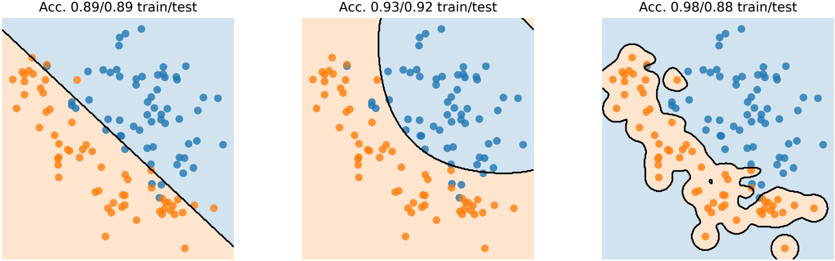
- Learning a ML model = on the train set where you know the output of the model
- The test set is **never available**, used only to deploy the model
- A validation set is often used to **calibrate the model** (choose hyperparameters), and **evaluate the generalization properties** of your model

Underfitting and overfitting

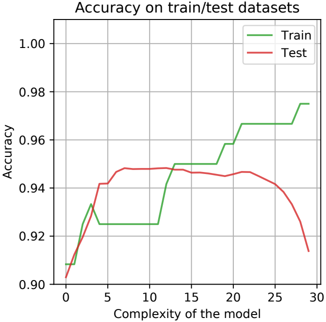


Underfitting and overfitting



Complexity of a model

- Under-fitting when the model is too simple.
- Over-fitting occurs when the model is too complex
- Training data performance is not a good proxy for testing performance.
- We want to predict well on new data!
- Parameter and model validation.



Empirical risk minimization

Train by minimizing the train error

To find f the idea is to **minimize the averaged error** on the training samples:

$$\min_f \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\mathbf{x}_i)) + \lambda \,\mathrm{Reg}(f) \tag{ERM}$$

- It is called **empirical risk minimization (ERM)**
- Given the loss, finds the "best" f on the training data
- Teacher/student analogy
- Same idea applies for unsupervised problem (minimizing reconstruction error)

... but we want generalization !

- We want f to be good outside the training samples
- Add regularization ! (limit the complexity of f)

Plan

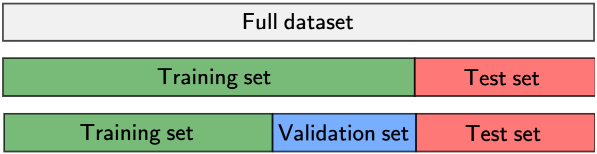
Model selection and validation

Bias-complexity tradeoff

$$\text{excess risk} = \text{estimation error} + \text{approximation error}$$

Conlusion: we have to select a model that is not too complex but not too simple !

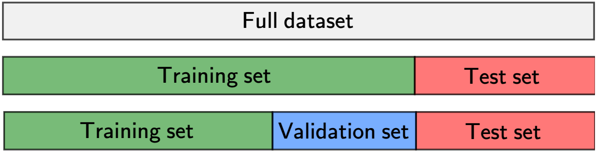
Splitting the data



Principle of Hold-Out cross-validation

- Split the training data in a training and validation sets (non overlapping).
- Train different models (different methods and/or parameters) on the train data.
- Evaluate performance on the validation data and select the method/parameters with best performance.

Splitting the data



Principle of Hold-Out cross-validation

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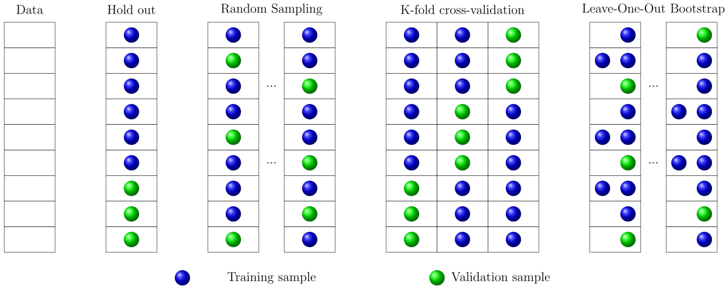
Final estimator

- After selecting the optimal parameters, one should retrain the estimator on the whole training dataset using the optimal method/parameters.

