Machine Learning

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Standard programming

Solving a task with a computer

- input and output definition
- algorithm design
- implementation

Examples

- jpeg image converter
- interactive 3D world
- computational fluid dynamics
- chess program
- spam filtering (with e.g. SpamAssassin)

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100% human design

Machine learning

Machine programming

- climbing one step in abstraction
- designing programs with a program
- output: a program that solves a task
- input?

Machine learning

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Learning from examples

- input: a set of pairs (input, output)
- output: a program g
- if ($\mathbf{x}$, $\mathbf{y}$) is in the set, g should output $\mathbf{y}$ if given $\mathbf{x}$ as input (i.e., $g(\mathbf{x}) = \mathbf{y}$)
- this is called supervised learning
- example: produce SpamAssassin using tagged emails!

Minimal formal model

Data spaces

- $\mathcal{X}$: input space ($\mathbf{X} \in \mathcal{X}$)
- $\mathcal{Y}$: output space ($\mathbf{Y} \in \mathcal{Y}$)
  - if $|\mathcal{Y}| < \infty$: classification
  - if $\mathcal{Y} = \mathbb{R}$: regression

Programs

- mathematical version: a function g from $\mathcal{X}$ to $\mathcal{Y}$
- running the program: $g(\mathbf{X}) = \mathbf{Y}$
- preferred term: model

Machine learning program

- input: a data set $\mathcal{D} = \{(\mathbf{X}_i, \mathbf{Y}_i)\}_{1 \leq i \leq N}$ (or a data sequence)
- output: a function from $\mathcal{X}$ to $\mathcal{Y}$ (a model)

Is machine learning feasible?

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Yes!

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Yes!

- strong theoretical guarantees
- Probably Approximately Correct (PAC) framework
  - we look for g (the task solving program/model) in some class of models
  - is the class is not too complex, g can be recovered approximately with high probability given a reasonable amount (N) of input data
- Asymptotic framework
  - in addition the class of models can grow in complexity with the data size
  - then the best possible g (no restriction) can be reached asymptotically (almost surely in some cases): this is a consistency property

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How?

Neighbors

Additional hypothesis

- $\mathcal{X}$ is equipped with a dissimilarity d
- d is a dissimilarity on $\mathcal{X}$ iff:
  1. d is a function from $\mathcal{X} \times \mathcal{X}$ to $\mathbb{R}^+$
  2. $\forall \mathbf{X}, \mathbf{X}',\ d(\mathbf{X}, \mathbf{X}') = d(\mathbf{X}', \mathbf{X})$
  3. $\forall \mathbf{X}, \mathbf{X}',\ \mathbf{X} \neq \mathbf{X}' \Leftrightarrow d(\mathbf{X}, \mathbf{X}') > 0$

Neighbors

- $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$
- nn is the function from $\mathcal{X} \times \{1, \ldots, N\}$ to $\{1, \ldots, N\}$ such that

$$(1) \qquad d(\mathbf{x}, \mathbf{X}_{nn(\mathbf{x},1)}) \leq d(\mathbf{x}, \mathbf{X}_{nn(\mathbf{x},2)}) \leq \cdots \leq d(\mathbf{x}, \mathbf{X}_{nn(\mathbf{x},N)})$$

$$(2) \quad \text{if } d(\mathbf{x}, \mathbf{X}_{nn(\mathbf{x},k)}) = d(\mathbf{x}, \mathbf{X}_{nn(\mathbf{x},k+1)}) \text{ then } nn(\mathbf{x}, k) < nn(\mathbf{x}, k+1)$$

- denoted $nn_{\mathcal{D}}$ if needed

K nearest neighbors

Finite output space

- when $|\mathcal{Y}| < \infty$
- given as input the data set $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$ and the parameter K, the K nearest neighbors (K-nn) machine learning program outputs g_{K-nn} defined by

$$g_{K-nn}(\mathbf{x}) = \arg\max_{\mathbf{y} \in \mathcal{Y}} \left| \left\{ k \in \{1, \ldots, K\} \,|\, \mathbf{Y}_{nn_{\mathcal{D}}(\mathbf{x},k)} = \mathbf{y} \right\} \right|$$

- in simple terms: $g_{K-nn}(\mathbf{x})$ is the most common value of $\mathbf{y}$ in the examples that are the K closest ones to $\mathbf{x}$

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Consistency

- if $\mathcal{X}$ is a finite dimensional Banach space and $|\mathcal{Y}| = 2$
- then the K-nn method is consistent if K depends on N, K_N, in such a way that $K_N \to \infty$ and $\frac{K_N}{N} \to 0$

In practice?

Algorithm choice

- numerous ML algorithms
- with parameters (e.g., K for the K-nn method)
- How to chose the “best” model?

Efficiency

- computational efficiency
- data efficiency

And many other issues...

