Introduction to statistical learning

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Outline

- 15 hours for this introduction.
- Materials: slides + exercises with R available here
  https://lrouviere.github.io/intro-machine-learning/
- 4 parts:
  1. Setting for statistical learning
  2. Parametric vs non parametric approaches
  3. Penalized regressions
  4. Trees and random forests
- Prerequisites: basics in probability, statistics (law of large numbers, estimation, bias, variance...) and data mining (linear model, logistic model, linear discriminant analysis...).

Part I

Mathematical setting for SL

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Statement

- Due to the digital revolution, we are faced with more and more complex data.
- Usual algorithms are not always efficient for these kind of data.

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Statement

- Due to the digital revolution, we are faced with more and more complex data.
- Usual algorithms are not always efficient for these kind of data.
- It is necessary to provide efficient algorithms which (automatically) learn from data.

History - see [Besse and Laurent,]

Period	Memory	Order of magnitude
1940-70	Byte	$n = 30, p \leq 10$
1970	MB	$n = 500, p \leq 10$
1980	MB	Machine Learning (computer science)
1990	GB	Data-Mining
2000	TB	$p > n$, statistical learning
2010	PB	n and p large, cloud, cluster...
2013	??	Big data
2017	??	Artificial Intelligence

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Computer resources $\Longrightarrow$

- Data Mining (patterns in large datasets, outliers...).
- Statistical learning (algorithms that can automatically learn from the data) $\Longrightarrow$ data decides, not the user!

Statistical learning

- Find algorithms that can automatically learn from the data.
- It is not the user who choose both an algorithm and/or the parameters, it is the data which decides.
- But...

Statistical learning

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- It is not the user who choose both an algorithm and/or the parameters, it is the data which decides.
- But...the user should tell to the computer how to do that.

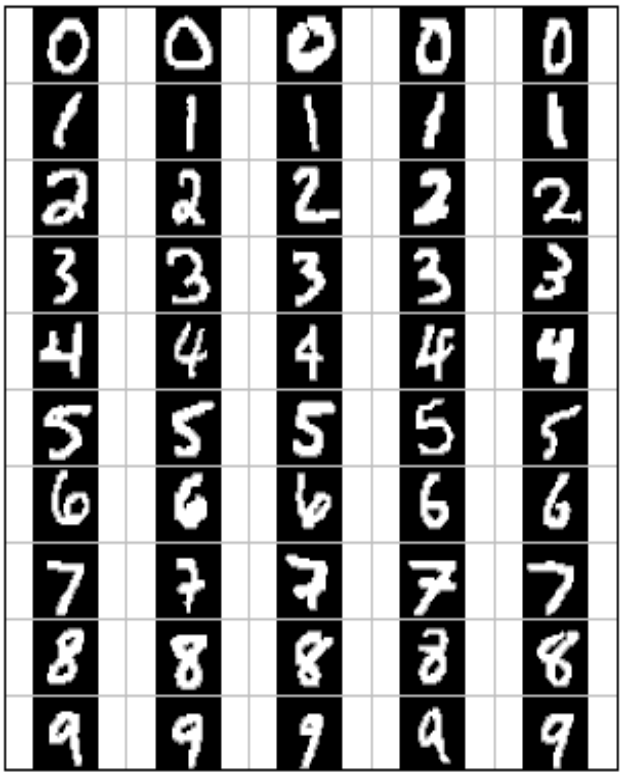
Conclusion

It is necessary to master the basics of machine learning algorithms.

Handwritten recognition

Statistical learning

Understand and learn a behavior from examples.



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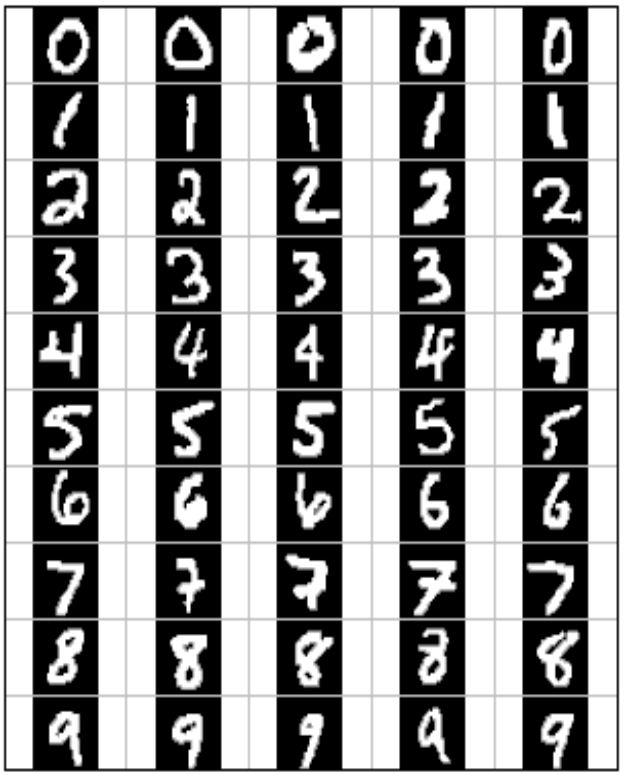
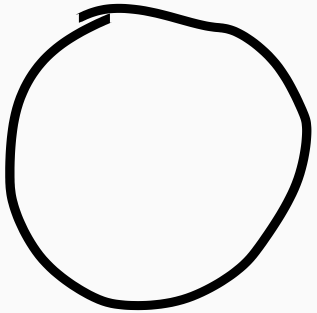
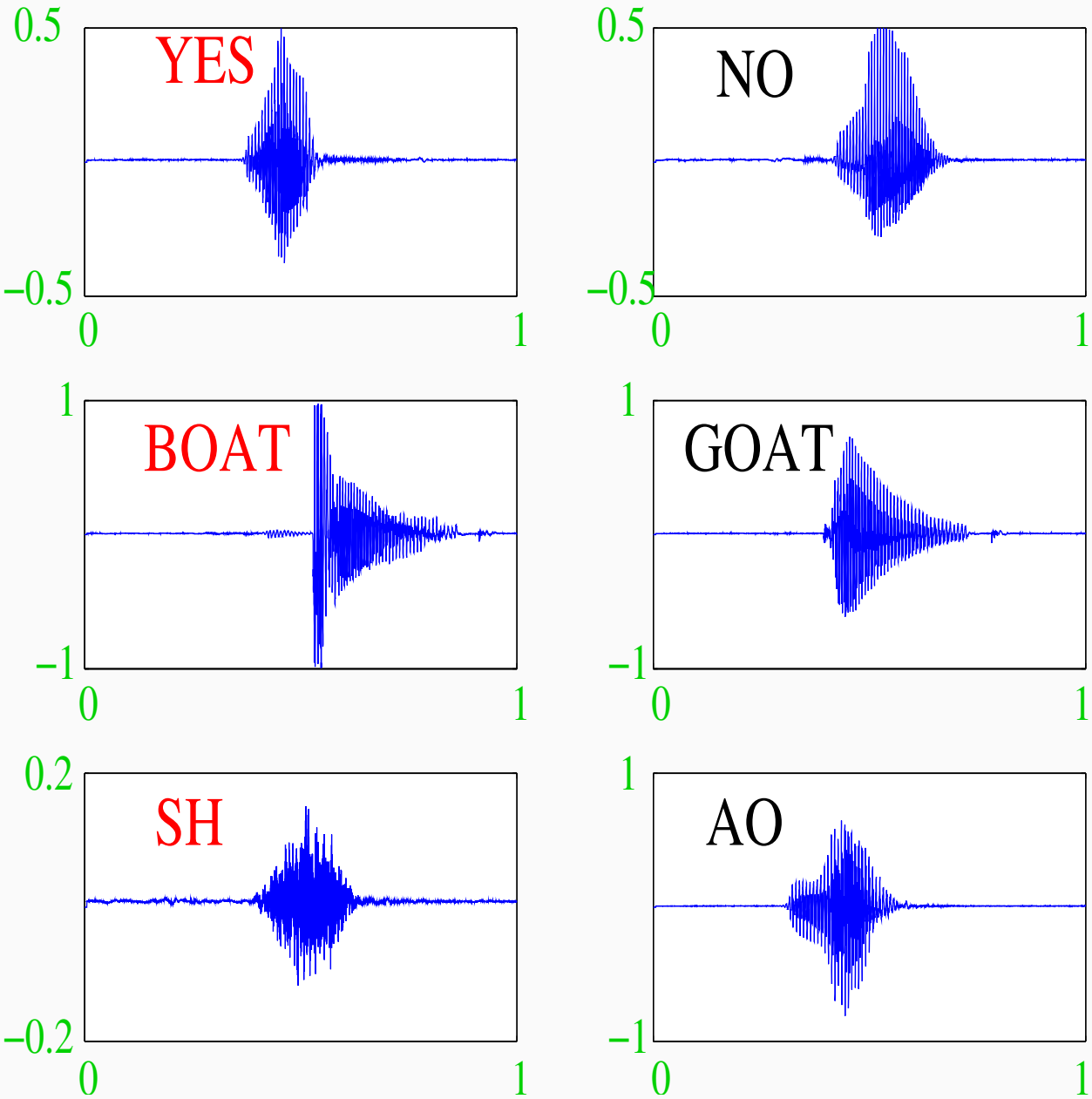




What is the number? 0, 1, 2...?

Speech recognition



Ozone prediction

- During one year, we have measured ozone concentration in a city (`V4`) ;
- Other meteorological variables are available (temperature, nebulosity, wind...).

```
> head(Ozone)
  V1 V2 V3 V4   V5 V6 V7 V8    V9  V10 V11   V12 V13
1  1  1  4  3 5480  8 20 NA    NA 5000 -15 30.56 200
2  1  2  5  3 5660  6 NA 38    NA   NA -14    NA 300
3  1  3  6  3 5710  4 28 40    NA 2693 -25 47.66 250
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Question

Can we explain and predict ozone concentration for tomorrow given meteorological predictions?

Spam detection

- For 4 601 emails, we have identified 1813 spams.
- In addition to this class label there are 57 variables indicating the frequency of some words and characters in the e-mail.

```
> spam[1:5,c(1:8,58)]
  make address  all num3d  our over remove internet type
1 0.00    0.64 0.64     0 0.32 0.00   0.00     0.00 spam
2 0.21    0.28 0.50     0 0.14 0.28   0.21     0.07 spam
3 0.06    0.00 0.71     0 1.23 0.19   0.19     0.12 spam
4 0.00    0.00 0.00     0 0.63 0.00   0.31     0.63 spam
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Question

From these informations, can we automatically detect if a new e-mail is (or not) a spam?

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  - k-means algorithms;
  - Mixture models...

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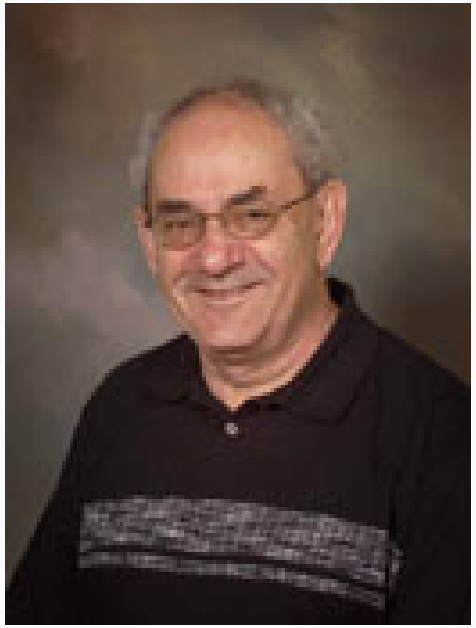
Wide range of applications

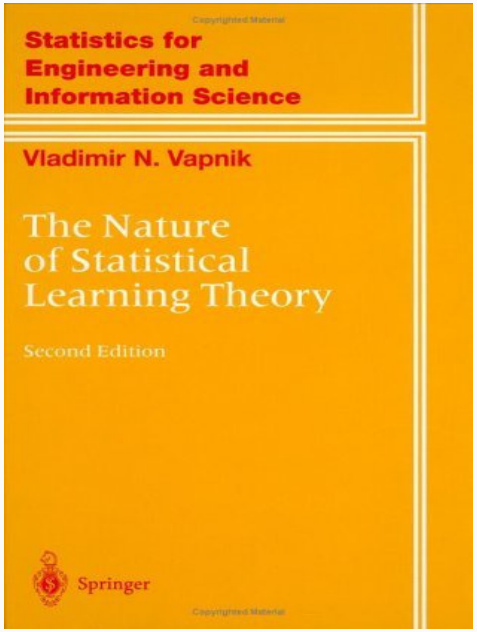
finance, economy, marketing, biology, medecine...

Theory for statistical learning

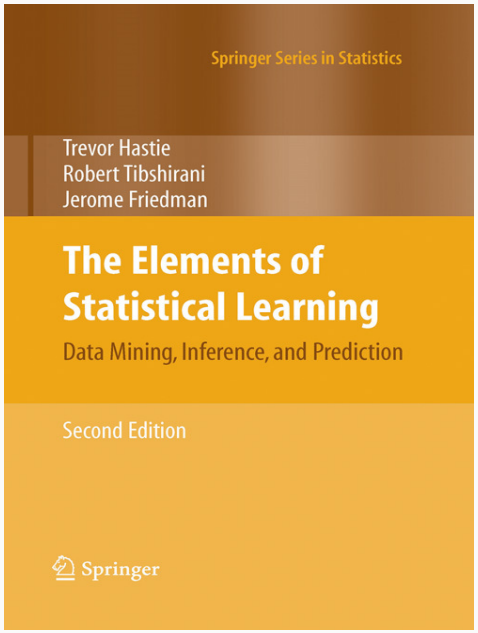
References

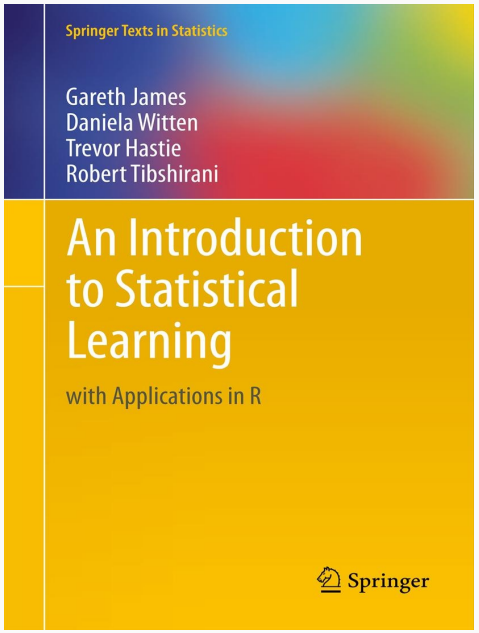
- Reference book: [Vapnik, 2000]





The Elements of Statistical Learning [Hastie et al., 2009, James et al., 2015]





- Available (with datasets, R commands...) at:

  https://web.stanford.edu/~hastie/ElemStatLearn/

  http://www-bcf.usc.edu/~gareth/ISL/

- This course is largely based on these two books.

Outline

Regression vs supervised classification

- Input/output data: $d_n = (x_1, y_1), \ldots, (x_n, y_n)$ where $x_i \in \mathcal{X}$ are the inputs $y_i \in \mathcal{Y}$ the outputs.

Goal

1. Explain connections between inputs x_i and outputs y_i;
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Vocabulary

- When the output $\mathcal{Y}$ is continuous, we are faced with a regression problem.
- When the output is categorical ($\mathrm{Card}(\mathcal{Y})$ finite), it is a supervised classification problem.

Examples

- Most of the presented problems are supervised learning problems: we have to predict an output y by inputs x:

y_i	x_i	
Number	picture	Super. Class.
Word	curve	Super. Class.
Spam	word frequencies	Super. Class
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Remark

- One output y_i.
- Wide range of input objects x_i (continuous, categorical, curves, pictures...).

Mathematical framework (begin)

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Interpretation

$\ell(y, y')$ measure the cost (error) between one prediction y' and one observation y.

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- Technical problem: this function is random $\Longrightarrow$ (very) difficult to minimize.

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Risk of a machine

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- Such a function $f^\star$ (if it exists) is called the optimal machine for the cost function ℓ.

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- Interpretation: the risk of f_n comes closer to the optimal risk as n grows.

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Important conclusion

In practice, it is crucial to choose a relevant cost function for the problem we are faced.

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- Indeed, $\forall f : \mathcal{X} \to \mathbb{R}$, we have

$$\mathcal{R}(f^\star) = \mathbf{E}[(Y - f^\star(X))^2] \leq \mathbf{E}[(Y - f(X))^2] = \mathcal{R}(f).$$

Universal consistency

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f_n is universally consistant if

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for any distribution of (X, Y).

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- The winner (called the Bayes rule) is

$$f^\star(x) = \begin{cases} -1 & \text{if } \mathbf{P}(Y = -1 | X = x) \geq \mathbf{P}(Y = 1 | X = x) \\ 1 & \text{otherwise.} \end{cases}$$

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$$f^\star(x) = \begin{cases} -1 & \text{if } \mathbf{P}(Y = -1 | X = x) \geq \mathbf{P}(Y = 1 | X = x) \\ 1 & \text{otherwise.} \end{cases}$$

- For any classification rule f,

$$\mathcal{R}(f^\star) = \mathbf{P}(f^\star(X) \neq Y) \leq \mathbf{P}(f(X) \neq Y) = \mathcal{R}(f).$$

Universal consistency

- Problem: $f^\star$ is unknown in practice. We have to find $f_n(x) = f_n(x, \mathcal{D}_n)$ such that $f_n(x) \approx f^\star(x)$.

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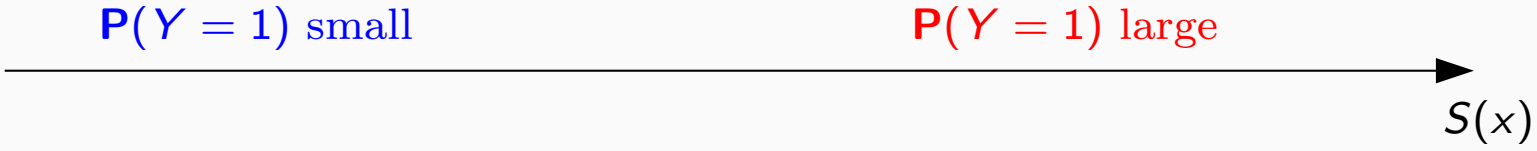
$\Longrightarrow$ See Exercise 1 - IML0.

Outline

Scoring function

- Always in binary classification ($\mathcal{Y} = \{-1, 1\}$).
- But... instead of a classification rule $f : \mathcal{X} \to \{-1, 1\}$, we want to find a function $S : \mathcal{X} \to \mathbb{R}$ such that



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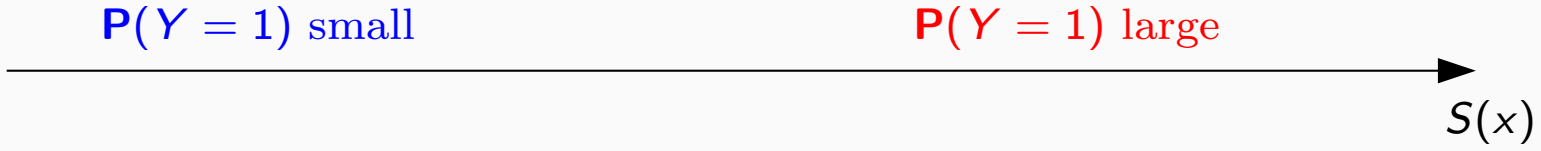
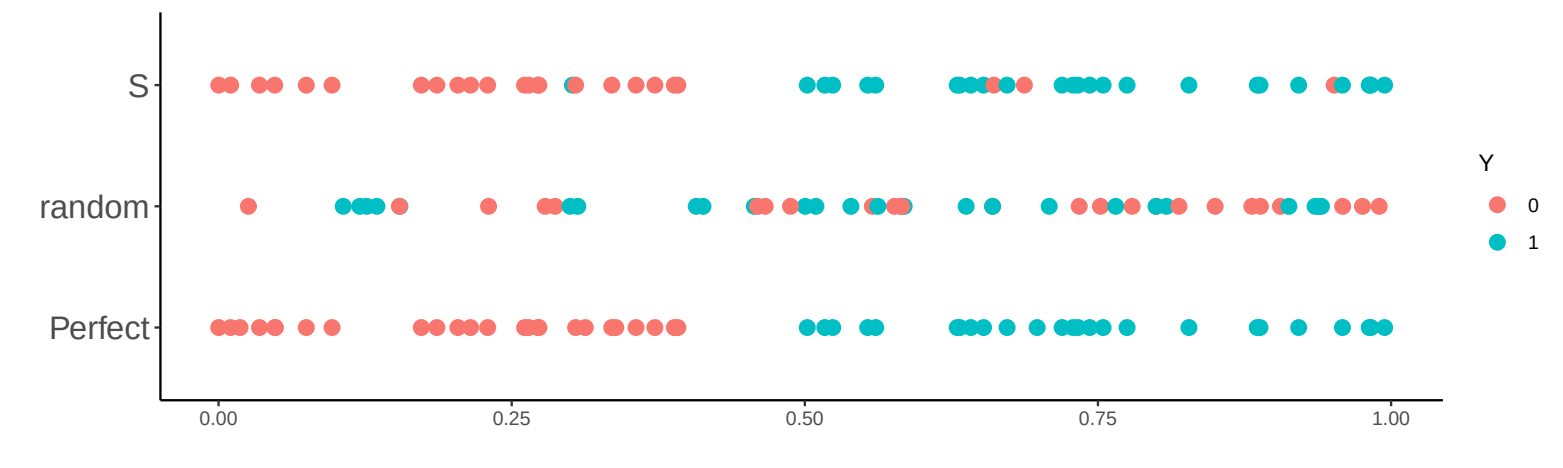


- Such a function is a score function: instead of predicting the label y of a new $x \in \mathcal{X}$, we provide a score $S(x)$ with
  - large values if we think that x is 1;
  - small values if we think that x is -1.