Different ways to split the data



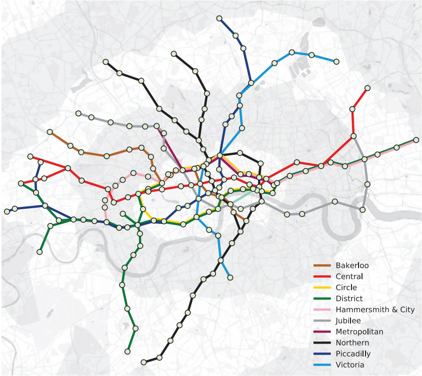
Data splitting for cross-validation Arlot and Celisse 2010

- The training data is split in non-overlapping training/validation sets.
- **Hold-Out** uses a unique split and computes the performance on the validation set.
- More robust cross-validation approaches actually investigate several splits of the data and compute the average performance:
  - **K-fold** (split in K sets and use one split as test for all k)
  - Random sampling (aka **Shuffle split**) draws several random splittings.
- Scikit-learn implementation : `sklearn.model_selection.cross_validate`

Plan

Motivating examples

- Traffic forecasting (e.g. ETA estimation): GNN for Google Maps Derrow-Pinion et al. 2021.



Motivating examples

- Traffic forecasting (e.g. ETA estimation): GNN for Google Maps Derrow-Pinion et al. 2021.
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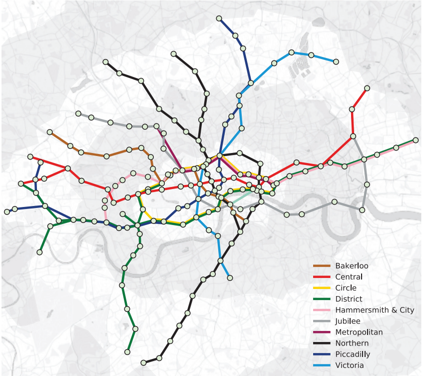
- Drug Repositioning: action of drugs and their interactions $\rightarrow$ graph Barabási, Gulbahce, and Loscalzo 2011.



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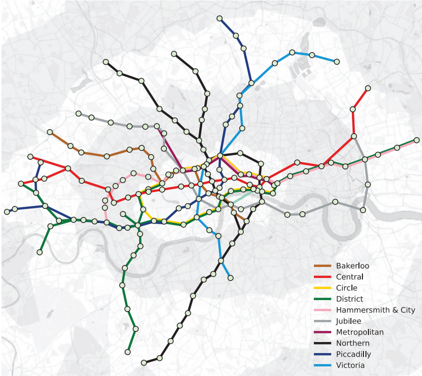

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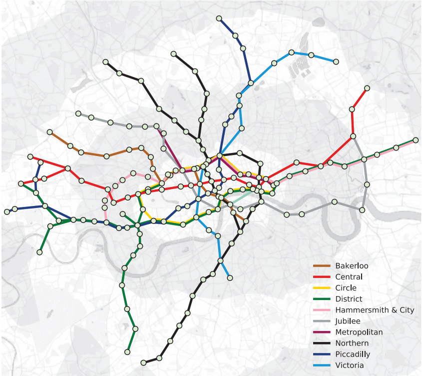

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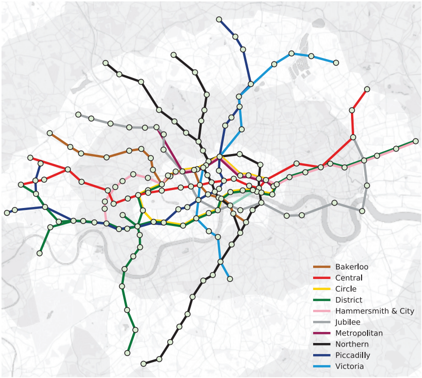
- and more...



What is a graph ?

Definition

A graph $G = (V, E)$ is defined as a set of **vertices** V, which are connected by a set of **edges** $E \subset V \times V$.