Machine learning vs AI

Artificial Intelligence

> *Artificial Intelligence (AI) is intelligence displayed by machines, in contrast with the natural intelligence (NI) displayed by humans and other animals.*
>
> Wikipedia AI page

Machine learning

- is about learning:
  - this is only a small part of intelligence!
  - a data set is needed: it is produced by humans (limited autonomy)
- ML is only a tool that might be useful (in the future!) to build real AI
- beware of syllogisms: what *can* be solved with human intelligence does not always *need* intelligence to be solved

Outline

Judging a ML algorithm

Supervised learning

- input: $\mathcal{D} = \{(\mathbf{X}_i, \mathbf{Y}_i)\}_{1 \leq i \leq N}$
- output: $g : \mathcal{X} \to \mathcal{Y}$
- "ideally" we would like that $\forall i, g(\mathbf{X}_i) = \mathbf{Y}_i$

Weakening the goal

- $\forall i, g(\mathbf{X}_i) = \mathbf{Y}_i$ is too strong
  - limited knowledge
  - intrinsic randomness
- approximate answers, i.e. $\forall i, g(\mathbf{X}_i) \simeq \mathbf{Y}_i$

Quality of an output

Loss function

A loss function l is

- a function from $\mathcal{Y} \times \mathcal{Y}$ to $\mathbb{R}^+$
- such that $\forall \mathbf{Y} \in \mathcal{Y}, \quad l(\mathbf{Y}, \mathbf{Y}) = 0$

Interpretation

$l(g(\mathbf{X}), \mathbf{Y})$ measures the loss incurred by the user of a model g when the true value $\mathbf{Y}$ is replaced by the value $g(\mathbf{X})$.

Weakening the goal

- $\forall i, g(\mathbf{X}_i) = \mathbf{Y}_i$ is replaced by
- $\forall i, l(g(\mathbf{X}_i), \mathbf{Y}_i)$ should be as small as possible

Examples

$\mathcal{Y} = \mathbb{R}$ (Regression)

- $l_2(p, t) = (p - t)^2$
- $l_1(p, t) = |p - t|$
- $l_{APE}(p, t) = \frac{|p-t|}{|t|}$

$|\mathcal{Y}| < \infty$ (Classification)

- $l_b(p, t) = \mathbf{1}_{p \neq t}$
- general case when $\mathcal{Y} = \{y_1, y_2\}$

$l(p,t)$	$t = y_1$	$t = y_2$
$p = y_1$	0	$l(y_1, y_2)$
$p = y_2$	$l(y_2, y_1)$	0

asymmetric costs are important in practice (think SPAM versus non SPAM)

Quality of a model

From local to global

- loss functions work at a local scale: what happens for *one* input
- we need a *global* assessment of a model g: how will the model behave if deployed?

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Empirical risk

- simple aggregation of local losses: average loss
- the empirical risk of a model g on a data set $\mathcal{D} = \{(\mathbf{X}_i, \mathbf{Y}_i)\}_{1 \leq i \leq N}$ for a loss function l is

$$\widehat{R}_l(g, \mathcal{D}) = \frac{1}{N} \sum_{i=1}^{N} l(g(\mathbf{X}_i), \mathbf{Y}_i) = \frac{1}{|\mathcal{D}|} \sum_{(\mathbf{x},\mathbf{y}) \in \mathcal{D}} l(g(\mathbf{x}), \mathbf{y})$$

- a good model has a low empirical risk

Data science intermezzo

Loss functions

- should not be chosen lightly
- have complex consequences, for instance
  - asymmetric losses can be seen as example weighting
  - APE loss induces underestimation
- a good data scientist knows how to translate objectives into loss functions

Empirical risk

- is only an average: does not rule out extreme behavior
- in particular, the actual loss can strongly vary with the "location" of $\mathbf{x}$ in $\mathcal{X}$
- reporting only the empirical risk is not sufficient!

Confusion matrix and co.

Confusion matrix

- when $\mathcal{Y}$ is finite, one should report a confusion matrix $\widehat{C}(\mathcal{D})$ with entries

$$\widehat{C}_{\mathbf{y},\mathbf{y}'} = |\{i \in \{1,\dots,N\} \mid g(\mathbf{X}_i) = \mathbf{y} \text{ and } \mathbf{Y}_i = \mathbf{y}'\}|$$

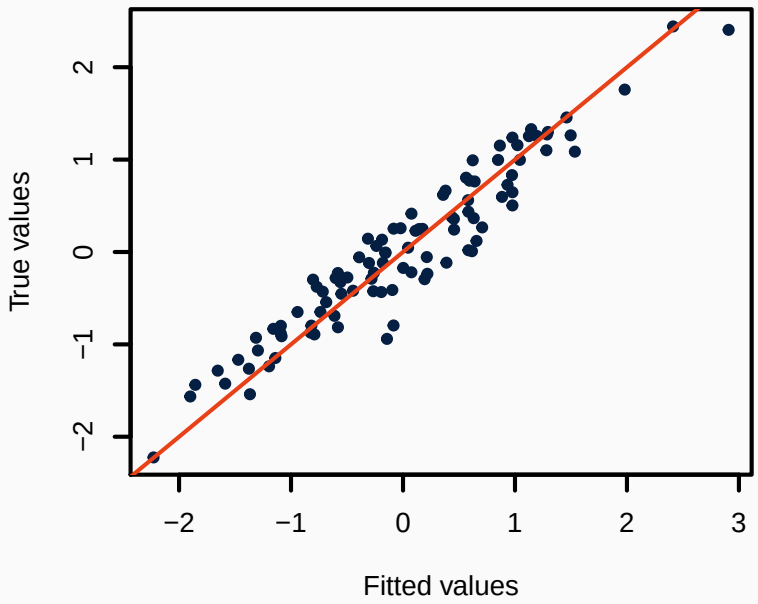
- $\widehat{C}_{\mathbf{y},\mathbf{y}'}$ counts the number of times g outputs $\mathbf{y}$ while it should output $\mathbf{y}'$
- transposed conventions have been used