Perfect and random scores



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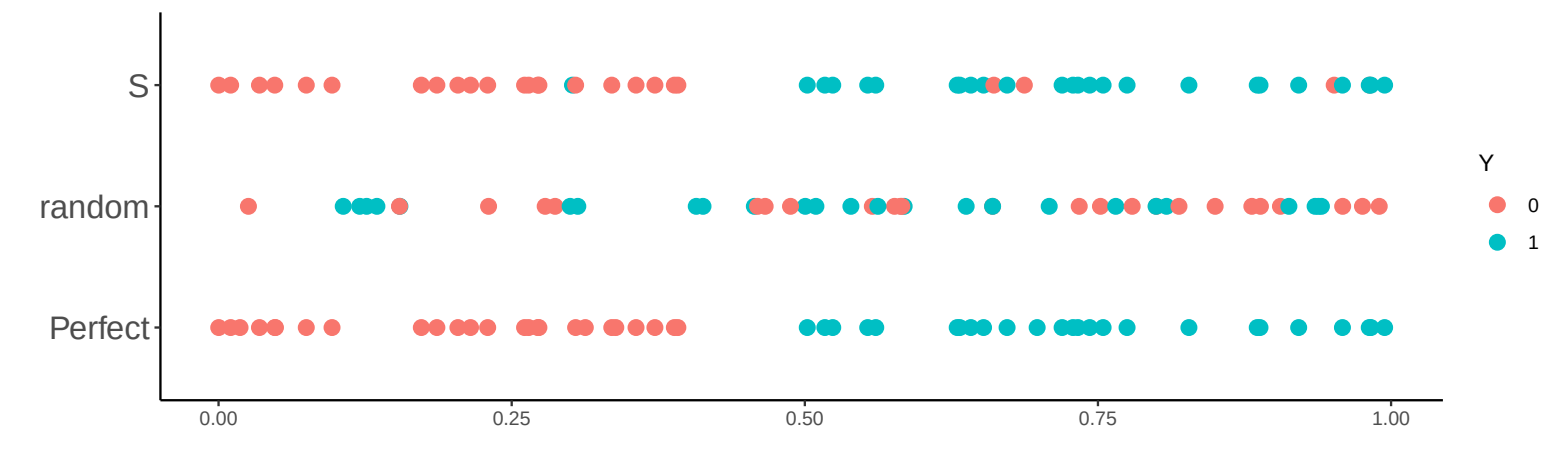

Definition

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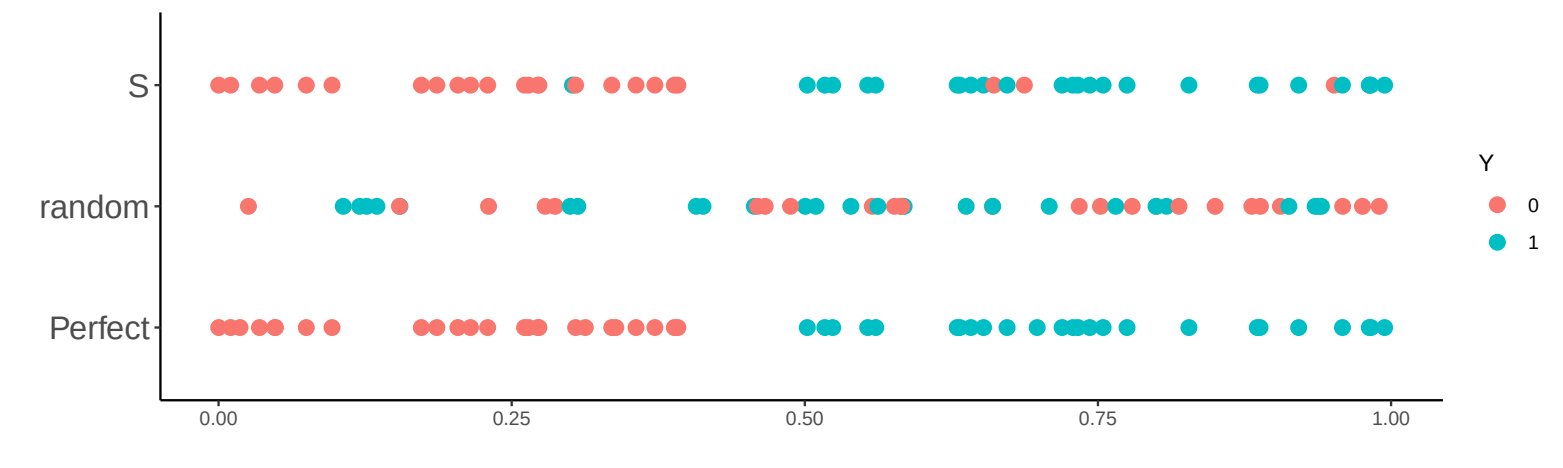

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- Random score: S is random if $S(X)$ and Y are independents.

Link between a score and a classification rule

- For a given score S and a threshold s, we obtain a classification rule:

$$f_s(x) = \begin{cases} 1 & \text{if } S(x) \geq s \\ -1 & \text{otherwise.} \end{cases}$$

- We have

	$f_s(X) = -1$	$f_s(X) = 1$
$Y = -1$	OK	E_1
$Y = 1$	E_2	OK

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- For any threshlod s, we can define 2 errors:

$$\alpha(s) = \mathbf{P}(f_s(X) = 1 | Y = -1) = \mathbf{P}(S(X) \geq s | Y = -1)$$

and

$$\beta(s) = \mathbf{P}(f_s(X) = -1 | Y = 1) = \mathbf{P}(S(X) < s | Y = 1).$$

We can also define

- Specificity: $sp(s) = \mathbf{P}(S(X) < s | Y = -1) = 1 - \alpha(s)$;
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Performance of a score

Visualize errors $\alpha(s)$ and $\beta(s)$ on a same graph for all thresholds s.

ROC curve

- **Idea**: define a 2-dimensionnel graph to represent errors $\alpha(s)$ and $\beta(s)$ for all values of s.

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The ROC curve of a score S is the parametrized curve defined by

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Remark

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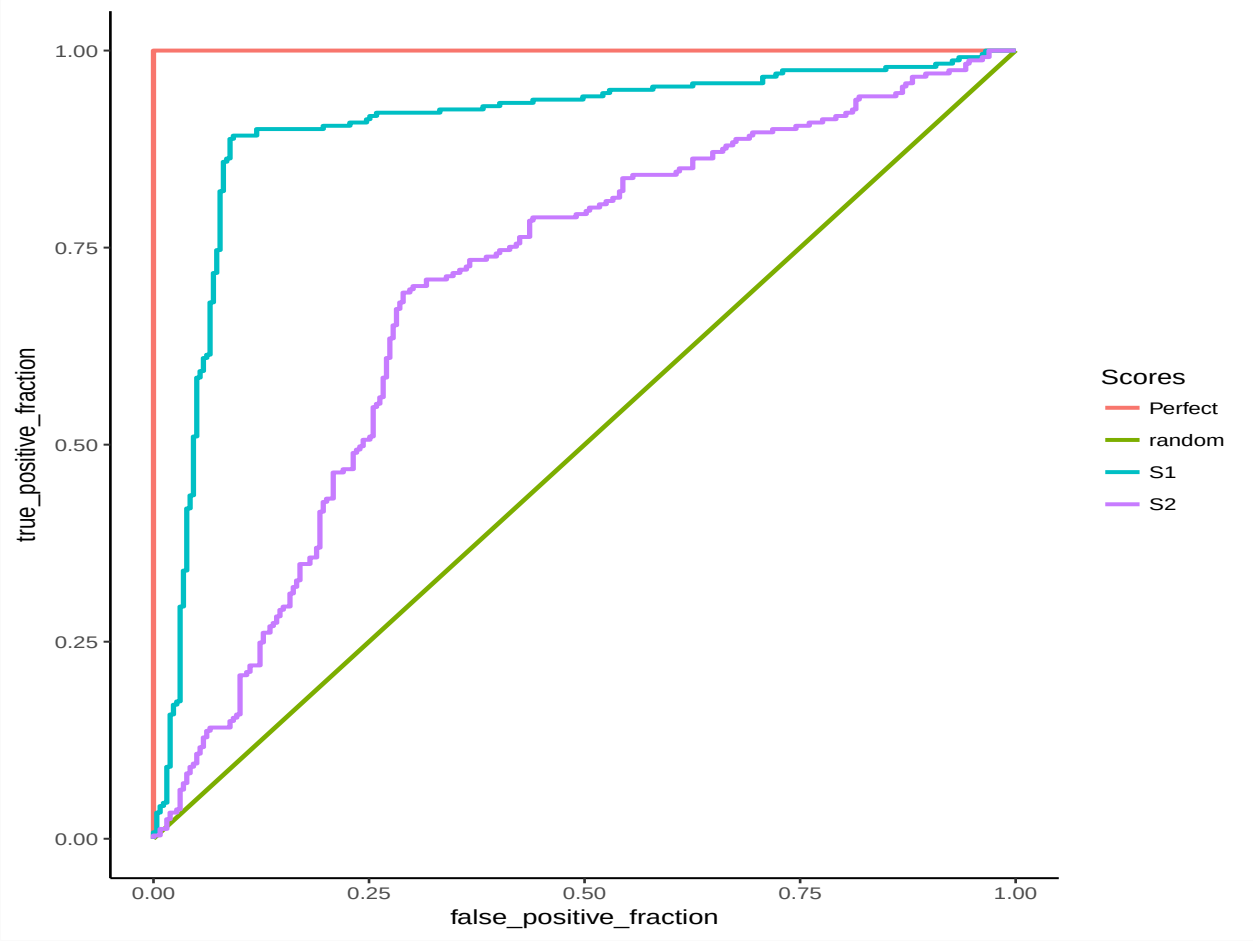
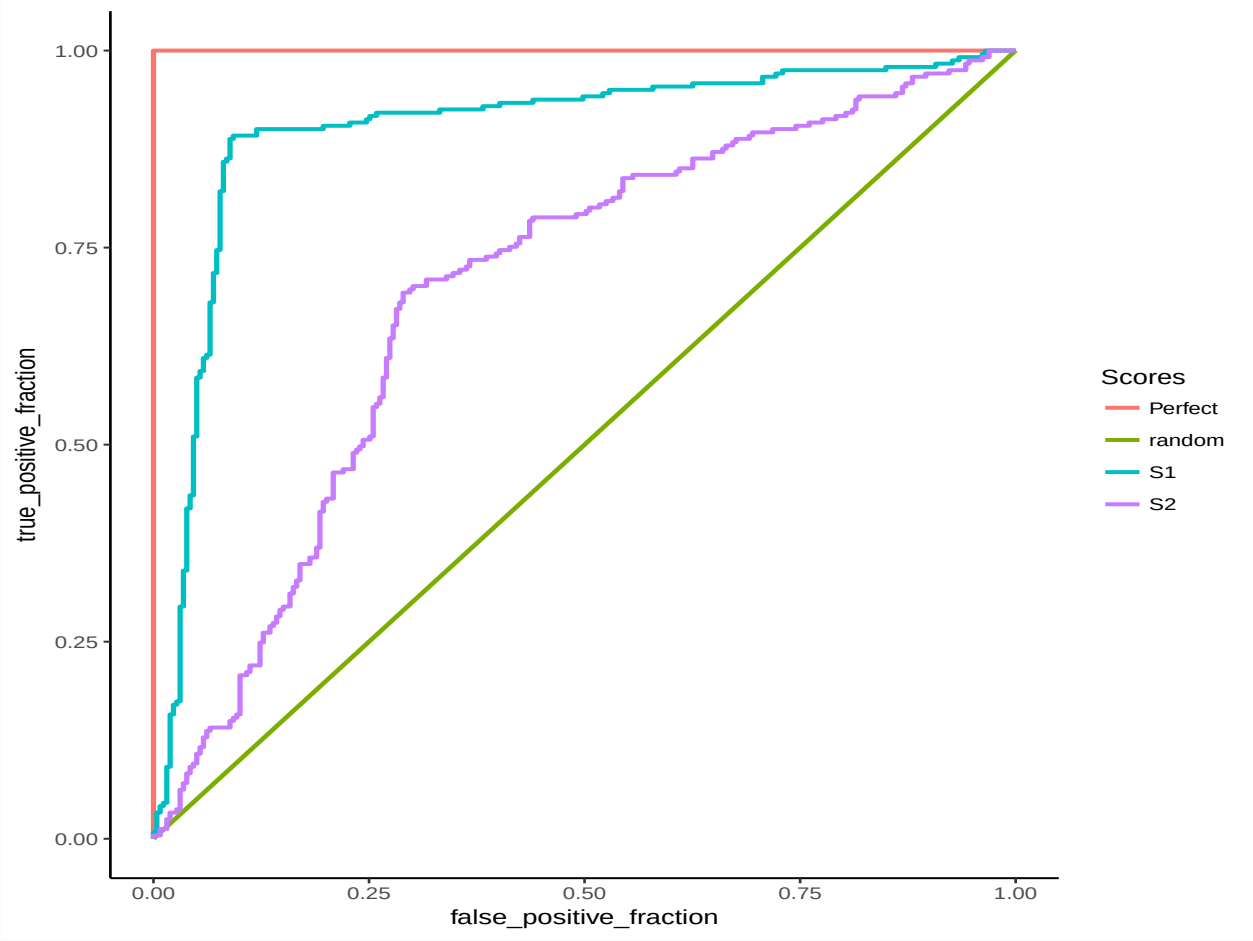

1.00
0.75
0.50
0.25
0.00
true_positive_fraction
0.00
0.25
0.50
0.75
1.00
false_positive_fraction
Scores
Perfect
random
S1
S2



Interpretation

We measure performance of a score by its ability to approach the line $y = 1$ as fast as possible.

AUC

Definition

- Area Under ROC for a score S, denoted $AUC(S)$ is often used to measure performance of a S.
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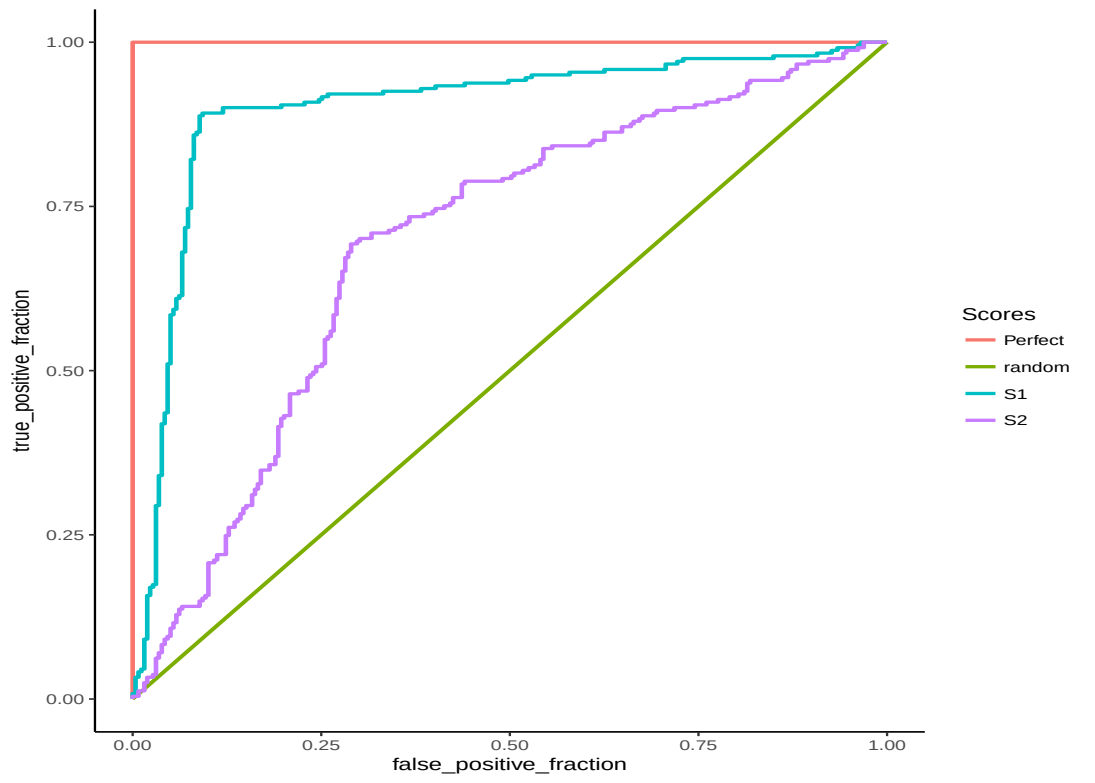
Conclusion

$AUC(S)$ measures the probability that S correctly orders two observations with different labels.

Example


1.00
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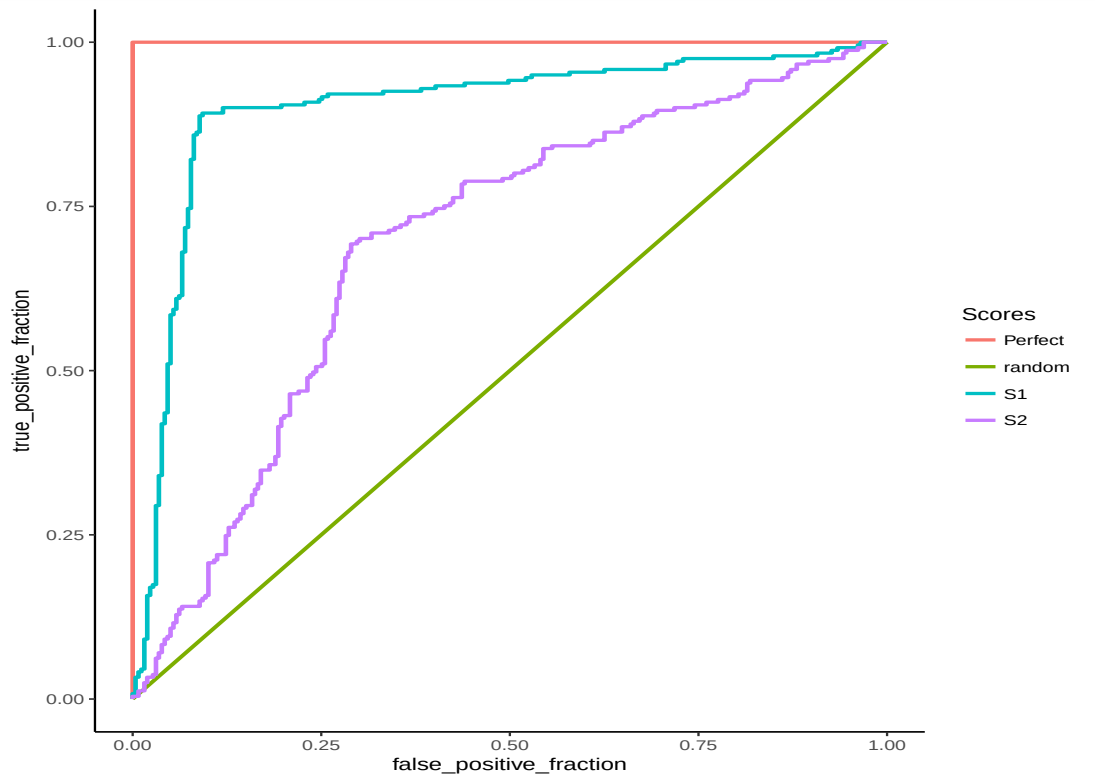


```
> df1 %>% group_by(Scores) %>% summarize(auc(D,M))
1 Perfect   1.0000000
2  random   0.5000000
3      S1   0.8999824
4      S2   0.6957177
```

Optimal score

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- Question: is there an optimal score $S^\star$ for this cost function?

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Consequence

We have to find a "good" estimate $S_n(x) = S_n(x, \mathcal{D}_n)$ of

$$S^\star(x) = \mathbf{P}(Y = 1|X = x).$$

Summary

	Cost $\ell(y, f(x))$	Risk $\mathbf{E}[\ell(Y, f(X))]$	Winner $f^\star$
Regression	$(y - f(x))^2$	$\mathbf{E}[Y - f(X)]^2$	$\mathbf{E}[Y \mid X = x]$
Binary class.	$\mathbf{1}_{y \neq f(x)}$	$\mathbf{P}(Y \neq f(X))$	Bayes rule
Scoring		$AUC(S)$	$\mathbf{P}(Y = 1 \mid X = x)$

Outline

Reminder

- n observations $(X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d in $\mathcal{X} \times \mathcal{Y}$.

Goal

Given a cost function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$, we search a machine $f_n(x) = f_n(x, \mathcal{D}_n)$ closed to the optimal machine $f^\star$ defined by

$$f^\star \in \operatorname*{argmin}_f \mathcal{R}(f)$$

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Question

Given a machine f_n, what can we say about its risk $\mathcal{R}(f_n)$?

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One solution

Cross validation or bootstrap approaches.

Validation hold hout

- The simplest approach.
- It consists in splitting the data $\mathcal{D}_n$ into:
  1. a learning or training set $\mathcal{D}_{n,train}$ used to learn a machine f_n ;
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Algorithm

Inputs. $\mathcal{D}_n$: data, $\{\mathcal{T}, \mathcal{V}\}$: a partition of $\{1, \ldots, n\}$.

1. Learn the machine with $\mathcal{D}_{n,train} = \{(X_i, Y_i) : i \in \mathcal{T}\} \Longrightarrow f_{n,train}$;
2. Compute $\widehat{\mathcal{R}}_n(f_n) = \frac{1}{|\mathcal{V}|} \sum_{i \in \mathcal{V}} \ell(Y_i, f_{n,train}(X_i))$.

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Comments

n_{train} and n_{test} should be large enough to

1. fit $f_{n,train}$;
2. estimate its risk $\mathcal{R}(f_{n,train})$.