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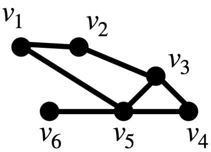
- Example of **undirected** graph

$$G = (V, E)$$



Adjacency matrix

$$\mathbf{A} = \begin{array}{c c} & \begin{array}{cccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \end{array} \\ v_1 & \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \end{array} = \mathbf{A}^\top$$

Adjacency matrix

The adjacency $\mathbf{A} \in \mathbb{R}^{|V| \times |V|}$ is defined as

$$[\mathbf{A}]_{ij} = \begin{cases} 1 \text{ if } (v_i, v_j) \in E (\text{often noted as } v_i \sim v_j) \\ 0 \text{ otherwise} \end{cases}$$

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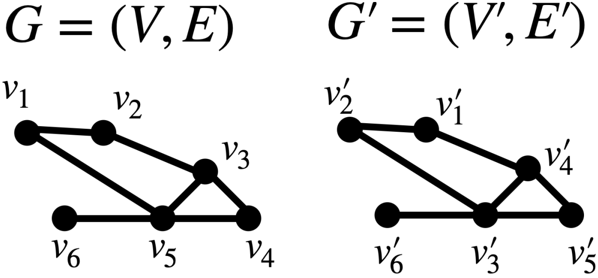
Isomorphic graphs

The definition depends on the ordering of the nodes.



$$\mathbf{A} = \mathbf{P}^\top \mathbf{A}' \mathbf{P}$$

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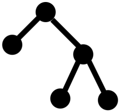
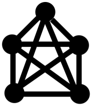
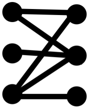
Some special structures



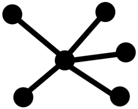
Tree



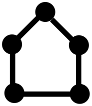
Complete graph



Bipartite graph



Star graph

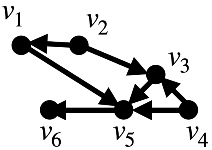


Circular graph

What is a graph ?

- Example of **directed** graph

$$G = (V, E)$$



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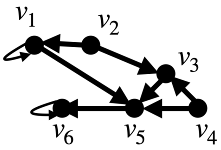
What is a graph ?

- Example of **directed** graph with **self-loops**.

$$G = (V, E)$$



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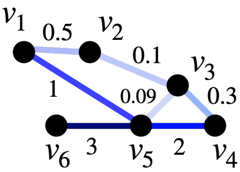
What is a graph ?

Weighted graph

A weighted graph $G = (V, E)$ associates non-negative weights to each edge.

- Example of **weighted** graph

$$G = (V, E)$$



Weight matrix

$$\mathbf{W} = \begin{pmatrix} 0 & 0.5 & 0 & 0 & 1 & 0 \\ 0.5 & 0 & 0.1 & 0 & 0 & 0 \\ 0 & 0.1 & 0 & 0.3 & 0.09 & 0 \\ 0 & 0 & 0.3 & 0 & 2 & 0 \\ 1 & 0 & 0.09 & 2 & 0 & 3 \\ 0 & 0 & 0 & 0 & 3 & 0 \end{pmatrix}$$

What is a graph ?

Degree of a node

The degree of a node v_i is

$$d_i = |\{v \in V : v \sim v_i\}| = \sum_{j=1}^{|V|} A_{ij}$$

The degree matrix is $\mathbf{D} = \mathrm{diag}(d_1, \cdots, d_{|V|})$.

What is a graph ?

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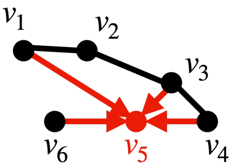
$$G = (V, E)$$



Adjacency matrix | Degree

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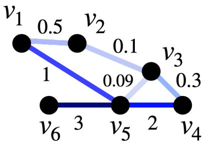
What is a graph ?

Degree of a node

The degree of a node v_i in a weighted graph is

$$d_i = \sum_{j=1}^{|V|} W_{ij}$$

$$G = (V, E)$$



$$\begin{array}{cc} & \text{Weight matrix} \\ \mathbf{W} = & \begin{pmatrix} 0 & 0.5 & 0 & 0 & 1 & 0 \\ 0.5 & 0 & 0.1 & 0 & 0 & 0 \\ 0 & 0.1 & 0 & 0.3 & 0.09 & 0 \\ 0 & 0 & 0.3 & 0 & 2 & 0 \\ 1 & 0 & 0.09 & 2 & 0 & 3 \\ 0 & 0 & 0 & 0 & 3 & 0 \end{pmatrix} \end{array} \quad \begin{array}{c} \text{Degree} \\ \begin{pmatrix} 1.5 \\ 0.6 \\ 0.49 \\ 2.3 \\ 4.09 \\ 3 \end{pmatrix} \end{array}$$

What is a graph ?