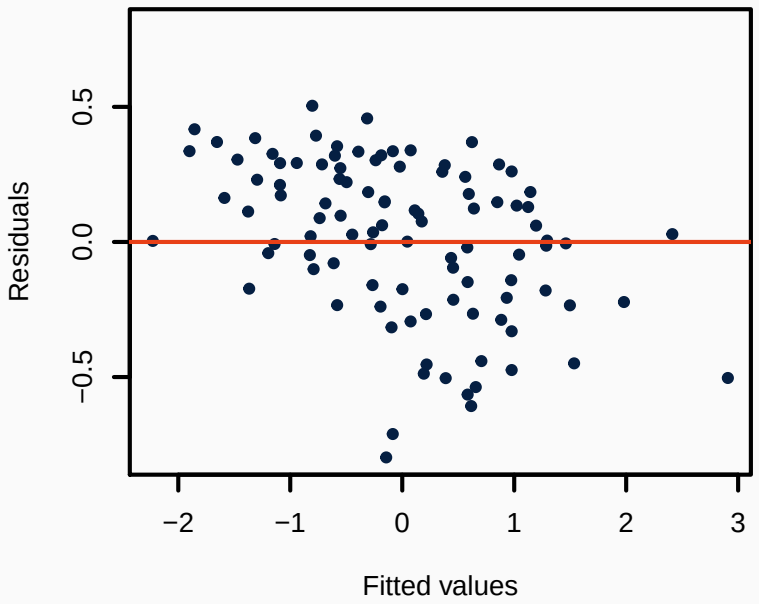
Positive and negative

- when $\mathcal{Y} = \{-1, 1\}$
- true positive: $g(\mathbf{X}_i) = \mathbf{Y}_i = 1$
- false negative: $g(\mathbf{X}_i) = -\mathbf{Y}_i = -1$
- etc.

Diagnostic plots

- when $\mathcal{Y} = \mathbb{R}$
- originally for linear regression (standard statistical model)
- some are useful for general regression models:
  - scatter plot of $\mathbf{Y}_i$ as a function of $g(\mathbf{X}_i)$
  - scatter plot of $\mathbf{Y}_i - g(\mathbf{X}_i)$ as a function of $g(\mathbf{X}_i)$ (residual plot)





Generalization

New data

- assume g is such as $\widehat{R}_l(g, \mathcal{D})$ is small
- what can we expect on a new data set $\widehat{R}_l(g, \mathcal{D}')$?
- generalization performances
- if g is learned on $\mathcal{D}$ and $\widehat{R}_l(g, \mathcal{D}) \ll \widehat{R}_l(g, \mathcal{D}')$, g is overfitting

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Mathematical model

- stationary behavior: $\mathcal{D} \simeq \mathcal{D}'$
- hypotheses:
  - observations are random variables with values in $\mathcal{X} \times \mathcal{Y}$
  - they are distributed according to a fixed and unknown distribution D
  - observations are independent

Risk

Data set revisited

- $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$
- $(\mathbf{X}_i, \mathbf{Y}_i) \sim D$
- $\mathcal{D} \sim D^N$ (product distribution)

Risk of a model

- The risk of g for the loss function l is

$$R_l(g) = \mathbb{E}_{(\mathbf{X},\mathbf{Y})\sim D}(l(g(\mathbf{X}), \mathbf{Y}))$$

- we should write $R_l(g, D)$
- the empirical risk $\widehat{R}_l(g, \mathcal{D})$ is a random variable
- if g is fixed or independent from $\mathcal{D}$, then $\widehat{R}_l(g, \mathcal{D}) \xrightarrow[|\mathcal{D}|\to\infty]{a.s.} R_l(g)$ (strong law of large numbers)

Formal definition of ML

Supervised learning

- input: a data set $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$ with $\mathcal{D} \sim D^N$ and a loss function l
- output: a function $g_{\mathcal{D}} : \mathcal{X} \to \mathcal{Y}$
- goal: ensure that $R_l(g_{\mathcal{D}})$ is as small as possible
- best risk

$$R_l^* = \inf_{g:\mathcal{X}\to\mathcal{Y}} R_l(g)$$

Consistency

a machine learning algorithm is universally (i.e. for any D)

- consistent if $\mathbb{E}_{\mathcal{D}\sim D^N}(R_l(g_{\mathcal{D}})) \xrightarrow[N\to\infty]{} R_l^*$
- strongly consistent if $R_l(g_{\mathcal{D}}) \xrightarrow[N\to\infty]{a.s.} R_l^*$

ML and statistical models

Statistical models

- specification for D (in general parametric)
- estimation with maximum likelihood
- numerous variants (especially Bayesian approaches)

Very different philosophies

- Machine Learning
  - performance oriented
  - universal consistency
  - limited post learning tuning, exploration, interpretation, etc.
- Statistical models
  - strong hypotheses
  - bad behavior under wrong specification
  - very rich framework for post estimation exploitation

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- Statistical models
  - strong hypotheses
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  - very rich framework for post estimation exploitation
- but many links!

Empirical risk minimization

A simple idea

- $R_l(g)$ cannot be computed as D is unknown
- but if $g \perp\!\!\!\perp \mathcal{D}$, $\widehat{R}_l(g, \mathcal{D}) \xrightarrow[|\mathcal{D}|\to\infty]{a.s.} R_l(g)$
- let's replace $R_l(g)$ by $\widehat{R}_l(g, \mathcal{D})$!