K fold cross-validation

- **Idea**: repeat validation hold out algorithm on each element of a data partition.

Algorithme - CV

Inputs. $\mathcal{D}_n$: data, K an integer ;

1. Define a random partition $\{\mathcal{I}_1, \ldots, \mathcal{I}_K\}$ of $\{1, \ldots, n\}$;
2. For $k = 1, \ldots, K$
   - 2.1 $\mathcal{I}_{train} = \{1, \ldots, n\} \backslash \mathcal{I}_k$ and $\mathcal{I}_{test} = \mathcal{I}_k$;
   - 2.2 Learn the machine with $\mathcal{D}_{n,app} = \{(X_i, Y_i) : i \in \mathcal{I}_{app}\} \Longrightarrow f_{n,k}$;
   - 2.3 Let $f_n(X_i) = f_{n,k}(X_i)$ for $i \in \mathcal{I}_{test}$;
3. **Output**

$$\widehat{\mathcal{R}}_n(f_n) = \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, f_n(X_i)).$$

Comments

- More useful than validation hold out when n is small.
- More accurate but more time consuming.
- K has to be chosen by the user (we often set $K = 10$).

Leave one out

- When $K = n$, we obtain leave one out cross validation.
- Risk is estimated by

$$\widehat{\mathcal{R}}_n(f_n) = \frac{1}{n}\sum_{i=1}^{n} \ell(Y_i, f_n^i(X_i))$$

where f_n^i stands for the machine defined on $\mathcal{D}_n$ after deleted the ith observation.

- Exercises 1-3, IML1.

Outline

- Most of statistical learning algorithms depends on parameters (λ).

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Examples

- number of input variables in linear and logistic models.
- penalty parameters for lasso and ridge regressions.
- depth for tree algorithms.
- number of nearest neighbors.
- bandwidth of kernel regression estimators.
- number of iterations for boosting algorithms.
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- The choice of theses parameters reveals crucial for the performance of the machine.

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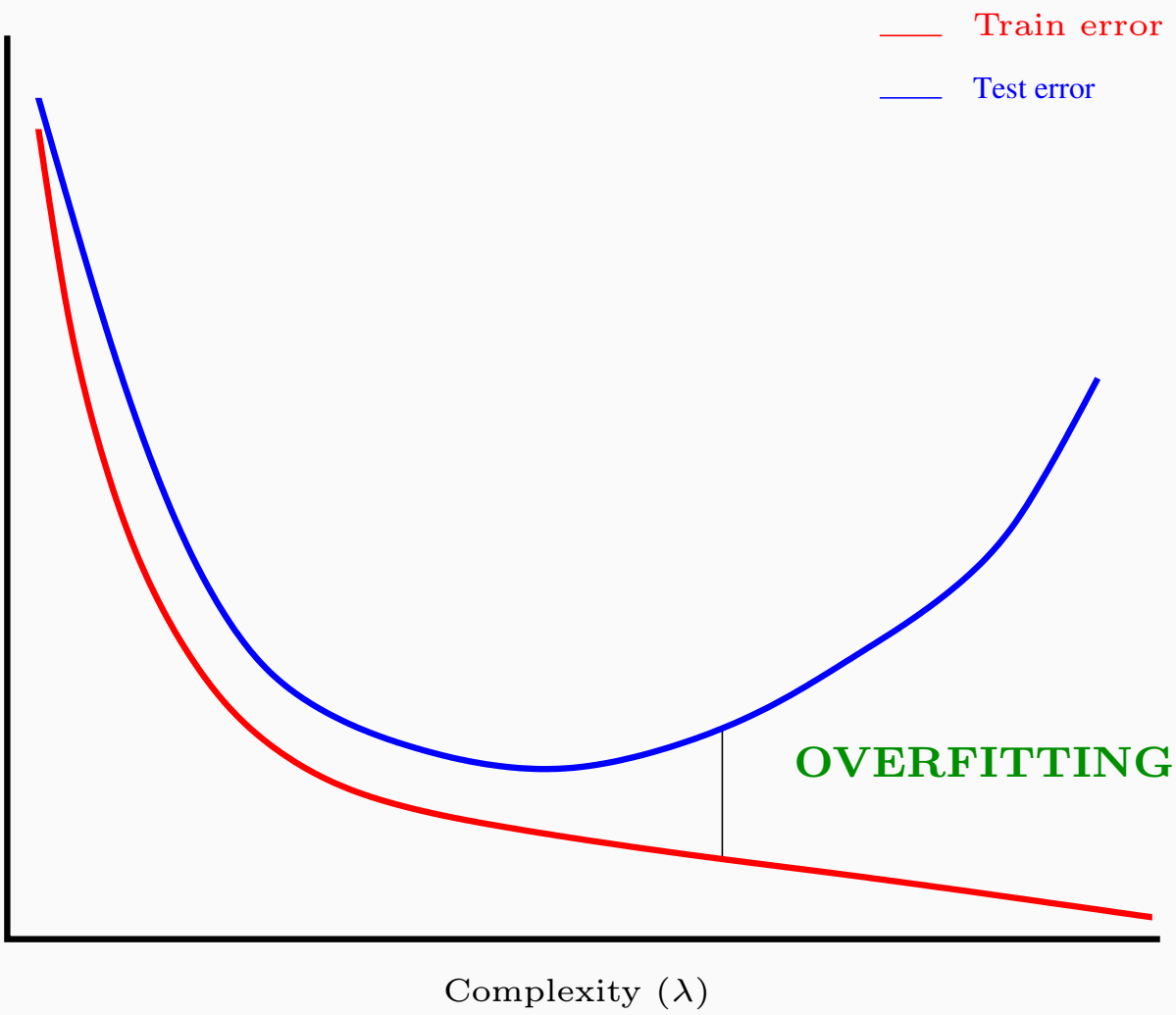
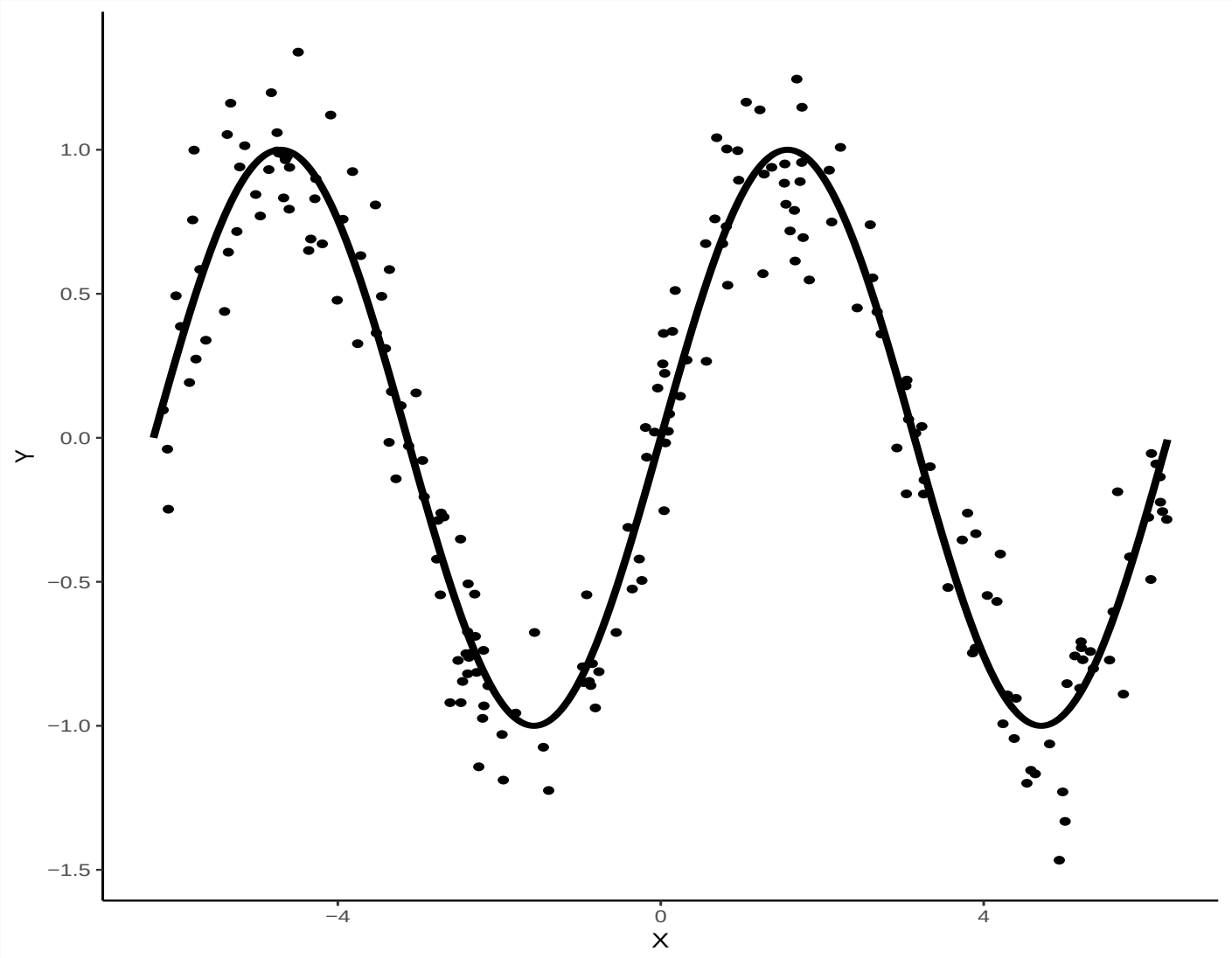
Overfitting

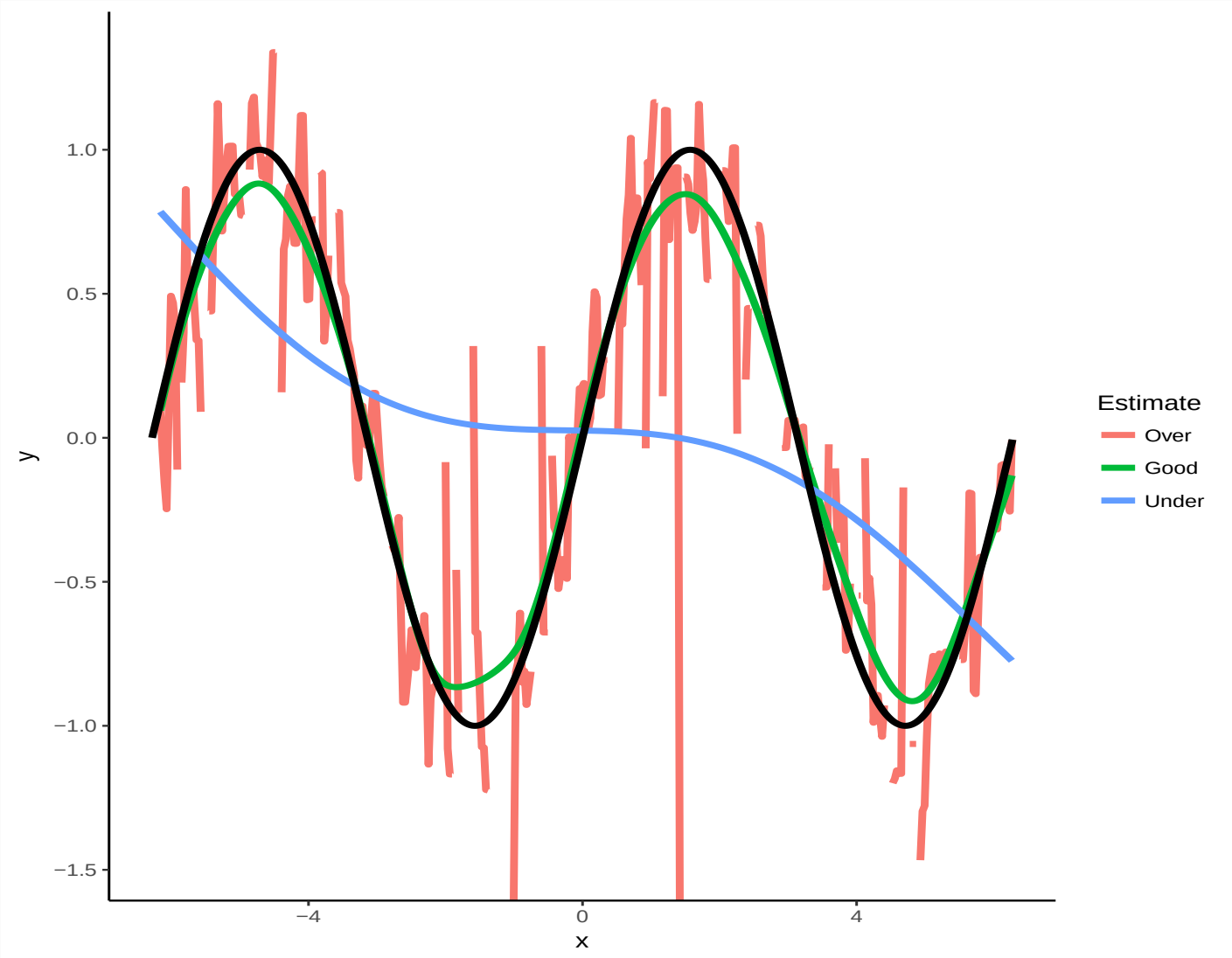
Good fitting on the training data (i.e. $f(X_i) = Y_i$) but poor predictive performances on new individuals.


Train error
Test error
OVERFITTING
Complexity (λ)

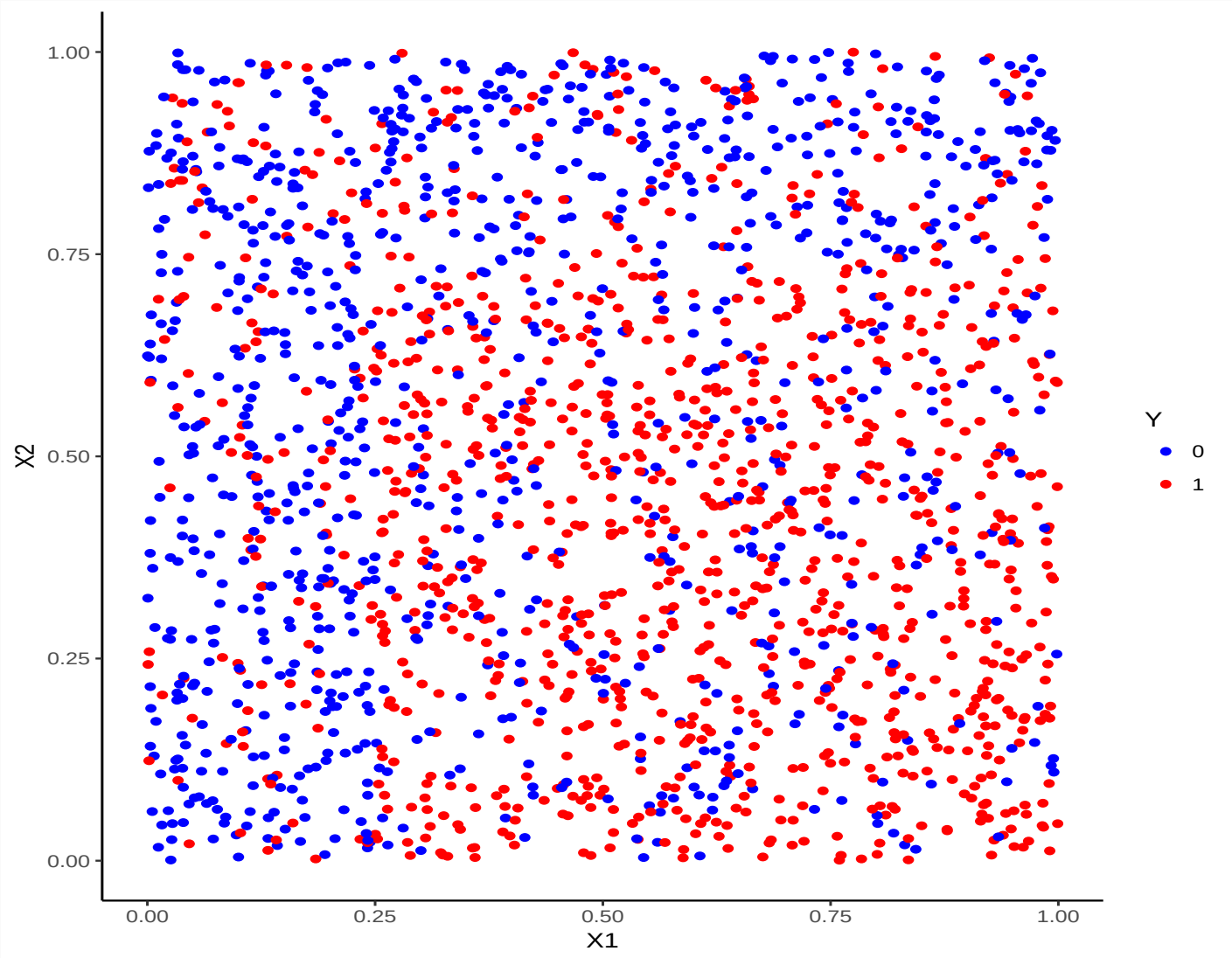
Overfitting for regression



Overfitting for regression



Overfitting for supervised classification



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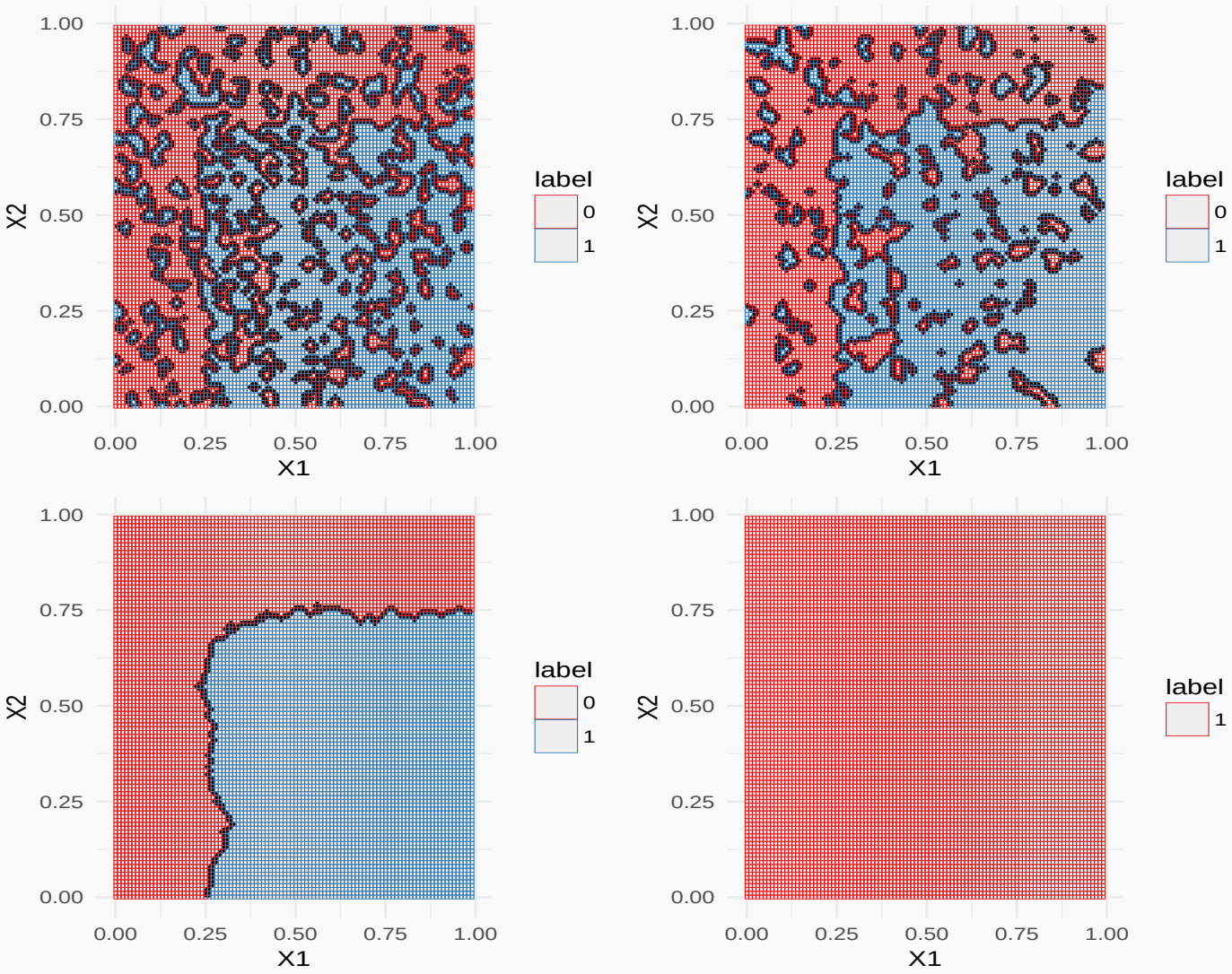

- Run application overfitting.app.

Outline

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Part II

Parametric versus nonparametric approaches

Outline

Mathematical framework

- n i.i.d observations $(X_1, Y_1), \ldots, (X_n, Y_n)$ in $\mathcal{X} \times \mathcal{Y}$.
- $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$ cost function.

Problem

Estimate

$$f^\star \in \operatorname*{argmin}_f \mathcal{R}(f) = \mathbf{E}[\ell(Y, f(X))]$$

by $f_n(.) = f_n(., \mathcal{D}_n)$.

Mathematical framework

- n i.i.d observations $(X_1, Y_1), \ldots, (X_n, Y_n)$ in $\mathcal{X} \times \mathcal{Y}$.
- $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$ cost function.

Problem

Estimate

$$f^\star \in \operatorname*{argmin}_f \mathcal{R}(f) = \mathbf{E}[\ell(Y, f(X))]$$

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- Modelize remains to fix a class of functions $\mathcal{F}$ and to assume that $f^\star \in \mathcal{F}$.