Laplacian matrix

The Laplacian matrix of a undirected graph is defined as

$$\mathbf{L} = \mathbf{D} - \mathbf{W} \text{ where } \mathbf{D} \text{ is the degree matrix}$$

Properties

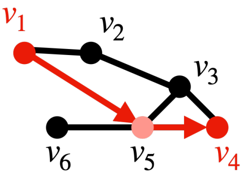
On the board

What is a graph ?

Shortest-path matrix

The shortest-path between $v, v' \in V$ is the path that connects v, v' such that the sum of the weights of its constituent edges is minimized.

$$G = (V, E)$$



Shortest-path matrix

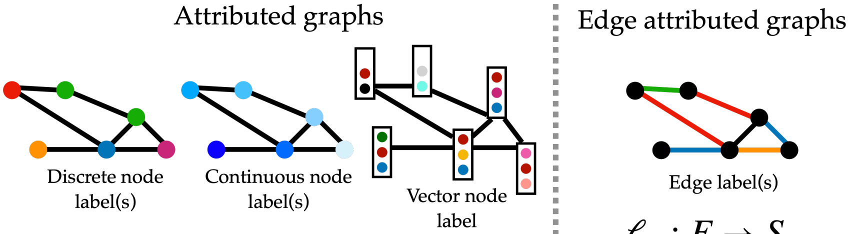
$$\mathbf{S} = \begin{pmatrix} 0 & 1 & 2 & 2 & 1 & 2 \\ 1 & 0 & 1 & 2 & 2 & 3 \\ 2 & 1 & 0 & 1 & 1 & 2 \\ 2 & 2 & 1 & 0 & 1 & 2 \\ 1 & 2 & 1 & 1 & 0 & 1 \\ 2 & 3 & 2 & 2 & 1 & 0 \end{pmatrix}$$

- Dijkstra's algorithm computes all the shortest paths from a single node in $O(|E| + |V| \log(|V|))$.
- All-pairs shortest paths with Floyd–Warshall algorithm in $O(|V|^3)$.

What is a graph ?

Attributed graphs

Most graphs encountered in ML also have **attributes**.



$$\ell_G : V \to S \ (\subset \mathbb{R}^N)$$

$$\ell_E : E \to S_E$$

ML vs structured data

Problems

ML vs structured data

Problems

- Can we encode a graph G as a vector $\in \mathbb{R}^d$ to use standard ML methods ?

ML vs structured data

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- How can we handle the combinatoric nature of graphs ?

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- Can we encode a graph G as a vector $\in \mathbb{R}^d$ to use standard ML methods ?
- Can we build ML methods with the raw representation of G ? How to adapt ML methods that work on vectors ?
- How can we handle the combinatoric nature of graphs ?
- ML outputs should be permutation invariant ? equivariant ?

ML vs structured data

Problems

- Can we encode a graph G as a vector $\in \mathbb{R}^d$ to use standard ML methods ?
- Can we build ML methods with the raw representation of G ? How to adapt ML methods that work on vectors ?
- How can we handle the combinatoric nature of graphs ?
- ML outputs should be permutation invariant ? equivariant ?
- When data $=$ vectors in one graph how can we take into account the structure of the graph ?

ML vs structured data

Problems

- Can we encode a graph G as a vector $\in \mathbb{R}^d$ to use standard ML methods ?
- Can we build ML methods with the raw representation of G ? How to adapt ML methods that work on vectors ?
- How can we handle the combinatoric nature of graphs ?
- ML outputs should be permutation invariant ? equivariant ?
- When data = vectors in one graph how can we take into account the structure of the graph ?
- When data = vectors can we find an (interesting) graph that represent these data ?

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