ERM algorithm

- choose a class of functions $\mathcal{G}$ from $\mathcal{X}$ to $\mathcal{Y}$
- define

$$g_{ERM,\mathcal{D}} = \arg\min_{g\in\mathcal{G}} \widehat{R}_l(g, \mathcal{D})$$

Empirical risk and learning

Empirical risk can be misleading

- for the 1-nn, in general:

$$\widehat{R}_l(g_{1-nn}, \mathcal{D}) = 0$$

  if g_{1-nn} has been constructed on $\mathcal{D}$
- indeed if all the $\mathbf{X}_i$ are distinct, $nn(\mathbf{X}_i, 1) = i$ and thus $g_{1-nn}(\mathbf{X}_i) = \mathbf{Y}_i$
- unrealistic value for $R_l(g_{1-nn})$

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Source of the problem

- the strong law of large numbers applies when the random variables are independent
- the $(l(g_{\mathcal{D}}(\mathbf{X}_i), \mathbf{Y}_i))_{1 \leq i \leq N}$ are dependent variables!

Methodology

Does ERM work?

- Yes!

Methodology

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- Yes!
- but one needs to control the complexity of the class of models $\mathcal{G}$
- this is a form of regularization: one cannot look for the model in an arbitrary class of models
- this will be addressed latter in the course

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Basic element for a solution

- apply the ML method to a data set $\mathcal{D}$, the learning set
- evaluate its risk on another independent data set $\mathcal{D}'$
- in summary: $\widehat{R}_l(g_{\mathcal{D}}, \mathcal{D}')$

Example

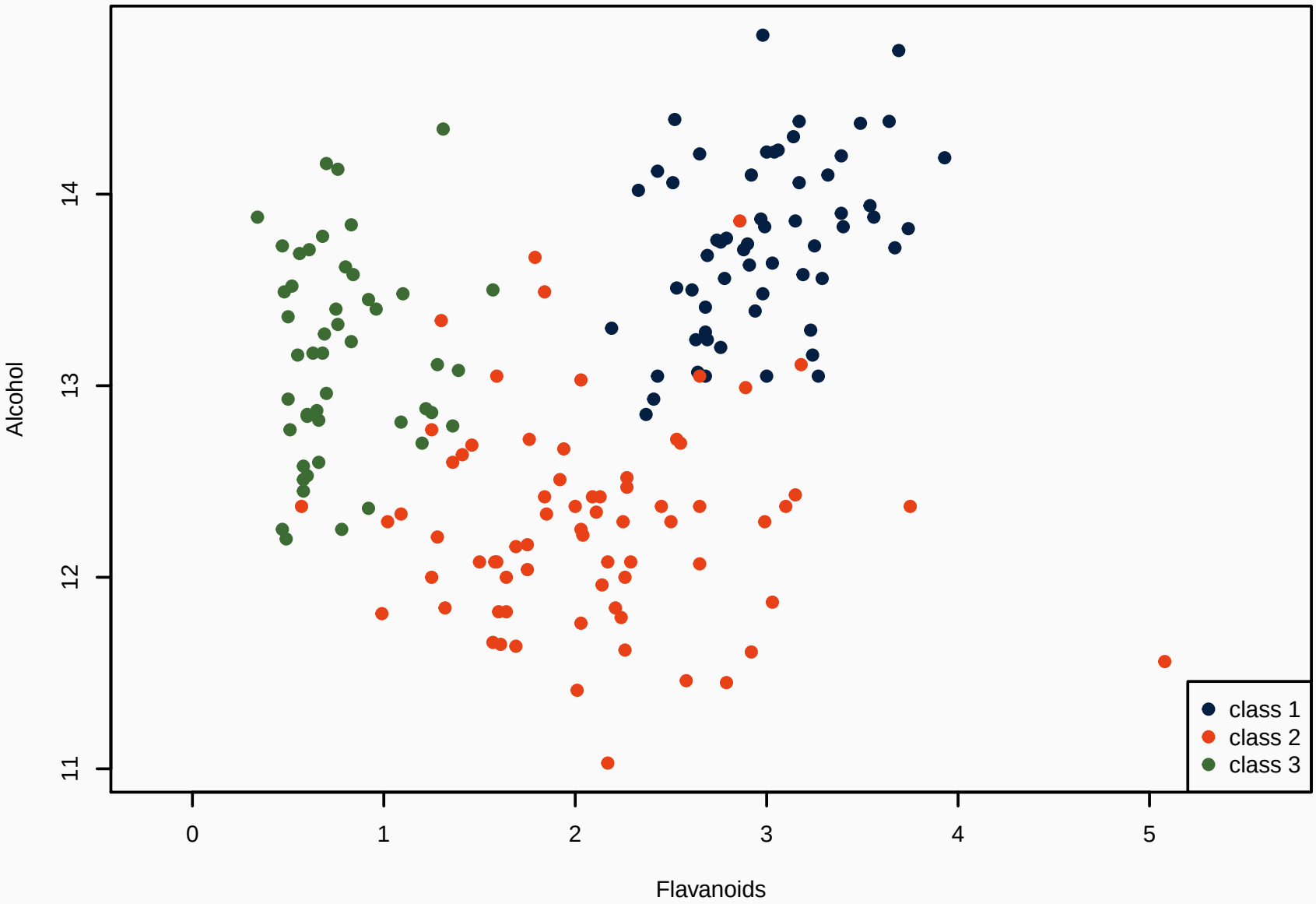
Data and loss

- chemical analysis of wines derived from three cultivars ($\mathcal{Y} = \{1, 2, 3\}$)
- 178 observations with 2 variables ($\mathcal{X} = \mathbb{R}^2$)
- $l(a, b) = \mathbf{1}_{a \neq b}$