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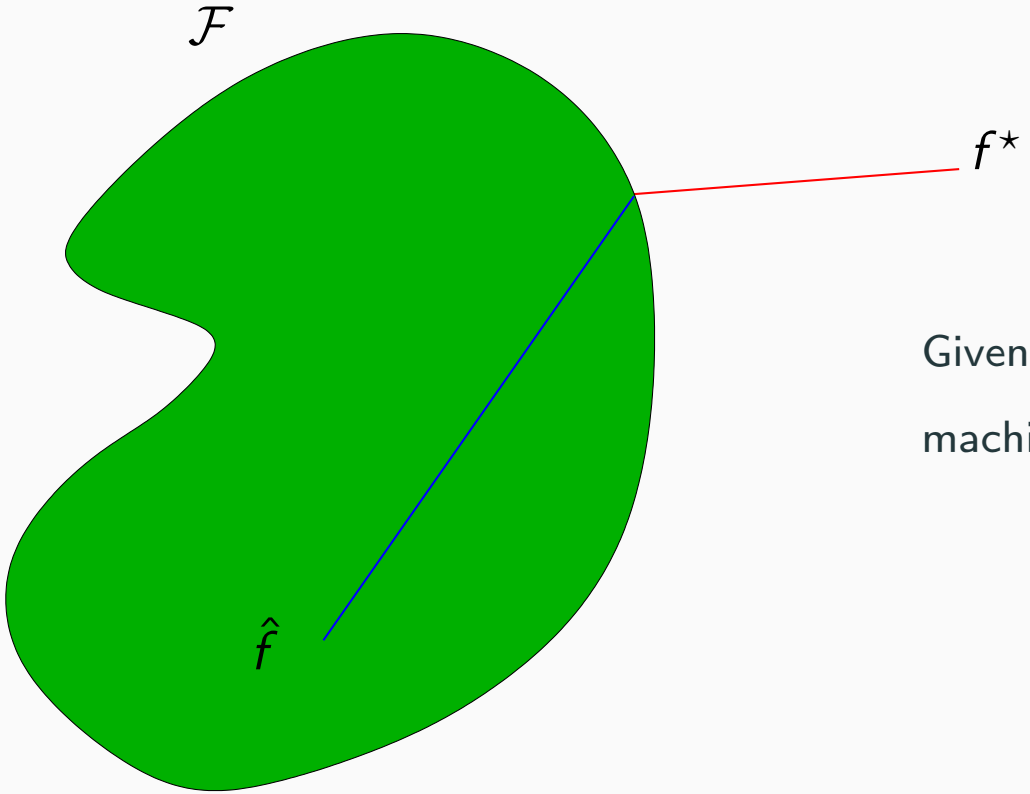
- Modelize = make an assumption.



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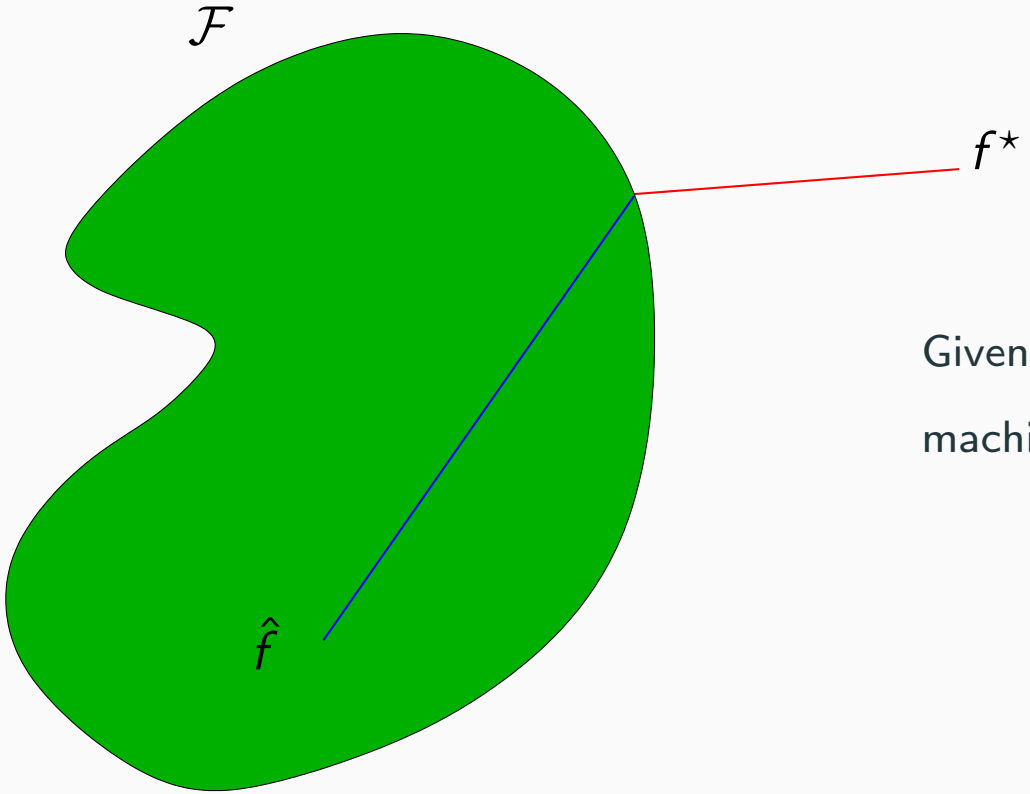
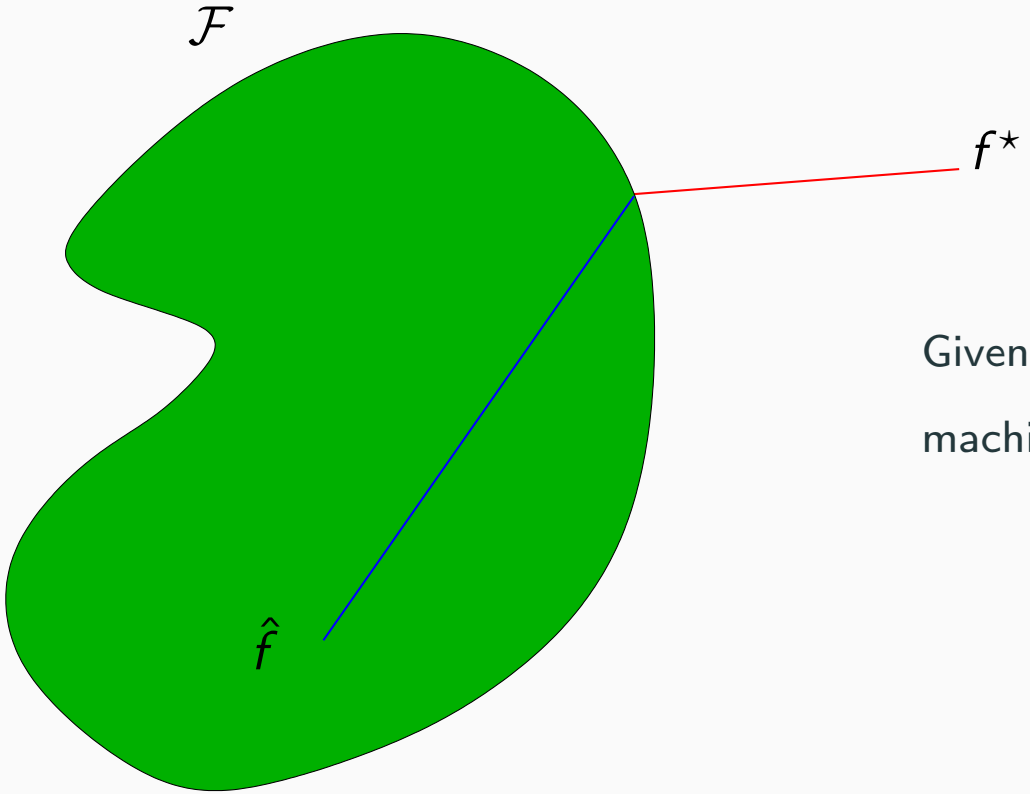


Given $(X_1, Y_1), \ldots, (X_n, Y_n)$, find the best machine $f \in \mathcal{F}$.

$$\mathcal{R}(\hat{f}) - \mathcal{R}^\star = \mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) + \inf_{f \in \mathcal{F}} \mathcal{R}(f) - \mathcal{R}^\star.$$

$$= \text{Estimation error} + \text{Approximation error}.$$



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Remarks

- These two terms vary in opposite directions.
- Statistician's job: trade-off between these two terms.

Parametric and non parametric

Definition

- If $\mathcal{F} = \{f_\theta : \theta \in \Theta\}$ with Θ of finite dimension, then the model is parametric.
- If $\mathcal{F}$ is an infinite dimensional space, then the model is non-parametric.

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- Loss of accuracy in NP models. In this part, we will study this loss.

Outline

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The linear model

- In regression with $\mathcal{X} = \mathbb{R}^d$, the linear model is the parametric reference model.
- This model makes the assumption that the regression function is linear:

$$m^\star(x) = \mathbf{E}[Y|X = x] = \beta_1 x_1 + \ldots + \beta_d x_d.$$

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$$m^\star(x) = \mathbf{E}[Y|X = x] = \beta_1 x_1 + \ldots + \beta_d x_d.$$

- Or equivalently

$$Y = \beta_1 X_1 + \ldots + \beta_d X_d + \varepsilon$$

where $\mathbf{E}[\varepsilon|X = x] = 0$ and $\mathbf{V}[\varepsilon|X = x] = \sigma^2$.

Remark

Estimate $m^\star \iff$ estimate $\beta \in \mathbb{R}^d$ (finite dimension $\implies$ parametric model).

Some properties

- Least squares estimates minimize

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (Y_i - (\beta_1 X_{i1} + \ldots + \beta_d X_{id}))^2.$$

The solution is given by

$$\hat{\beta}_n = (\mathbb{X}^t \mathbb{X})^{-1} \mathbb{X}^t \mathbb{Y}.$$

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- Regression function $m^\star$ is thus estimated by

$$\hat{m}_n(x) = \hat{\beta}_1 x_1 + \ldots + \hat{\beta}_d x_d.$$

Proposition

Under some technical assumptions, we prove that

- $\mathbf{E}[\hat{\beta}] = \beta$ *and* $\mathbf{V}[\hat{\beta}] = (\mathbb{X}^t\mathbb{X})^{-1}\sigma^2$.

We deduce that (exercise 2, IML0)

$$\mathbf{E}[\|\hat{\beta} - \beta\|^2] = \mathrm{O}\left(\frac{1}{n}\right) \quad \textit{and} \quad \mathbf{E}[(\hat{m}_n(x) - m^\star(x))^2] = \mathrm{O}\left(\frac{1}{n}\right).$$

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Remark

- Least squares estimates achieve the parametric rate $(1/n)$.
- Moreover, if errors terms $\varepsilon_i, i = 1 \ldots, n$ are Gaussian, we can compute the distribution of the least squares estimates (confidence intervals, test statistics...).
- See [Grob, 2003, Cornillon and Matzner-Løber, 2011] for more information.

Example

- Linear model to explain ozone concentration.

```
> model_lin <- lm(V4~V5+V6+V7+V8+V9+V10+V11+V12+V13,data=Ozone)
> summary(model_lin)
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) 59.9517553 38.3286940   1.564 0.119421
V5          -0.0139111  0.0072511  -1.918 0.056527 .
V6           0.0276862  0.1741433   0.159 0.873847
V7           0.0808740  0.0237694   3.402 0.000812 ***
V8           0.1503404  0.0692994   2.169 0.031272 *
V9           0.5253439  0.1247136   4.212 3.87e-05 ***
V10         -0.0010052  0.0003944  -2.549 0.011586 *
V11          0.0049796  0.0147772   0.337 0.736501
V12         -0.1543882  0.1192917  -1.294 0.197140
V13         -0.0033951  0.0048963  -0.693 0.488883
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Logistic model

- Logistic model is the "brother" of the linear model in the context of binary classification ($\mathcal{Y} = \{-1, 1\}$).
- This model makes the assumption that (the logit transformation of) the probability $p(x) = \mathbf{P}(Y = 1|X = x)$ is linear :

$$\mathrm{logit}\, p(x) = \log \frac{p(x)}{1 - p(x)} = \beta_1 x_1 + \ldots + \beta_d x_d = x^t \beta.$$

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$$\mathrm{logit}\, p(x) = \log \frac{p(x)}{1 - p(x)} = \beta_1 x_1 + \ldots + \beta_d x_d = x^t \beta.$$

- $\beta = (\beta_1, \ldots, \beta_d) \in \mathbb{R}^d \Longrightarrow$ parametric model.
- Unknown parameters $\beta_1, \ldots, \beta_d$ are estimated by maximizing the (log)-likelihood:

$$\mathcal{L}_n(\beta) = \sum_{i=1}^{n} \left\{ y_i x_i^t \beta - \log(1 + \exp(x_i^t \beta)) \right\}.$$

Some properties

Theorem [Fahrmeir and Kaufmann, 1985]

Under technical assumptions we have

1. the ML estimate $\{\hat{\beta}_n\}_n$ is consistant: $\hat{\beta}_n \xrightarrow{\mathbf{P}} \beta$;
2. the ML estimate $\{\hat{\beta}_n\}_n$ is asymptotically gaussian:

$$\sqrt{n}(\hat{\beta}_n - \beta) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \mathcal{I}^{-1}(\beta)).$$

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$$\mathbf{E}[\|\hat{\beta} - \beta\|^2] = O\left(\frac{1}{n}\right).$$

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$$\mathbf{E}[\|\hat{\beta} - \beta\|^2] = O\left(\frac{1}{n}\right).$$

Important remark

Again, the ML estimate achieves the parametric rate $(1/n)$.

Example

- In R, we can fit a logistic model with the glm function.

```
> model_log <- glm(type~.,data=spam,family=binomial)
> summary(model_log)$coefficients[1:5,]
              Estimate Std. Error    z value     Pr(>|z|)
(Intercept) -1.5686144  0.1420362 -11.043767 2.349719e-28
make        -0.3895185  0.2314521  -1.682933 9.238799e-02
address     -0.1457768  0.0692792  -2.104194 3.536157e-02
all          0.1141402  0.1103011   1.034806 3.007594e-01
num3d        2.2515195  1.5070099   1.494031 1.351675e-01
```

Outline

Presentation

- Logistic regression directly modelizes the parameter of the distribution of $Y|X = x$.
- Linear discriminant analysis do the opposite. It consists in
  - modelizing the distributions of $X|Y = j$ for $j = 1, \ldots, K$ by gaussian distributions $f_j(x)$.

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- Logistic regression directly modelizes the parameter of the distribution of $Y|X = x$.
- Linear discriminant analysis do the opposite. It consists in
  - modelizing the distributions of $X|Y = j$ for $j = 1, \ldots, K$ by gaussian distributions $f_j(x)$.
  - calculating the posterior distribution $Y|X = x$ with Bayes formula :

$$\mathbf{P}(Y = j|X = x) = \frac{\pi_j f_j(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$$

where $\pi_j = \mathbf{P}(Y = j), j = 1, \ldots, K$.

Example: Fisher's iris problem

- Explain iris species by lengths and widths of petals and sepals.

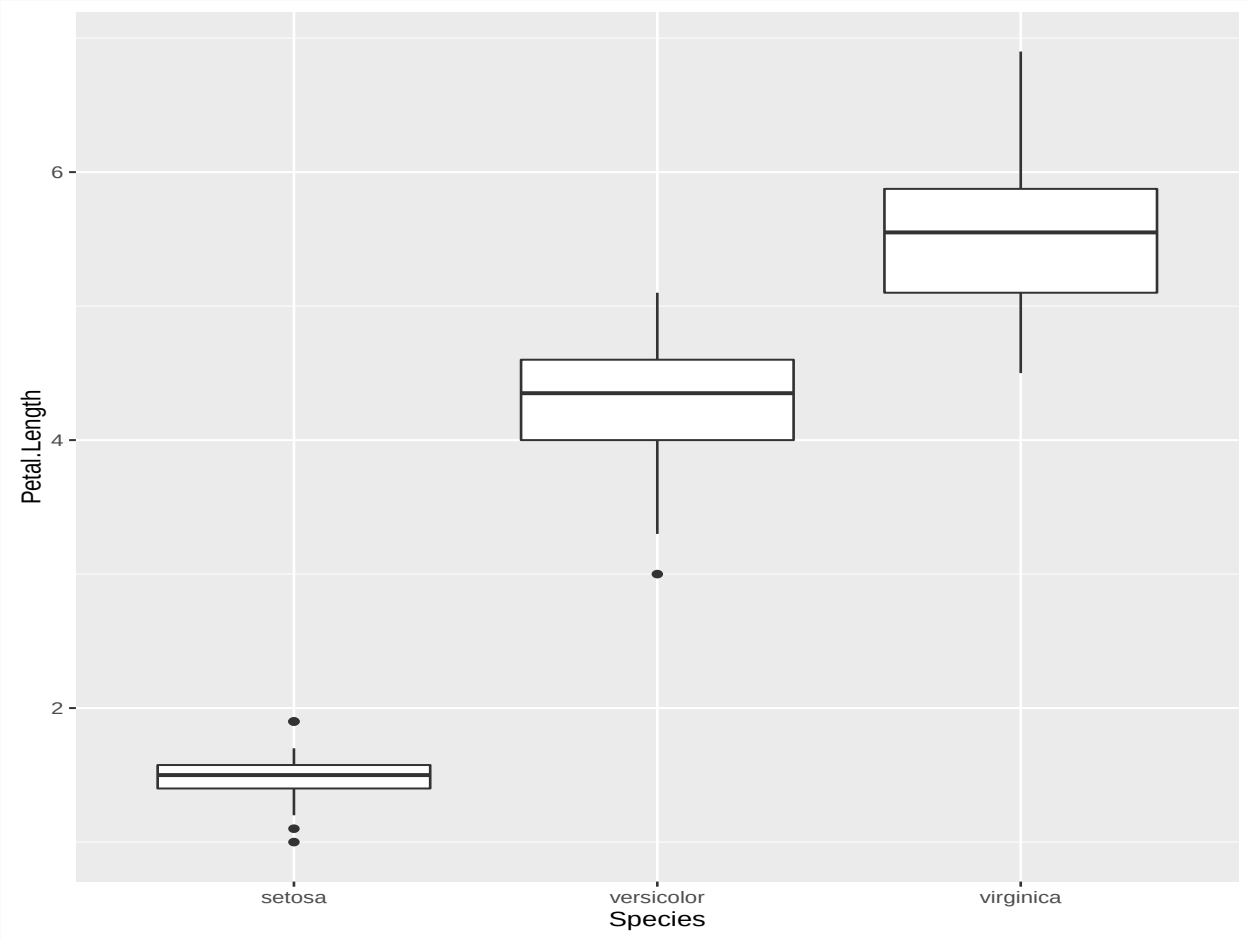
Example: Fisher's iris problem

- Explain iris species by lengths and widths of petals and sepals.
- 5 variables :
  - the target variable species (categorical).
  - lengths and widths of petals and sepals.

```
> summary(iris)
  Sepal.Length    Sepal.Width     Petal.Length    Petal.Width
 Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100
 1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300
 Median :5.800   Median :3.000   Median :4.350   Median :1.300
 Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199
 3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800
 Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500
       Species
 setosa    :50
 versicolor:50
 virginica :50
```

- We first want to explain Species by
- We can draw the following boxplot.

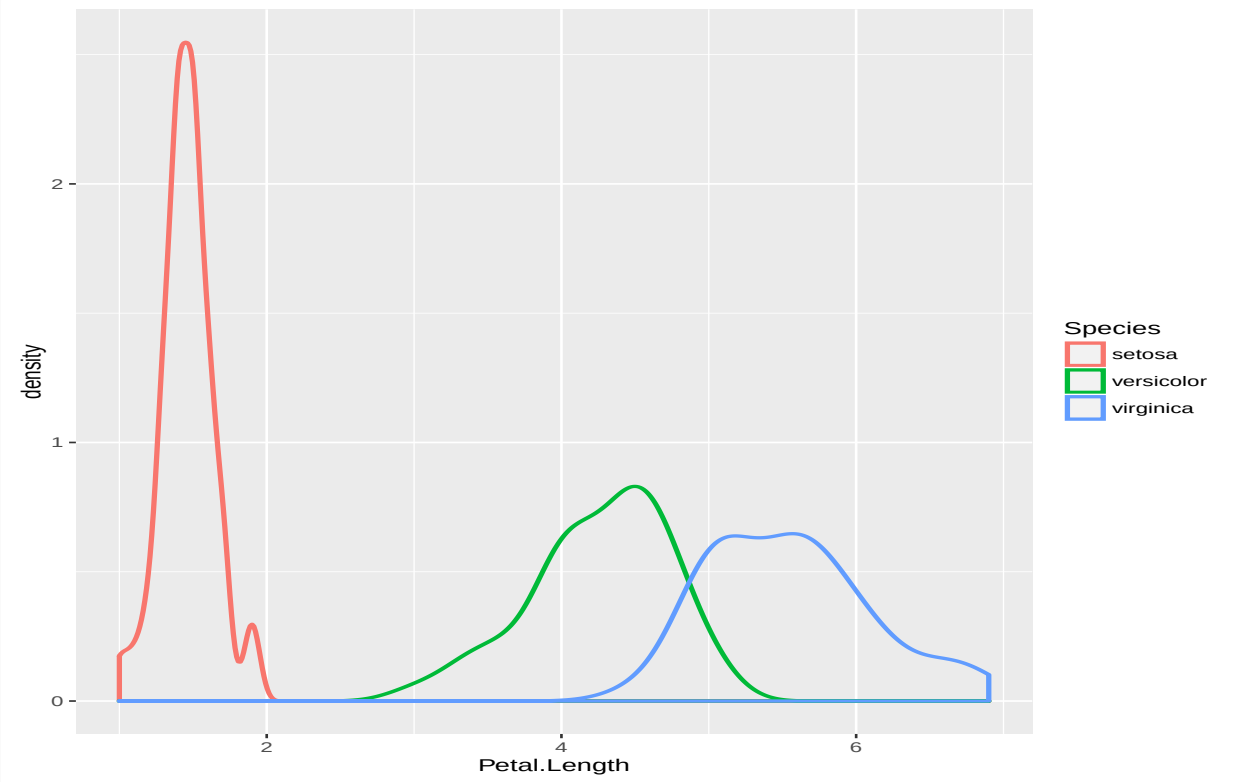
```
> ggplot(iris)+aes(x=Species,y=Petal.Length)+geom_boxplot()+theme_bw()
```



Visualize densities

- geom_density allows to visualize conditional distributions of $X|Y = j$, $j = 1, 2, 3$.