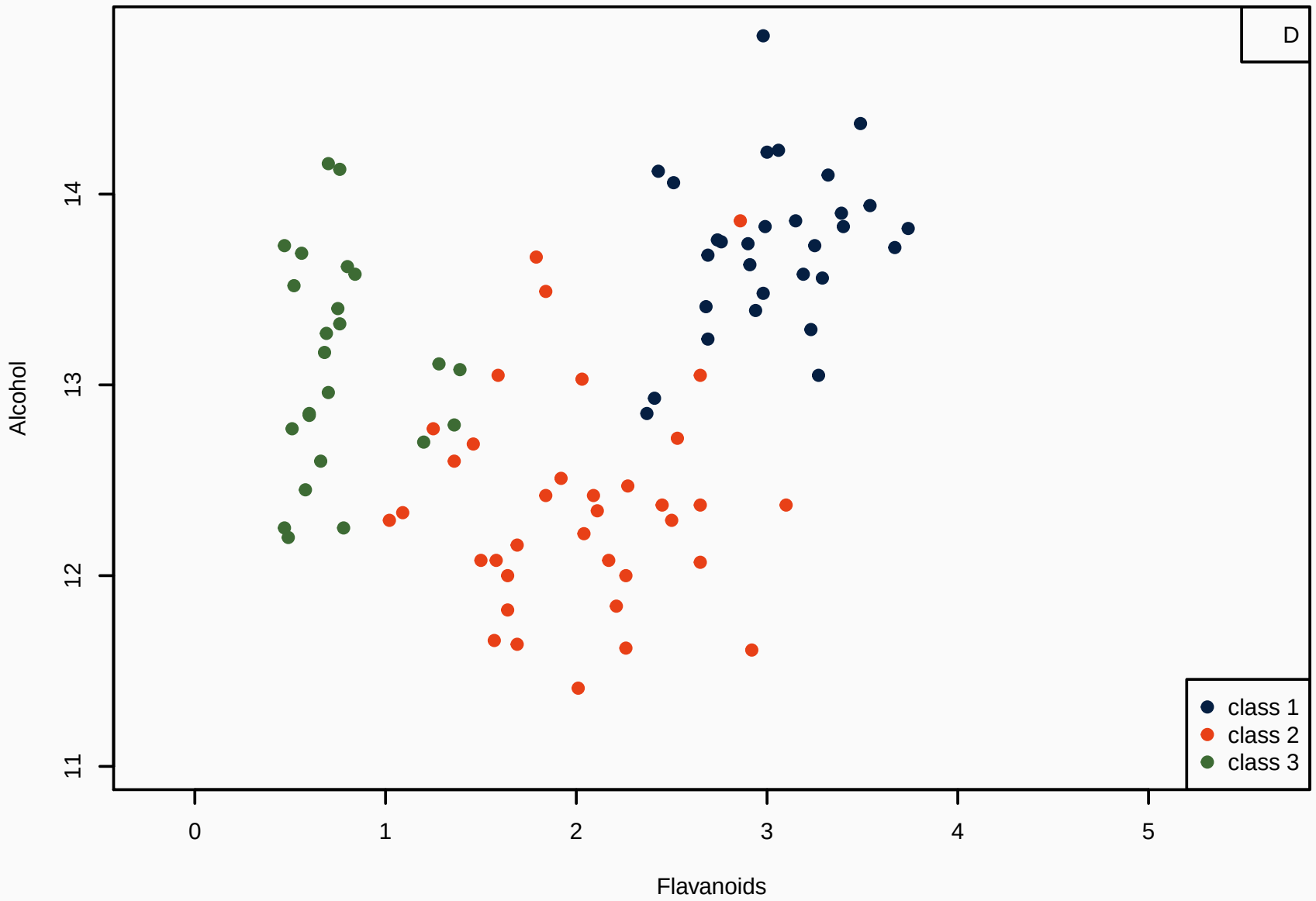
K-nn model

- use half the data for the learning set $\mathcal{D}$
- use the other half for empirical risk evaluation $\mathcal{D}'$

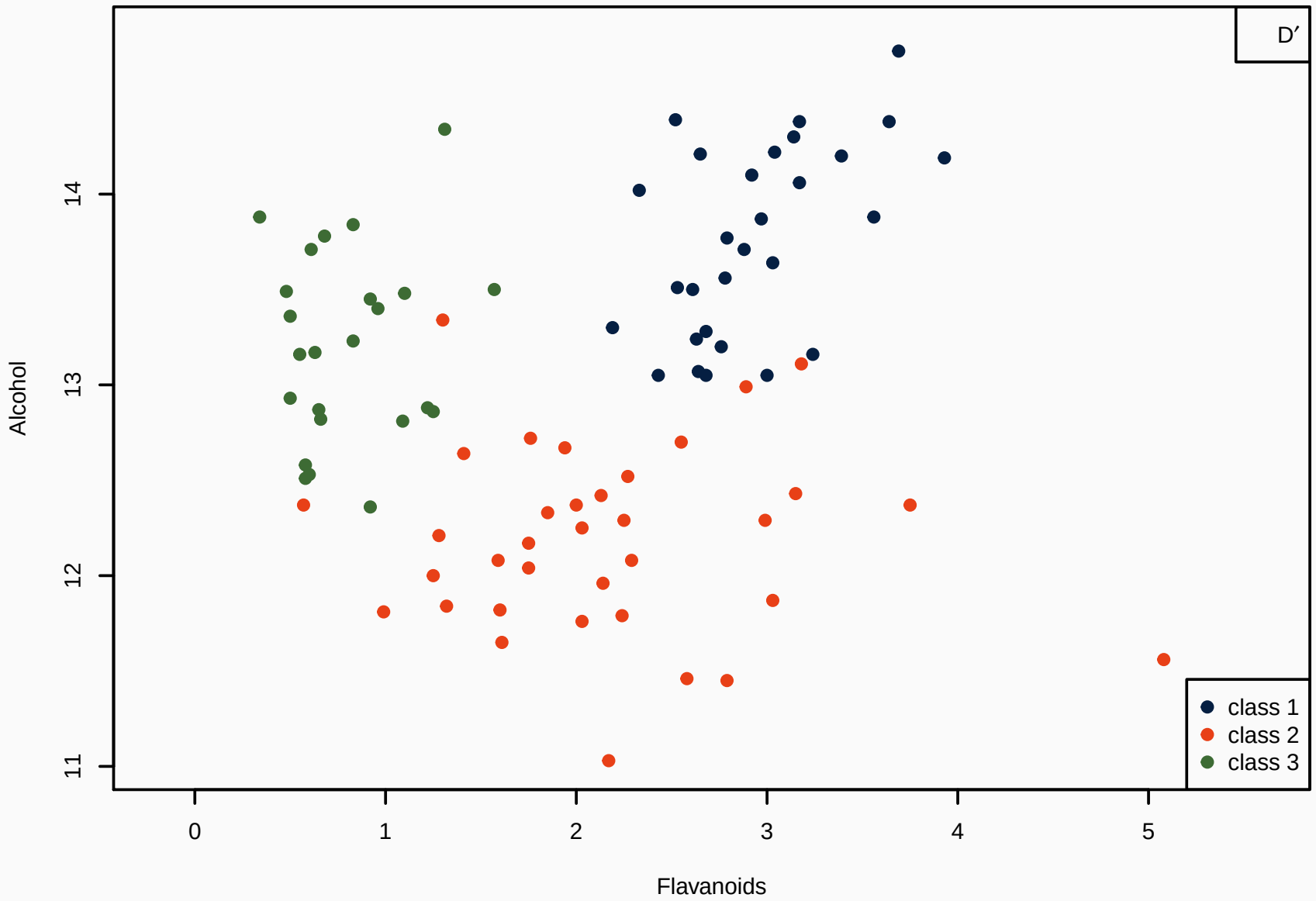
Example



Example


D
Alcohol
11
12
13
14
0
1
2
3
4
5
Flavanoids
class 1
class 2
class 3

Example


D′
Alcohol
14
13
12
11
0
1
2
3
4
5