```
> ggplot(iris)+aes(x=Petal.Length,color=Species)+geom_density(size=1)
```



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- Let $X =$Petal.Length and $Y=$ Species. We assume that distributions of X given $Y = k$ are Gaussians $\mathcal{N}(\mu_k, \sigma^2)$, $k = 1, 2, 3$.

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- Let $X =$Petal.Length and $Y=$ Species. We assume that distributions of X given $Y = k$ are Gaussians $\mathcal{N}(\mu_k, \sigma^2)$, $k = 1, 2, 3$.
- Densities of $X|Y = k$ are thus given by

$$f_{X|Y=k}(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma^2}\right).$$

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These quantities are naturally estimated by

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:Y_i=k} X_i, \quad \widehat{\sigma^2} = \frac{1}{n-2} \sum_{k=1}^{K} \sum_{i:Y_i=k} (X_i - \hat{\mu}_k)^2$$

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$$\hat{\pi}_k = \frac{n_k}{n} \quad \text{where} \quad n_k = \sum_{i=1}^{n} \mathbf{1}_{\{Y_i=k\}}.$$

Example with R

```
> library(MASS)
> model <- lda(Species~Petal.Length,data=iris)
> model
Call:
lda(Species ~ Petal.Length, data = iris)

Prior probabilities of groups:
    setosa versicolor  virginica
 0.3333333  0.3333333  0.3333333

Group means:
           Petal.Length
setosa            1.462
versicolor        4.260
virginica         5.552

Coefficients of linear discriminants:
                  LD1
Petal.Length 2.323774
```

Making predictions

- predict function allows to predict species of new iris:

```
> don_pred
    Sepal.Length Sepal.Width Petal.Length Petal.Width
           5.0         3.6          1.4         0.2
           5.5         2.4          3.7         1.0
           7.1         3.0          5.9         2.1
           6.7         3.3          5.7         2.5
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           6.7         3.3          5.7         2.5
```

- We just have to enter

```
> predict(model,newdata=don_pred)
$class
[1] setosa     versicolor virginica  virginica
Levels: setosa versicolor virginica
$posterior
          setosa   versicolor    virginica
    1.000000e+00 2.589892e-10 6.170197e-21
    3.123152e-06 9.997752e-01 2.217125e-04
    1.113402e-23 9.723296e-04 9.990277e-01
    9.198362e-22 3.913109e-03 9.960869e-01
```

- Goal: explain iris specie by the 4 explanatory variables `Sepal.Length`, `Sepal.Width`, `Petal.Length`, `Petal.Width`. We denote by X_1, X_2, X_3, X_4 these 4 variables and $X = (X_1, X_2, X_3, X_4)$.

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- The approach is similar to the previous case (1 variable)

  1. We model distributions of $X|Y = k$ by Gaussian multivariate distributions.

  2. We use Bayes formula to obtain posterior probabilities $\mathbf{P}(Y = k|X = x)$.

LDA: general case

- Distributions of $X|Y = k$ are are assumed to be Gaussians $\mathcal{N}(\mu_k, \Sigma)$ where $\mu_k \in \mathbb{R}^p$ and Σ is a $p \times p$ definite positive matrix. Densities of $X|Y = k$ are thus given by:

$$f_{X|Y=k}(x) = \frac{1}{(2\pi \det(\Sigma))^{p/2}} \exp\left(-\frac{1}{2}(x - \mu_k)^t \Sigma^{-1}(x - \mu_k)\right).$$

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- Posterior probabilities $\mathbf{P}(Y=k|X=x)$ are obtained thanks to the Bayes formula

$$\mathbf{P}(Y=k|X=x) = \frac{\pi_k f_{X|Y=k}(x)}{f(x)}$$

where $f(x)$, the density of X, is computed from $f_{X|Y=k}(x)$ and from prior probabilites $\pi_k = \mathbf{P}(Y=k)$.

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- We again need to estimate unknown parameters of the model:

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$$\hat{\pi}_k = \frac{n_k}{n} \quad \text{with} \quad n_k = \sum_{i=1}^{n} \mathbf{1}_{\{Y_i = k\}}.$$

Example with R

```
> full_model<- lda(Species~.,data=iris)
> full_model
Call:
lda(Species ~ ., data = iris)

Prior probabilities of groups:
    setosa versicolor  virginica
 0.3333333  0.3333333  0.3333333

Group means:
           Sepal.Length Sepal.Width Petal.Length Petal.Width
setosa            5.006       3.428        1.462       0.246
versicolor        5.936       2.770        4.260       1.326
virginica         6.588       2.974        5.552       2.026
```

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```
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Levels: setosa versicolor virginica

$posterior
          setosa   versicolor    virginica
5   1.000000e+00 1.637387e-22 1.082605e-42
82  9.648075e-16 9.999997e-01 3.266704e-07
103 1.231264e-42 2.592826e-05 9.999741e-01
145 4.048249e-46 2.524984e-07 9.999997e-01
```

Classification rule

- Reminder: LDA allows to estimate posterior probabilities:

$$\mathbf{P}(Y = k | X = x).$$

Classification rule

- Reminder: LDA allows to estimate posterior probabilities:

$$\mathbf{P}(Y = k|X = x).$$

- Classification rule: we choose the group which maximizes these probabilities

$$\widehat{g}(x) = k \quad \text{if and only if} \quad \mathbf{P}(Y = k|X = x) \geq \mathbf{P}(Y = j|X = x), \quad j \neq k.$$

- Boundary between 2 groups: set of points x such that $\mathbf{P}(Y = k|X = x) = \mathbf{P}(Y = j|X = x)$.

- Or

$$\begin{aligned}\log \frac{\mathbf{P}(Y=k|X=x)}{\mathbf{P}(Y=\ell|X=x)} &= \log \frac{f_k(x)}{f_\ell(x)} + \log \frac{\pi_k}{\pi_\ell} \\ &= \log \frac{\pi_k}{\pi_\ell} - \frac{1}{2}(\mu_k+\mu_\ell)^t \Sigma^{-1}(\mu_k-\mu_\ell) \\ &\quad + x^t \Sigma^{-1}(\mu_k-\mu_\ell) \qquad (1)\end{aligned}$$

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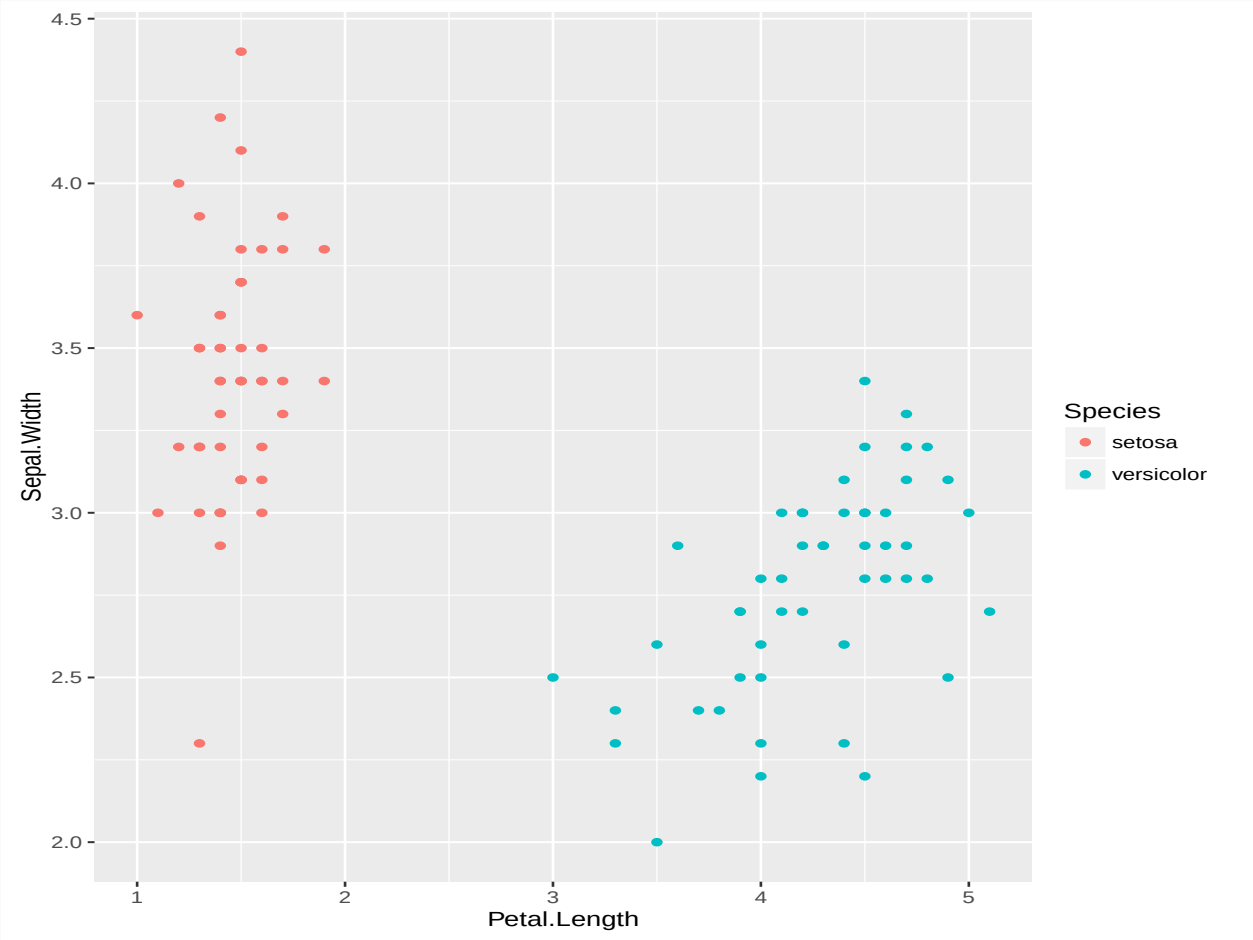
Conclusion

Bondary between 2 groups is linear!

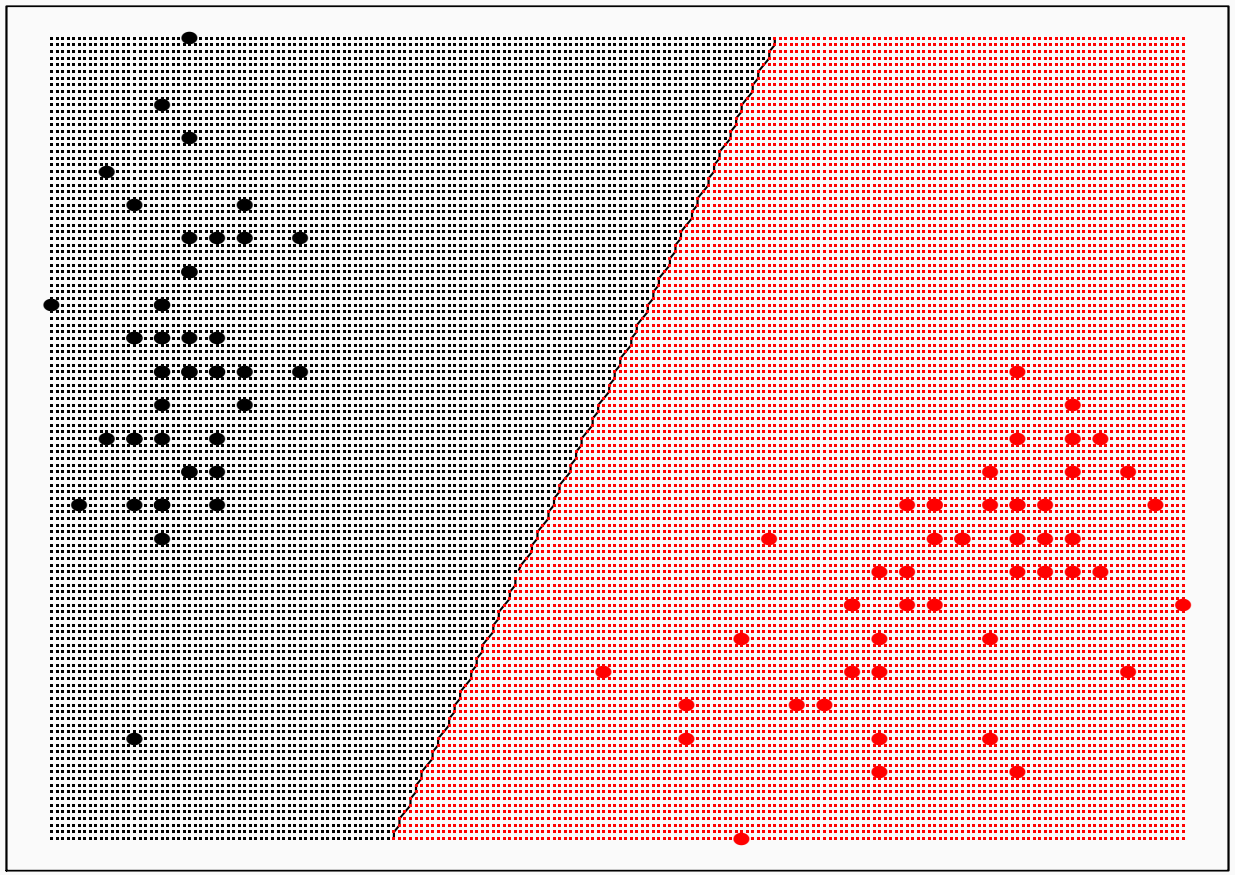
Example

- Boundary between "Setosa" and "Versicolor" for 2 variables.

```
> iris1 <- iris[iris$Species%in%c("setosa","versicolor"),c(3,2,5)]
> ggplot(iris1)+aes(x=Petal.Length,y=Sepal.Width,color=Species)+geom_point()
```



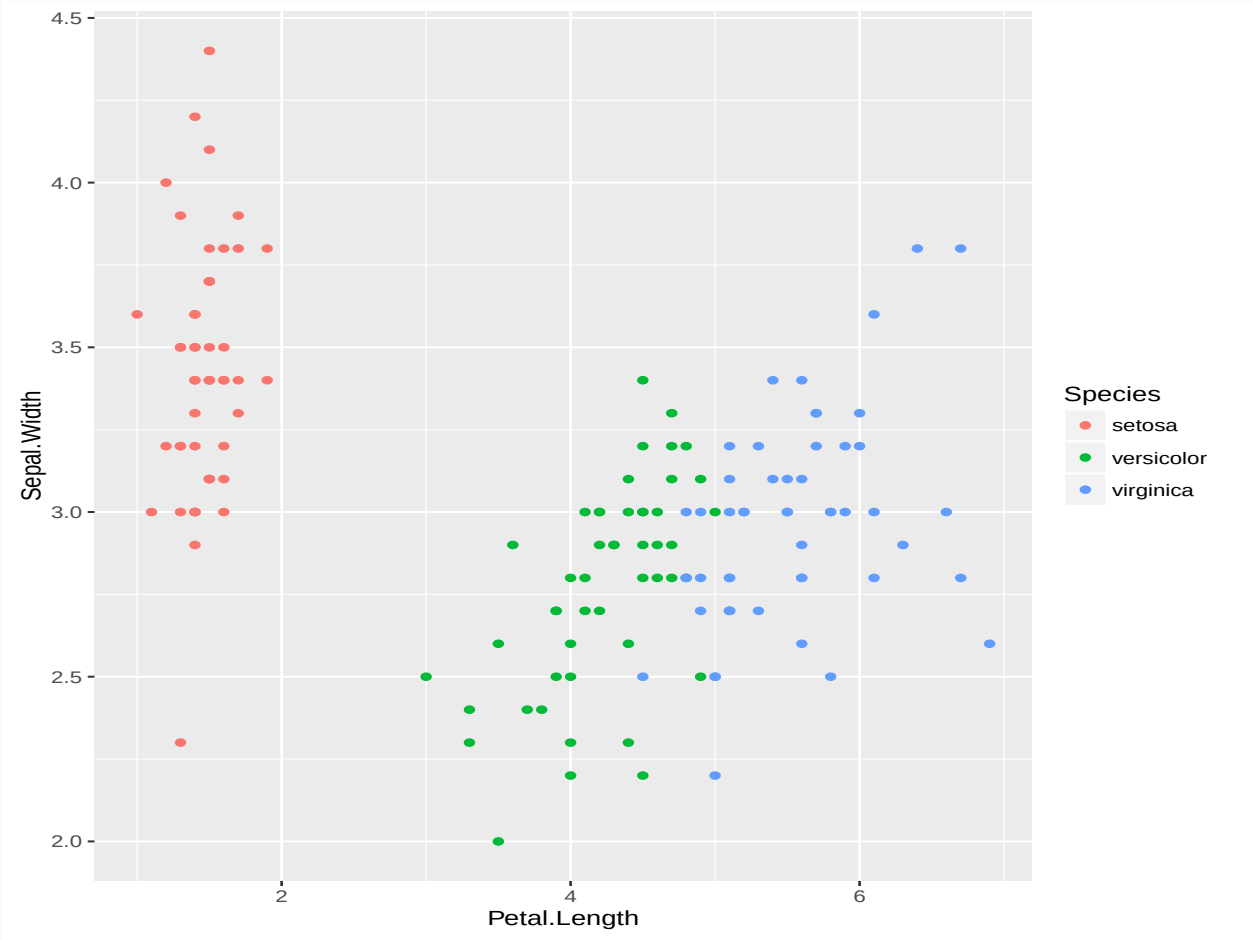
Boundary two classes



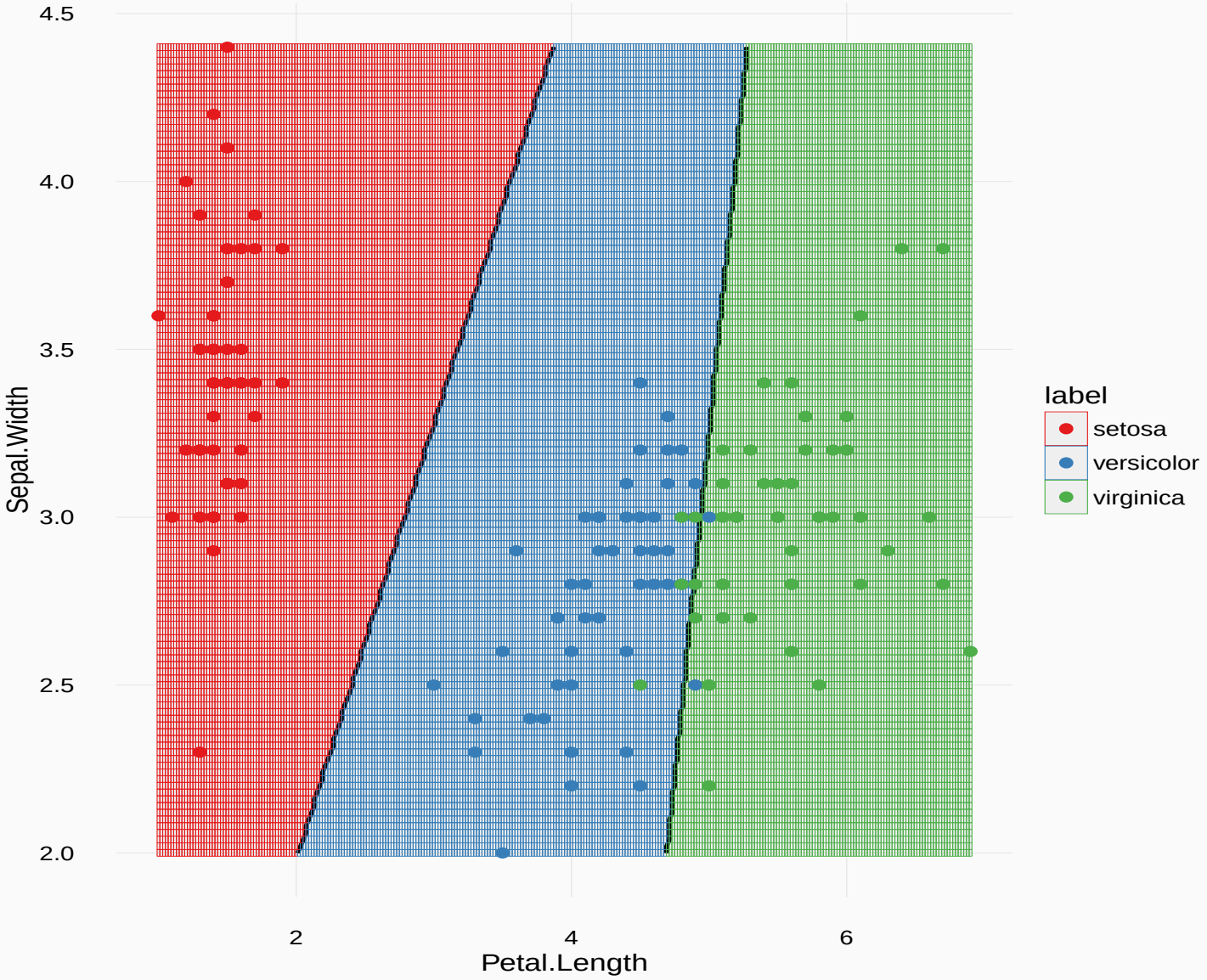
Example - 3 labels

- We do the same for the 3 species (3 classes).

```
> ggplot(iris)+aes(x=Petal.Length,y=Sepal.Width,color=Species)+geom_point()
```



Boundaries


4.5
4.0
3.5
3.0
2.5
2.0
Sepal.Width
2
4
6
Petal.Length
label
setosa
versicolor
virginica

Linear discriminant functions

Definition

Linear discriminant functions are defined by

$$\delta_k(x) = x^t \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^t \Sigma^{-1} \mu_k + \log \pi_k, \quad k = 1, \ldots, K.$$

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Propriété

Thanks to (1), we deduce

$$\operatorname*{argmax}_k \mathbf{P}(Y = k | X = x) = \operatorname*{argmax}_k \delta_k(x).$$

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$$\operatorname*{argmax}_k \mathbf{P}(Y = k | X = x) = \operatorname*{argmax}_k \delta_k(x).$$

Conclusion

Maximising posterior probabilities is similar to maximising linear discriminant functions.