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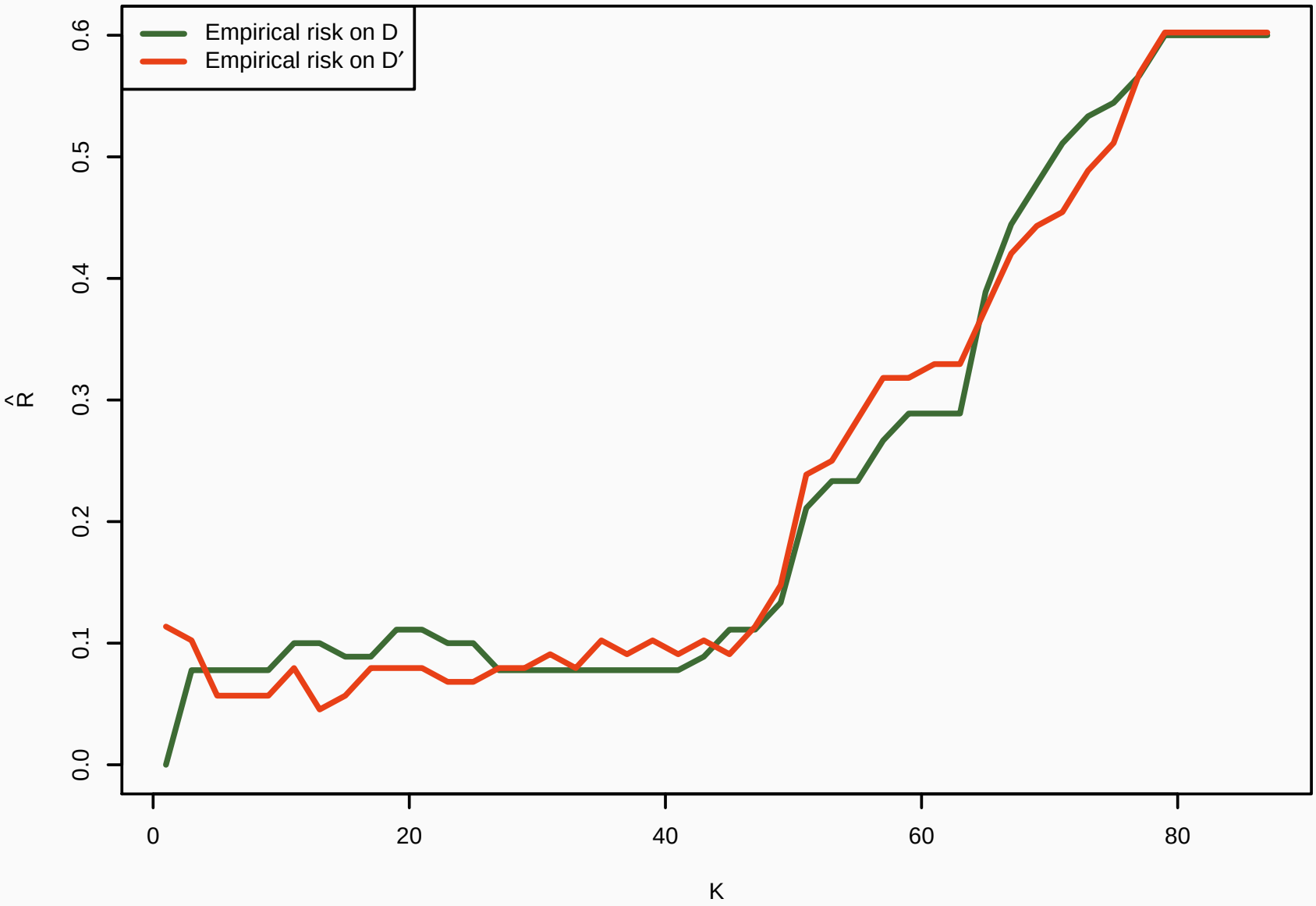
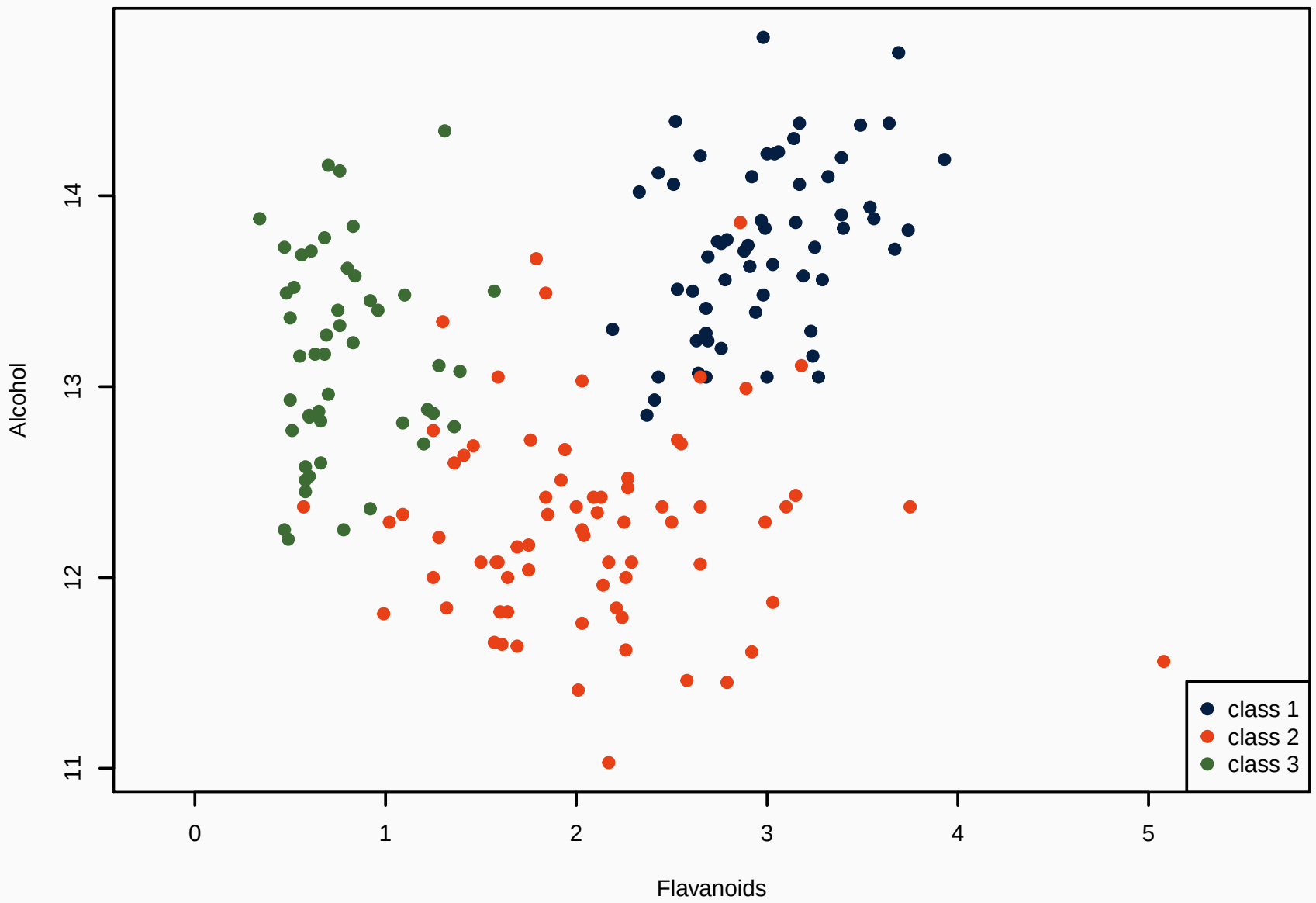
Results


Empirical risk on D
Empirical risk on D′
0.0
0.1
0.2
0.3
0.4
0.5
0.6
R̂
0
20
40
60
80
K

Outputs of the model



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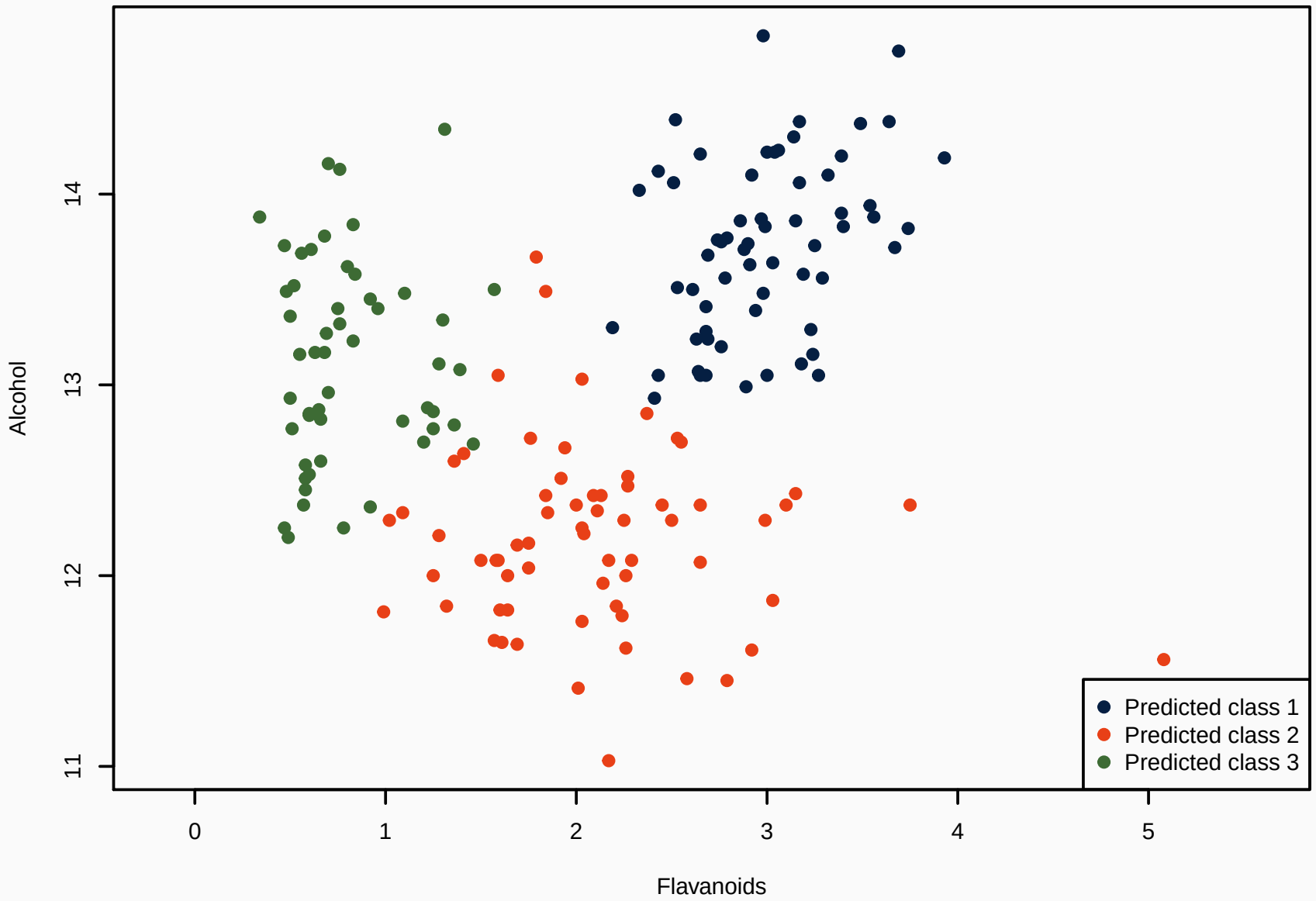

Basic general framework

1. split the data into $\mathcal{D}$ (learning), $\mathcal{D}'$ (validation) and $\mathcal{D}''$ (test)
2. for each machine learning algorithm $\mathcal{A}$ under study
   - 2.1 for each value θ of the parameters of the algorithm
     - 2.1.1 compute the model using θ on $\mathcal{D}$, $g_{\mathcal{A},\theta,\mathcal{D}}$
     - 2.1.2 compute $\widehat{R}_l(g_{\mathcal{A},\theta,\mathcal{D}}, \mathcal{D}')$
3. chose the best algorithm with the best parameter, $\mathcal{A}^*$ and θ^* (according to $\widehat{R}_l(., \mathcal{D}')$)
4. compute the best model $g^* = g_{\mathcal{A}^*,\theta^*,\mathcal{D}\cup\mathcal{D}'}$
5. compute $\widehat{R}_l(g^*, \mathcal{D}'')$

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Goals of this course

- describe state-of-the-art alternative for the algorithms
- study some theoretical aspects, e.g. empirical risk minimization
- describe better frameworks

Other learning contexts

Unsupervised learning

- $\mathcal{D} = ((\mathbf{X}_i)_{1 \leq i \leq N})$
- no target value!
- goal: “understanding” the data
- in practice, many concrete goals such as
  - finding clusters
  - finding frequent patterns
  - finding outliers
  - modeling the data distribution
  - etc.

Semi-supervised learning

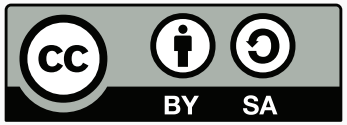
- a data set $\mathcal{D} = ((\mathbf{X}_i, \mathbf{Y}_i))_{1 \leq i \leq N}$
- another data set $\mathcal{D} = ((\mathbf{X}'_i)_{1 \leq i \leq N'})$
- standard supervised learning goal

Other learning contexts

Reinforcement learning

- completely different context:
  - an agent and its environment with associated states
  - a set of actions the agent can take
  - probabilistic transitions: when the agent takes an action, the global state changes as a consequence, possibly in a stochastic way
  - immediate reward: the reward gained by taking an action
- goal: computing an optimal policy
  - a policy maps states to actions
  - the value of a policy is the expected total reward obtained by following it
  - “easy” if everything is known
- learning: discovering the optimal policy by performing actions

Licence



Version

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