Outline

Local averaging

Idea

- Parametric models require strong assumptions on the function to estimate.
- Nonparametric approaches try to be less restrictive.

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- Parametric models require strong assumptions on the function to estimate.
- Nonparametric approaches try to be less restrictive.
- These methods consists of studying the data on a neighborhood of the points where we want to estimate the target function.

- For both regression and supervised classification, nonparametric approaches rely on local averaging:

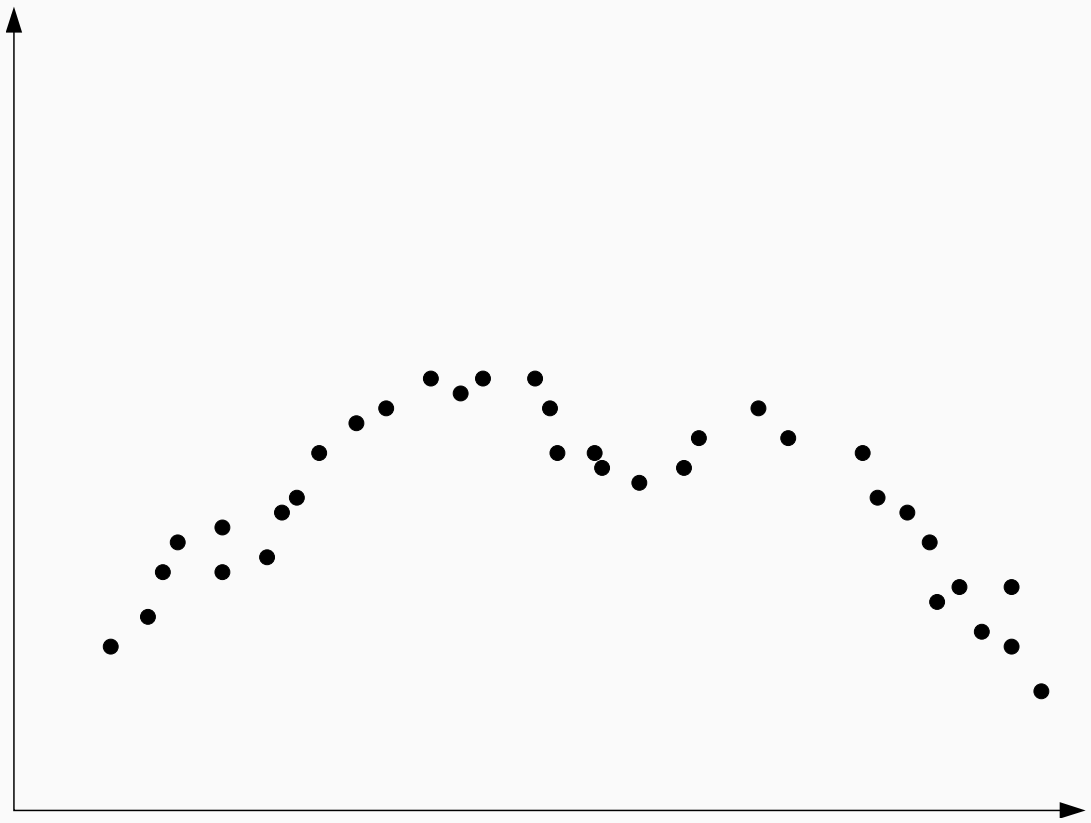
$$\widehat{f}_n(x) = \sum_{i=1}^{n} W_{ni}(x) Y_i$$

  where the weights W_{ni} depend on the algorithm.
- W_{ni} large if X_i is closed to x.

Outline

Kernel estimate

- $(X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d. with the same law as (X, Y).
- Goal: estimate $m^\star(x) = \mathbf{E}[Y|X = x]$.



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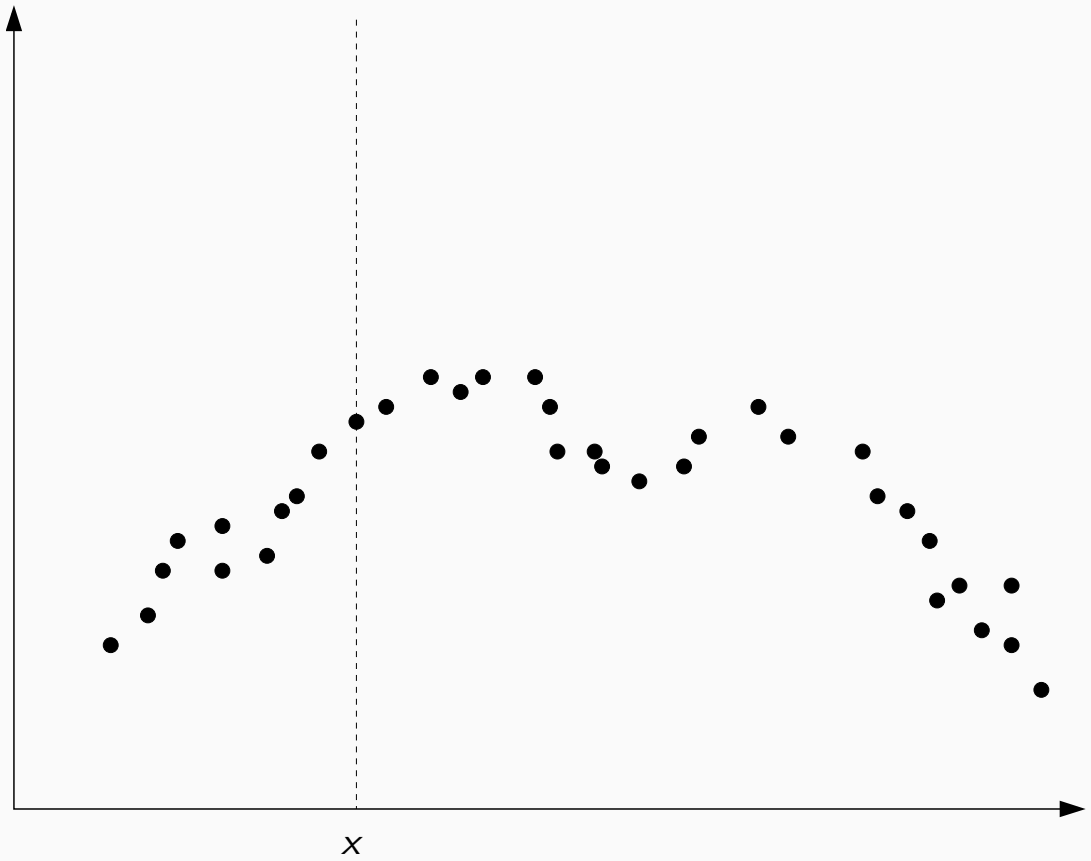

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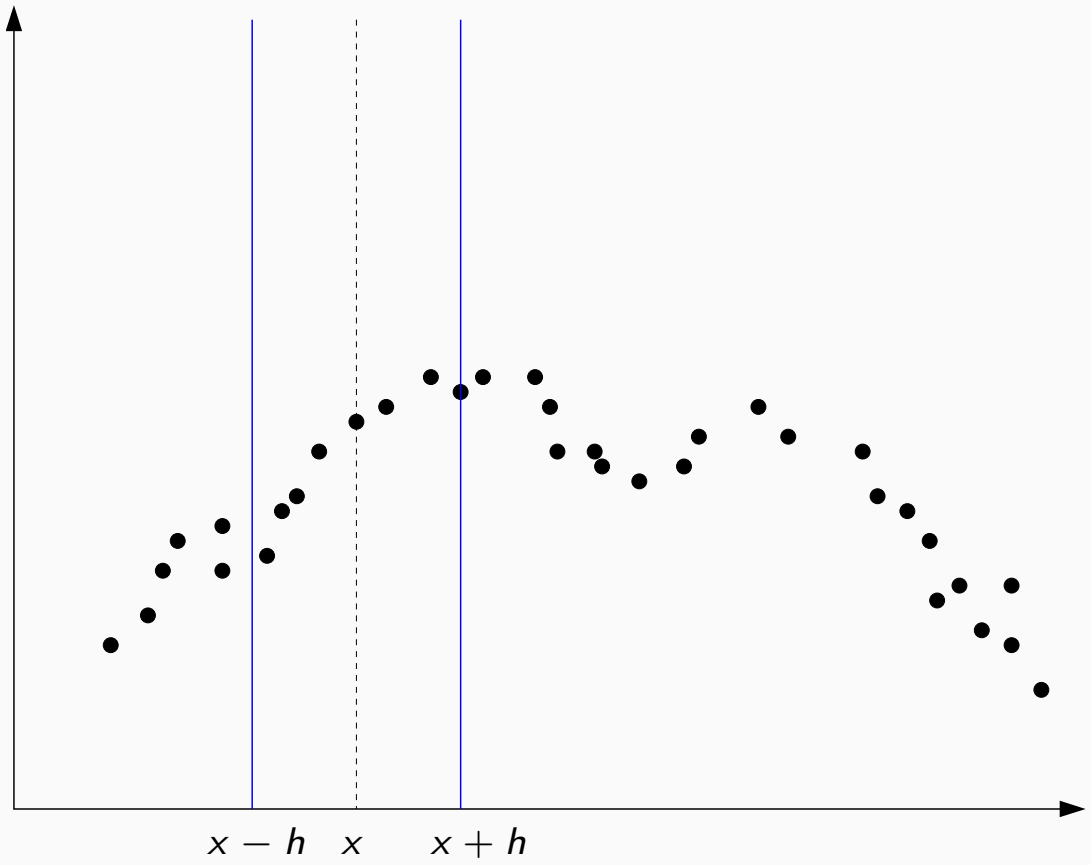

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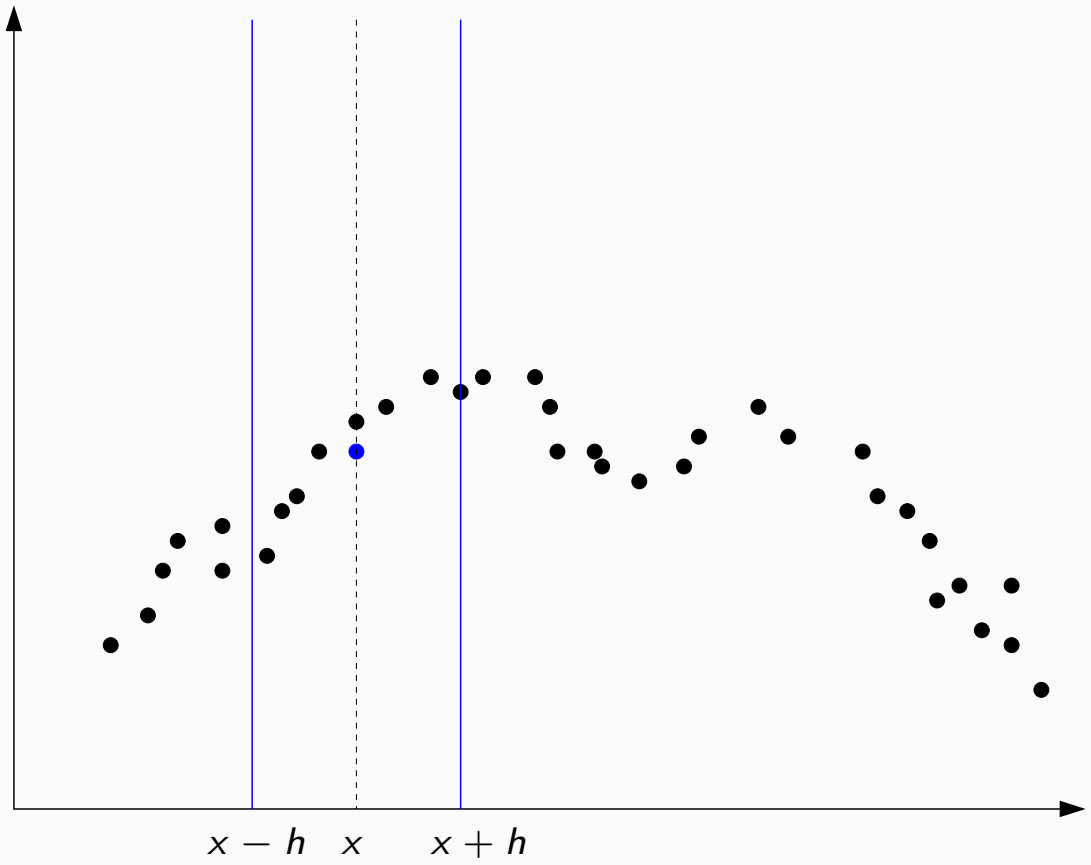

- The estimator

$$\widehat{m}_n(x) = Average(Y_i : X_i \in [x-h, x+h]) = \frac{\sum_{i=1}^{n} \mathbf{1}_{x-h \leq X_i \leq x+h} Y_i}{\sum_{i=1}^{n} \mathbf{1}_{x-h \leq X_i \leq x+h}}.$$

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Definition

Let $h > 0$ and $K : \mathcal{X} \to \mathbb{R}^+$. The kernel estimate with bandwidth h and kernel K is defined by

$$\widehat{m}_n(x) = \frac{\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right) Y_i}{\sum_{i=1}^{n} K\left(\frac{X_i - x}{h}\right)}.$$

Choice of the bandwidth

- Usual kernels when $\mathcal{X} = \mathbb{R}^d$:
  1. Uniform: $K(x) = \mathbf{1}_{\|x\| \leq 1}$;
  2. Gaussian: $K(x) = \exp(-\|x\|^2)$;
  3. Epanechnikov: $K(x) = \frac{3}{4}(1 - \|x\|^2)\mathbf{1}_{\|x\| \leq 1}$.

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- The choice of the bandwidth h reveals crucial for the performance of the estimate:
  1. h large: steady estimator, low variance, high bias;
  2. h small: unsteady estimator ("overfitting"), high variance, small bias.

Conclusion

h governs the complexity of the estimate.

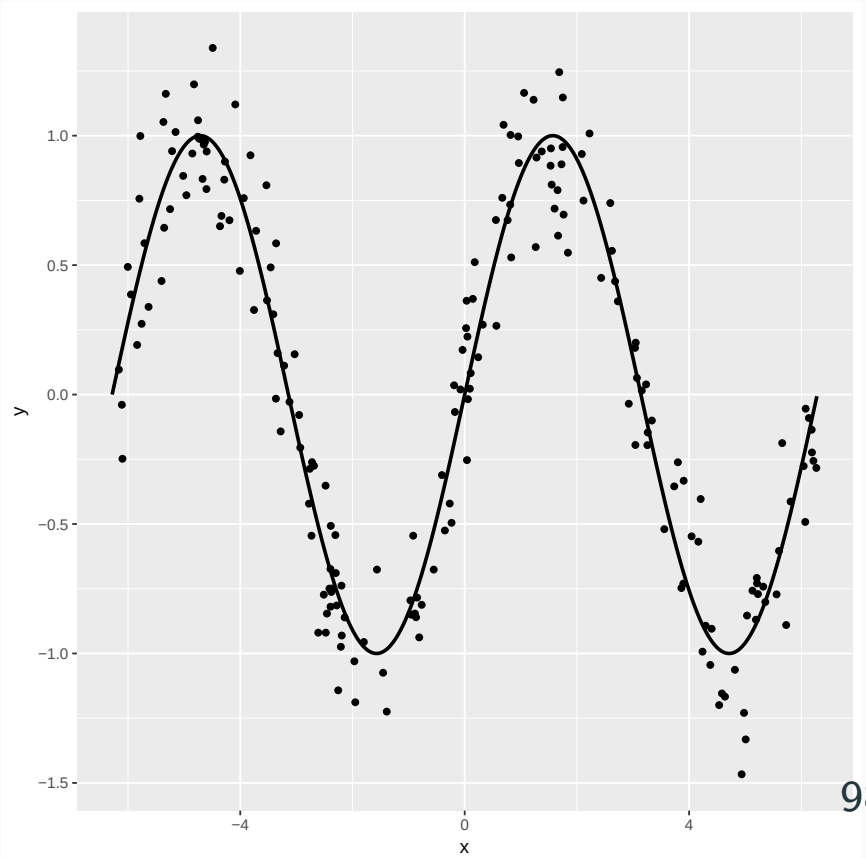
Example

- We generate data $(X_i, Y_i), i = 1, \ldots, n = 200$ according to the model

$$Y_i = \sin(X_i) + \varepsilon_i, \quad i = 1, \ldots, n$$

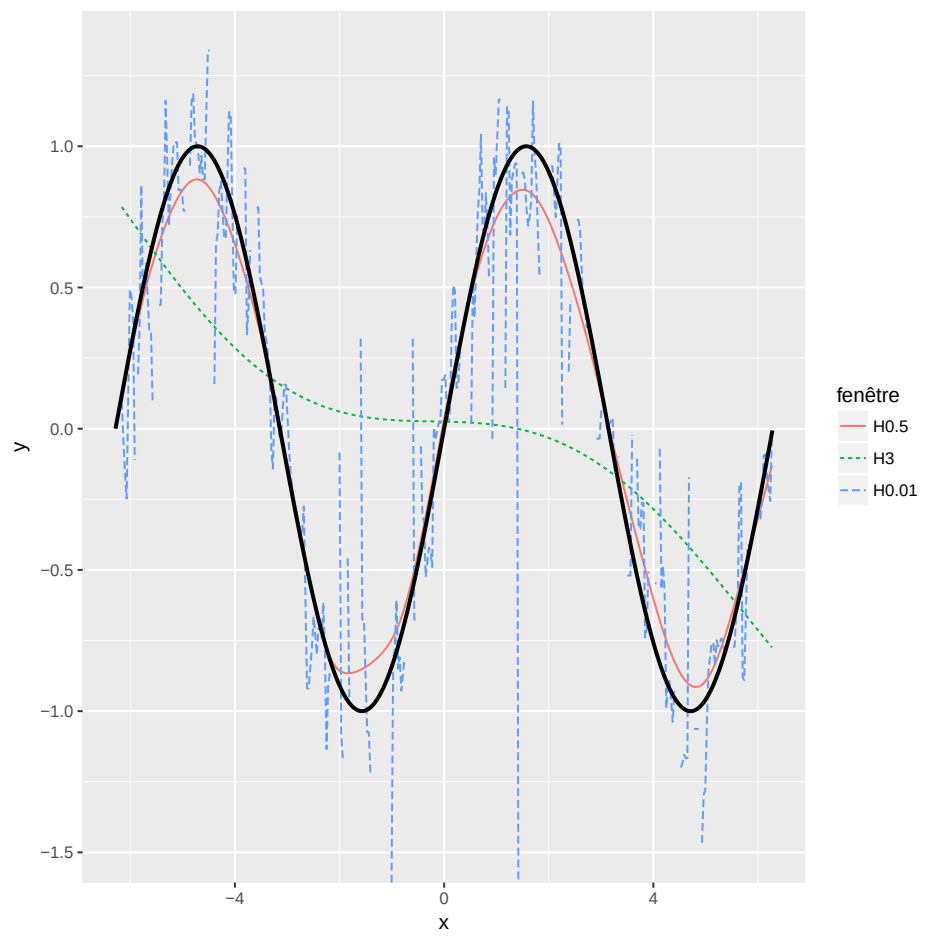
where X_i has a uniform distribution on $[-2\pi, 2\pi]$, ε_i has a Gaussian distribution $\mathcal{N}(0, 0.2^2)$.

```
> n <- 200; set.seed(1234)
> X <- runif(n,-2*pi,2*pi)
> set.seed(5678)
> eps <- rnorm(n,0,0.2)
> Y <- sin(X)+eps
> df <- data.frame(X=X,Y=Y)
> x <- seq(-2*pi,2*pi,by=0.01)
> df1 <- data.frame(x=x,y=sin(x))
> ggplot(df1)+aes(x=x,y=y)+
  geom_line(size=1)+
  geom_point(data=df,aes(x=X,y=Y))
```



- locpoly function from kernSmooth package allows to fit kernel estimates.

```
> h1 <- 0.5;h2 <- 3;h3 <- 0.01
> fx1 <-locpoly(X,Y,bandwidth=h1)
> fx2 <-locpoly(X,Y,bandwidth=h2)
> fx3 <-locpoly(X,Y,bandwidth=h3)
> df1 <- data.frame(x=x,y=sin(x))
> df2 <- data.frame(x=fx1$x,
    "H0.5"=fx1$y,"H3"=fx2$y,
    "H0.01"=fx3$y)
> df22 <- melt(df2,id.vars=1)
> names(df22)[2:3] <- c("fenêtre",
              "y")
> ggplot(df22)+aes(x=x,y=y)+
       geom_line(aes(color=fenêtre,
        lty=fenêtre))+geom_line
      (data=df1,aes(x=x,y=y),size=1)
```



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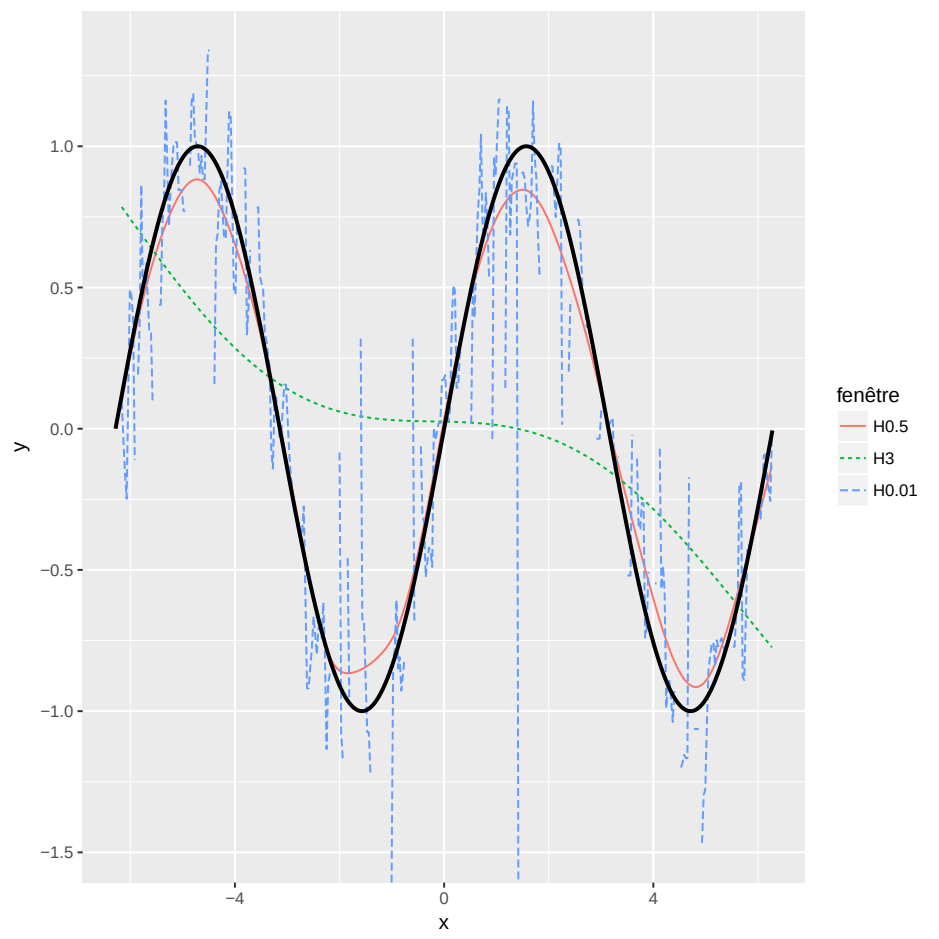

- Exercise 4-IML1.

Nearest neighbors algorithm

Definition

Let $k \leq n$ an integer. The k-nearest neighbors estimate is defined by

$$\hat{m}_n(x) = \frac{1}{k} \sum_{i \in \mathrm{knn}(x)} Y_i$$

where for $x \in \mathcal{X}$

$$\mathrm{knn}(x) = \{i : X_i \text{ is among the knn of } x \text{ among } \{X_1, \ldots, X_n\}\}.$$

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Once again, the choice of k reveals crucial for the performance of the:

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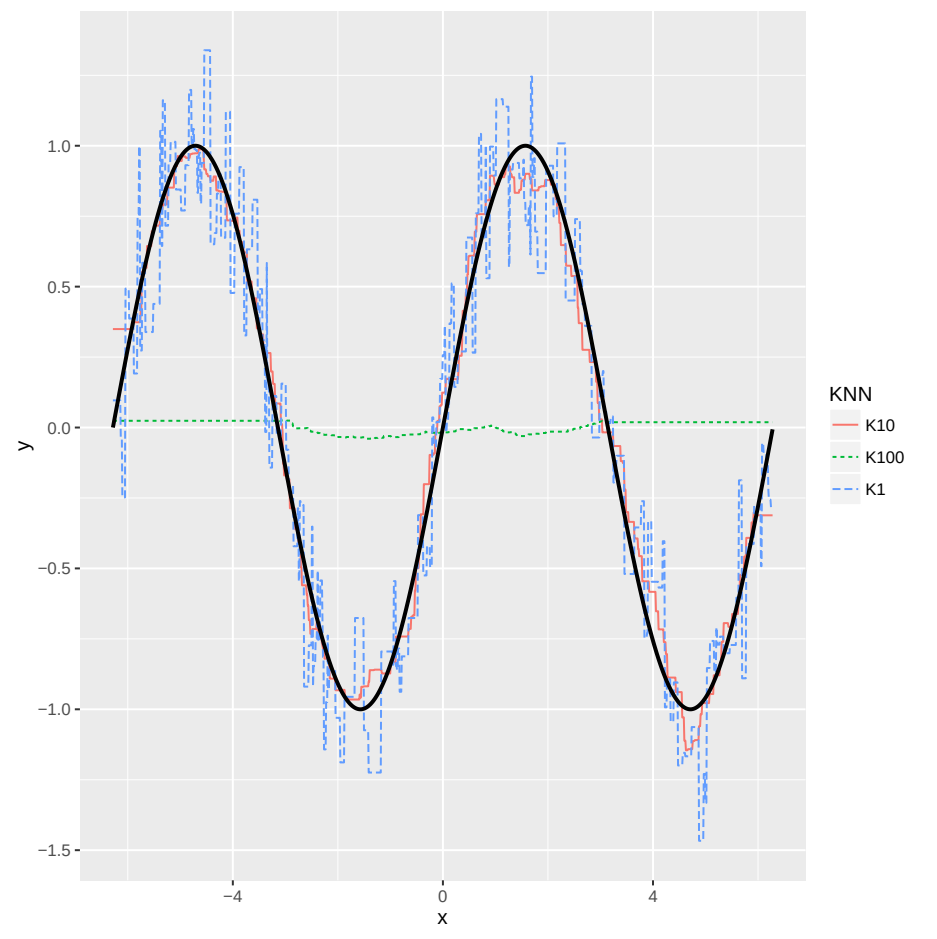
$\Longrightarrow$ k governs the complexity of the model.

Example

- knn.reg function from FNN package allows to fit k-nearest neighbors estimate.

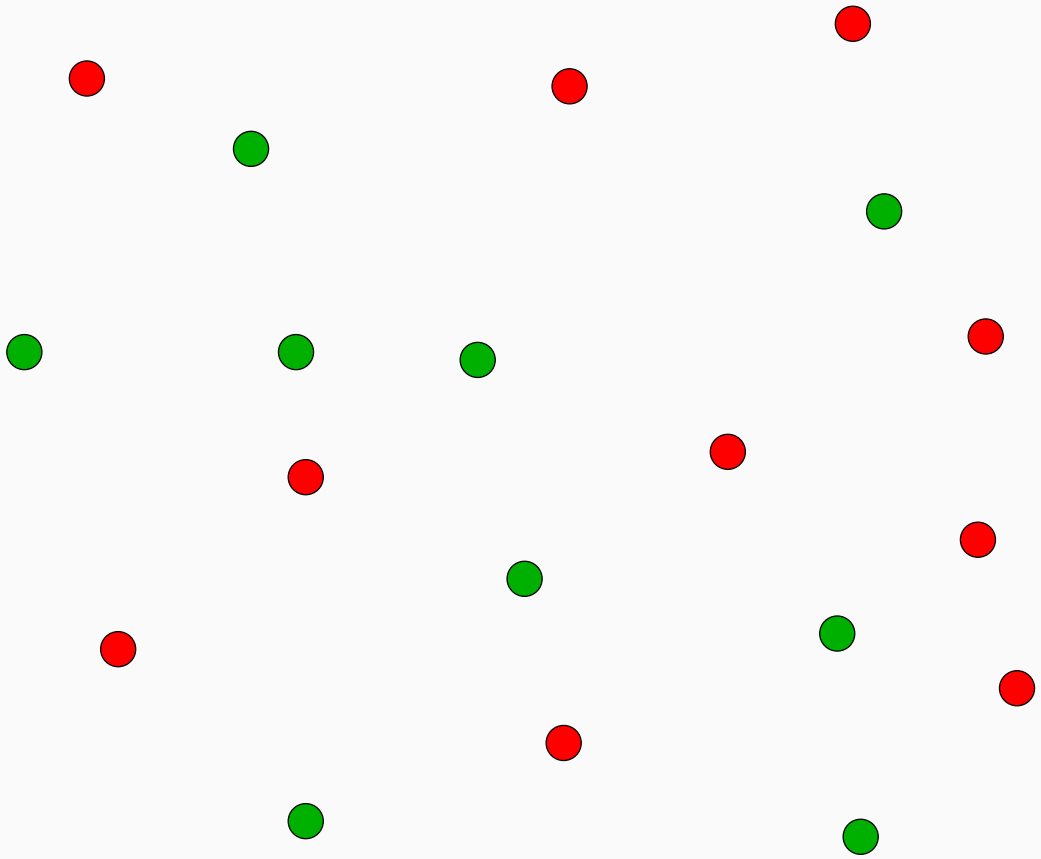
```
> k1 <- 10; k2 <- 100; k3 <- 1
> fx1 <- knn.reg(X,as.matrix(x),y=Y,k=k1)
> fx2 <- knn.reg(X,as.matrix(x),y=Y,k=k2)
> fx3 <- knn.reg(X,as.matrix(x),y=Y,k=k3)
> df1 <- data.frame(x=x,y=sin(x))
> df2 <- data.frame(x=x,"K10"=fx1$pred,
            "K100"=fx2$pred,"K1"=fx3$pred)
> df22 <- melt(df2,id.vars=1)
> names(df22)[2:3] <- c("KNN","y")
> ggplot(df22)+aes(x=x,y=y)+
  geom_line(aes(color=KNN,lty=KNN))+
  geom_line(data=df1,aes(x=x,y=y),size=1)
```



Supervised classification

- Kernel and nearest neighbors estimates have been presented in regression ($\mathcal{Y} = \mathbb{R}$).
- Approaches are similar in supervised classification::
  1. neighborhoods are defined in the same way;
  2. (only) change: instead of averaging the Y_i in a neighborhood of x, we make a majority vote.

Kernel for supervised classification



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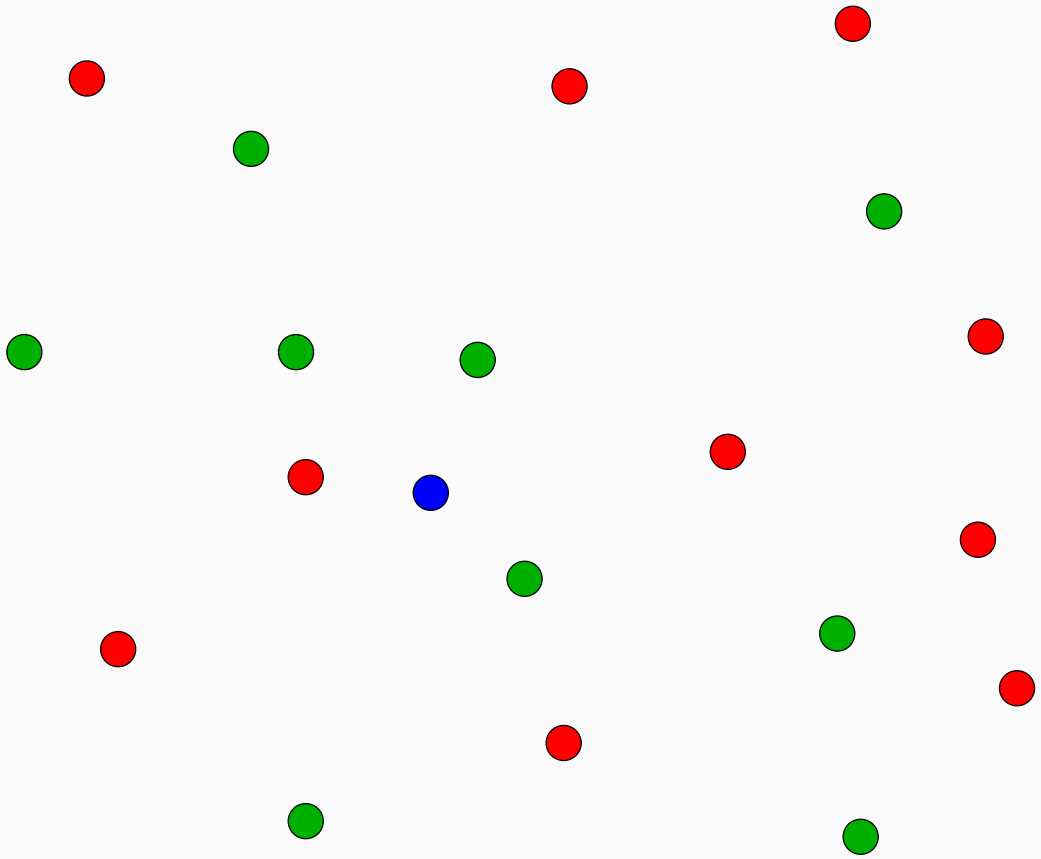

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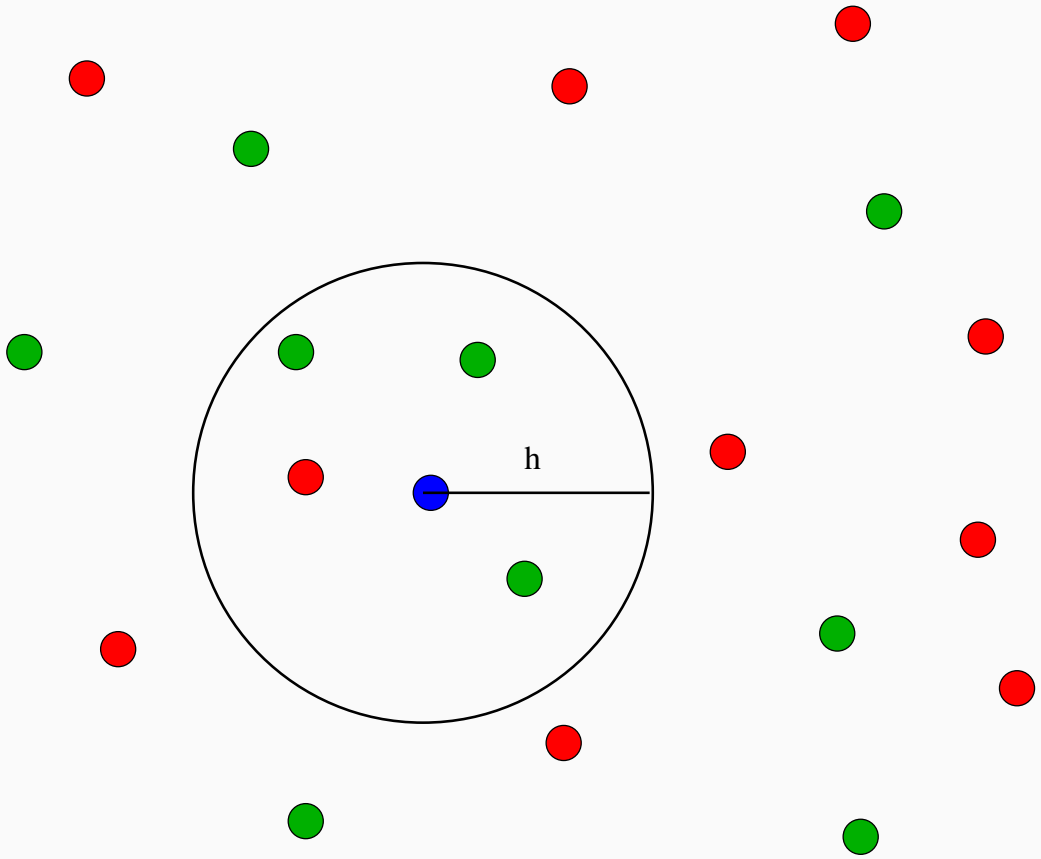

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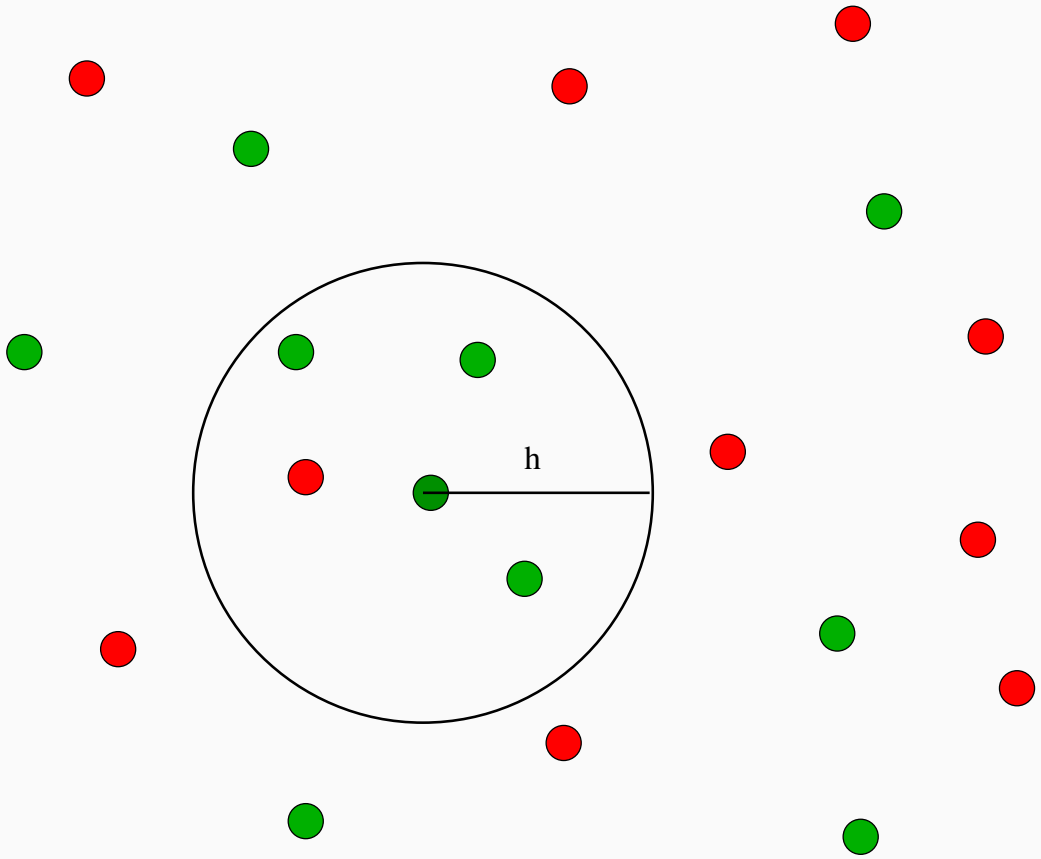
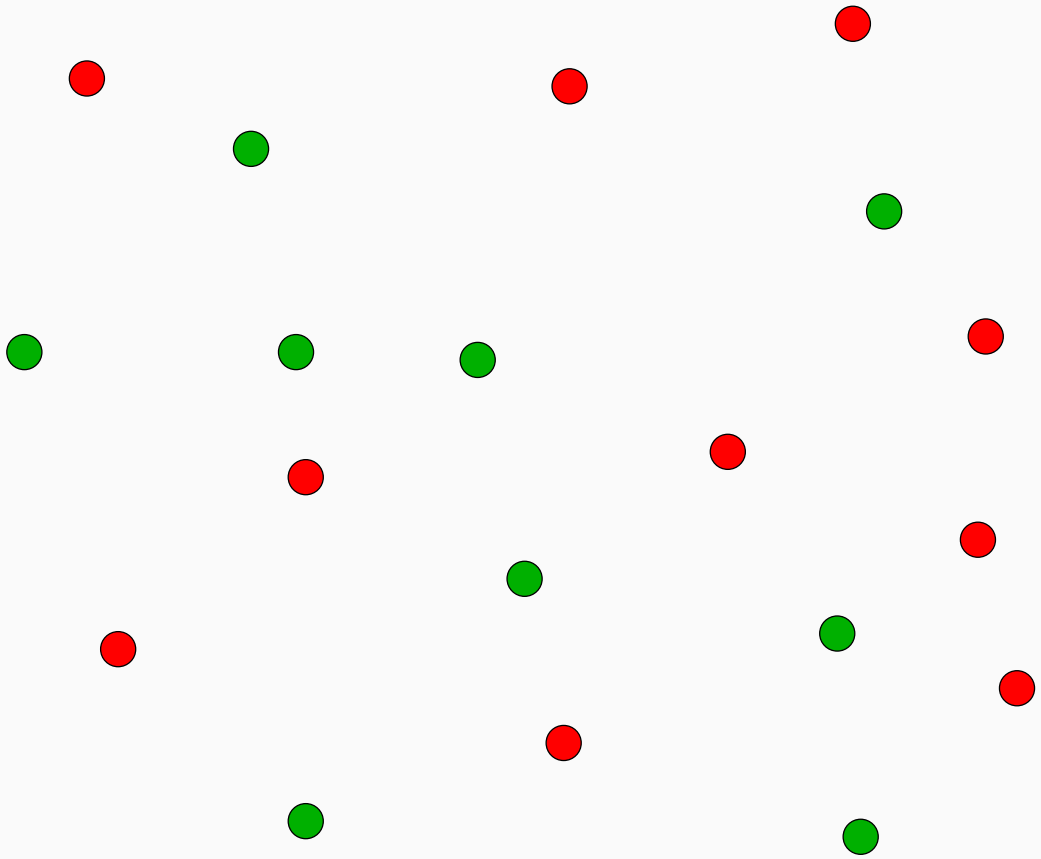


k-nn for supervised classification



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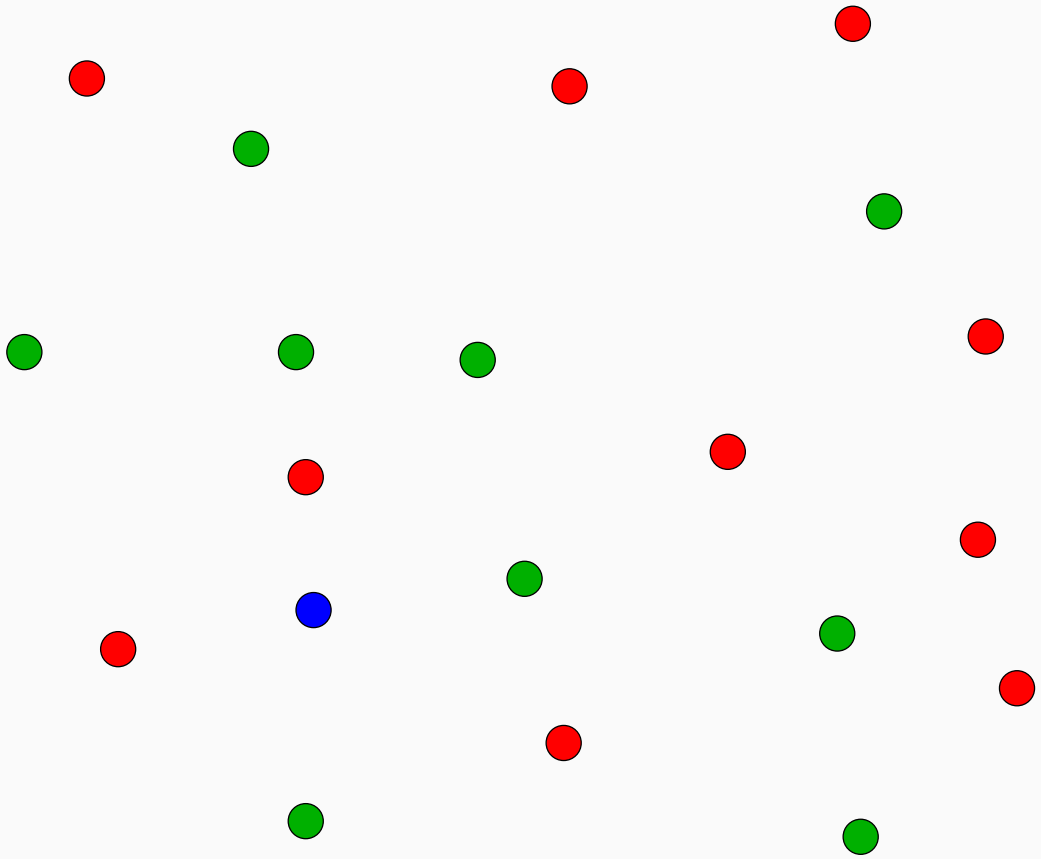

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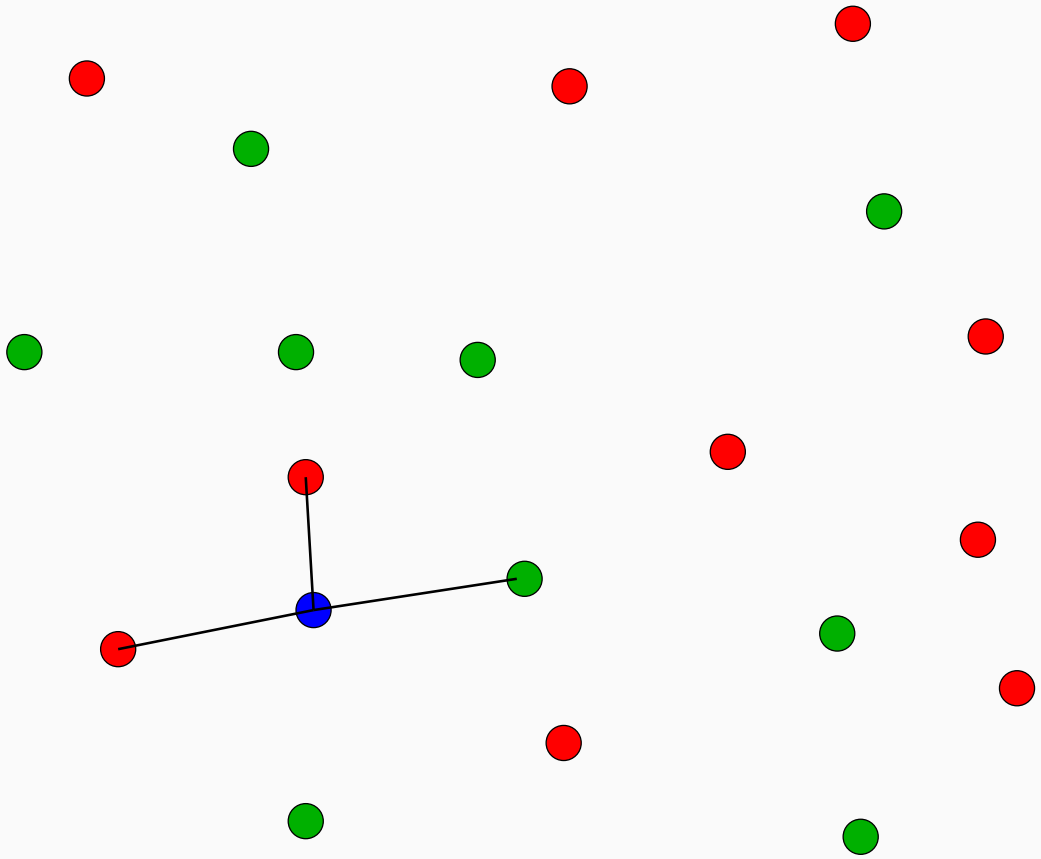

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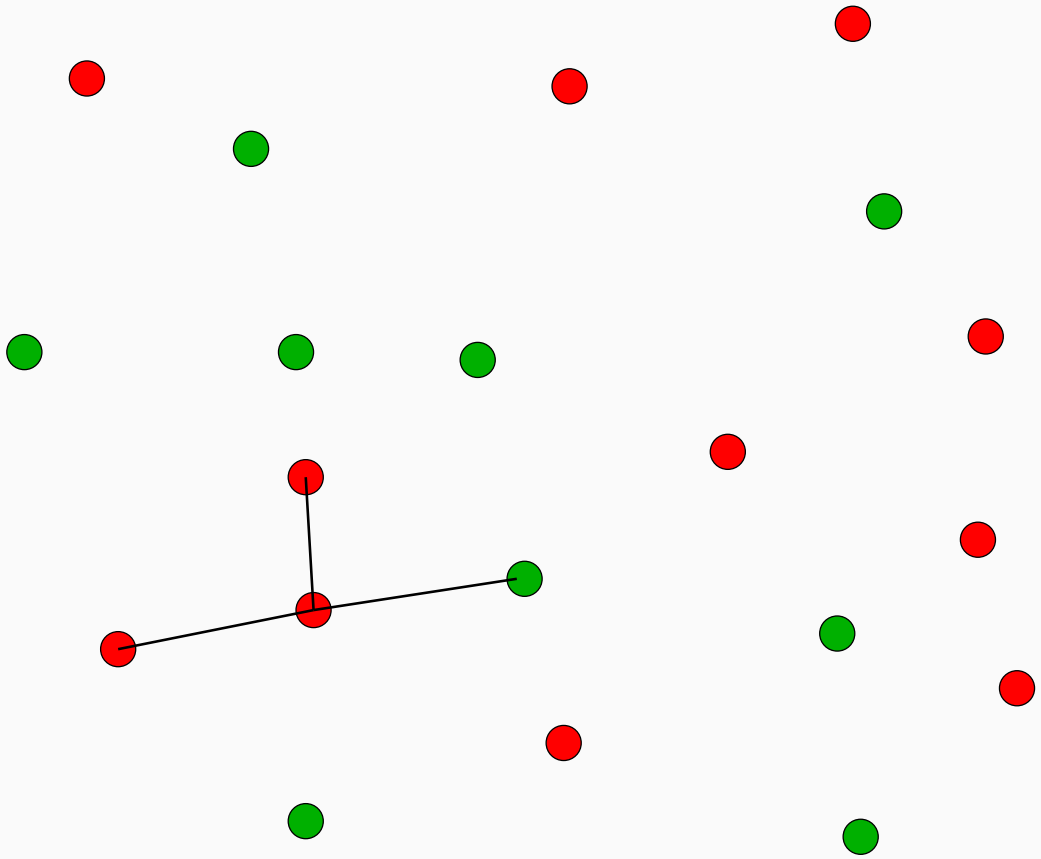

The k-nn rule

- Let $k \leq n$, the k-nn rule apply a majority vote to assess the group of new individuals:

$$\hat{g}_n(x) = MV(Y_i : i \in knn(x)) = \operatorname*{argmax}_{k \in \mathcal{Y}} \sum_{i \in \text{knn}(x)} \mathbf{1}_{Y_i = k}$$

where $\text{knn}(x) = \{i : X_i \text{ is among the knn of } x \text{ among } \{X_1, \ldots, X_n\}\}$.

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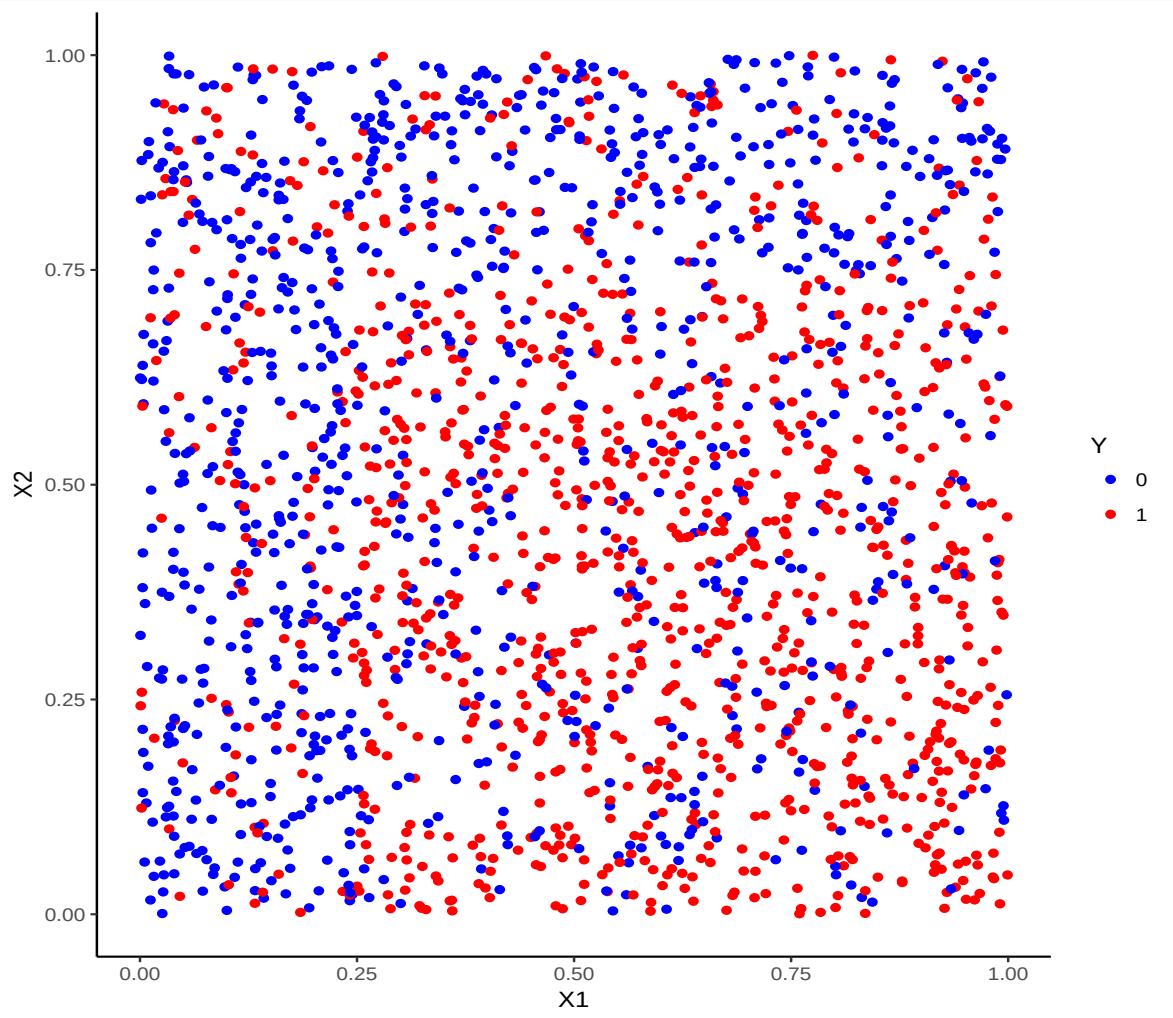
Remark

As for regression, the choice of k reveals crucial for the performance of the estimate:

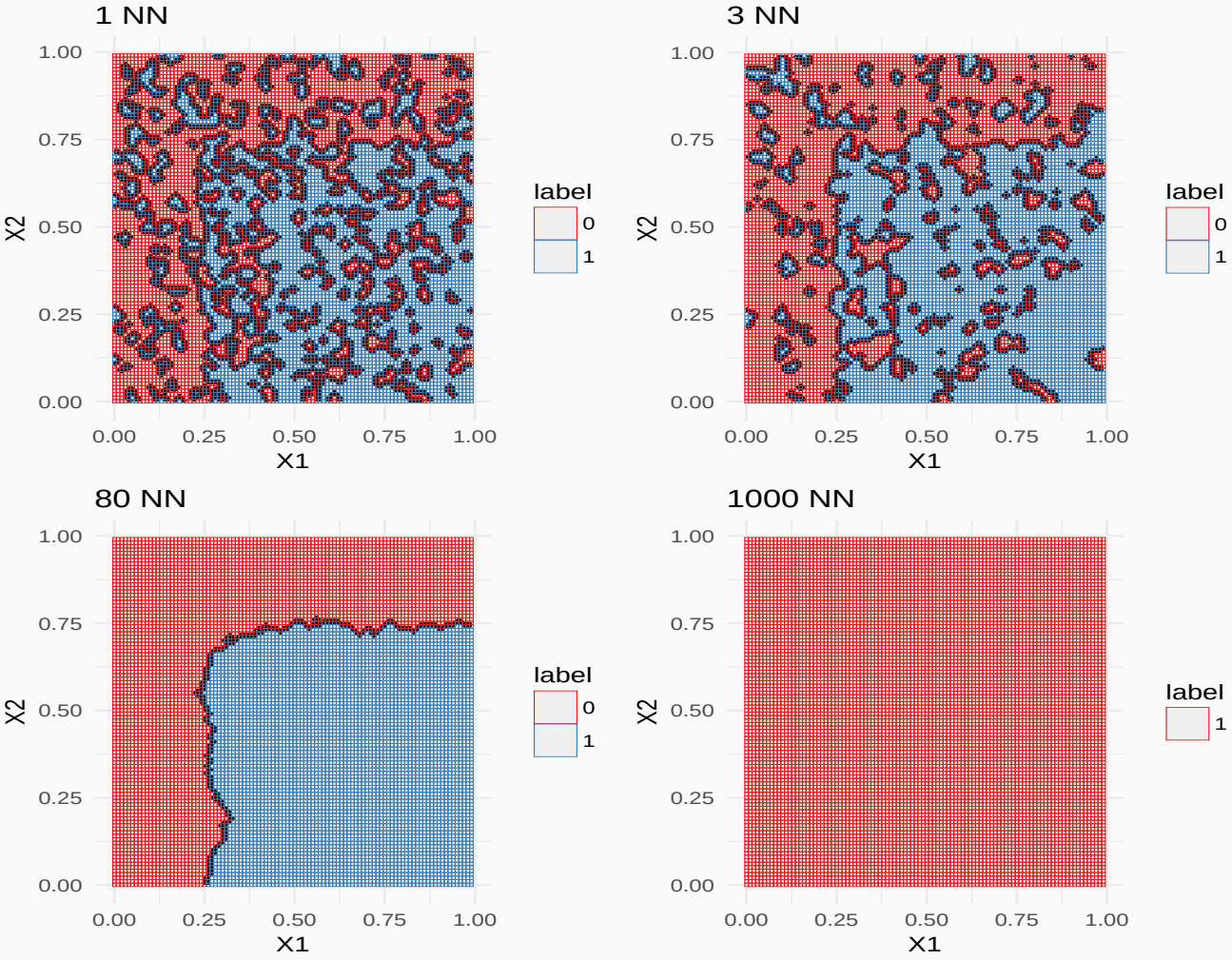
1. k large: "steady" estimate, small variance, large bias;
2. k small: "overfitting", large variance, small bias.

Example

- Goal: explain a binary variable Y by 2 continuous variables X_1 and X_2. We have $n = 2\,000$ observations.



k-nn rules



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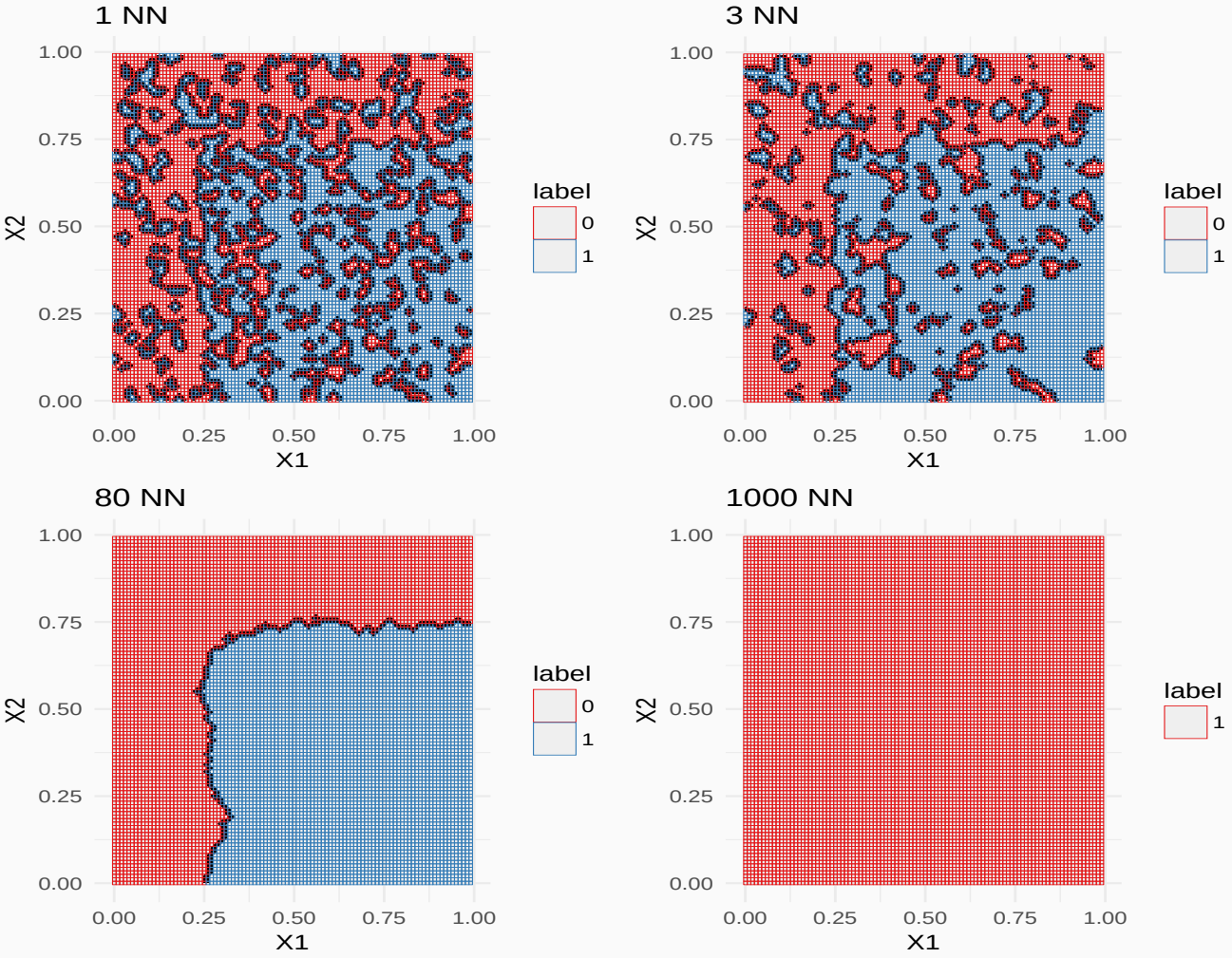

Conclusion

We clearly visualize how the choice of k is important.

Consistency [Györfi et al., 2002]

- For both regression and supervised classification, kernel rules and nearest neighbors rules are universally consistant (under weak assumptions).

Theorem [Stone, 1977]

If $k \to \infty$ and $k/n \to 0$, then the k-nn rule is universally consistant.

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- For both regression and supervised classification, kernel rules and nearest neighbors rules are universally consistant (under weak assumptions).

Theorem [Stone, 1977]

If $k \to \infty$ and $k/n \to 0$, then the k-nn rule is universally consistant.

Theorem [Devroye and Krzyżak, 1989]

If $h \to 0$ and $nh^d \to +\infty$, then the kernel rule universally consistant.

Outline

Rate of consistency [Györfi et al., 2002]

Nonparametric methods (always) suffer from the curse of dimensionality: as the dimension d increases, we have less and less observations in the neighborhoods of $x \Longrightarrow$

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Nonparametric methods (always) suffer from the curse of dimensionality: as the dimension d increases, we have less and less observations in the neighborhoods of $x \implies$ less and less accurate $\implies$ slower convergence rate.

Theorem

We consider the regression problem (explain Y by $X_1, \ldots, X_d$) and denote by m_n the k-nn estimate. Under technical assumptions, the quadratic risk of m_n satisfies (see exercise 3-IML0)

$$\mathcal{R}(m_n) = \mathrm{O}\left(n^{-\frac{2}{d+2}}\right).$$

Rate of consistency [Györfi et al., 2002]

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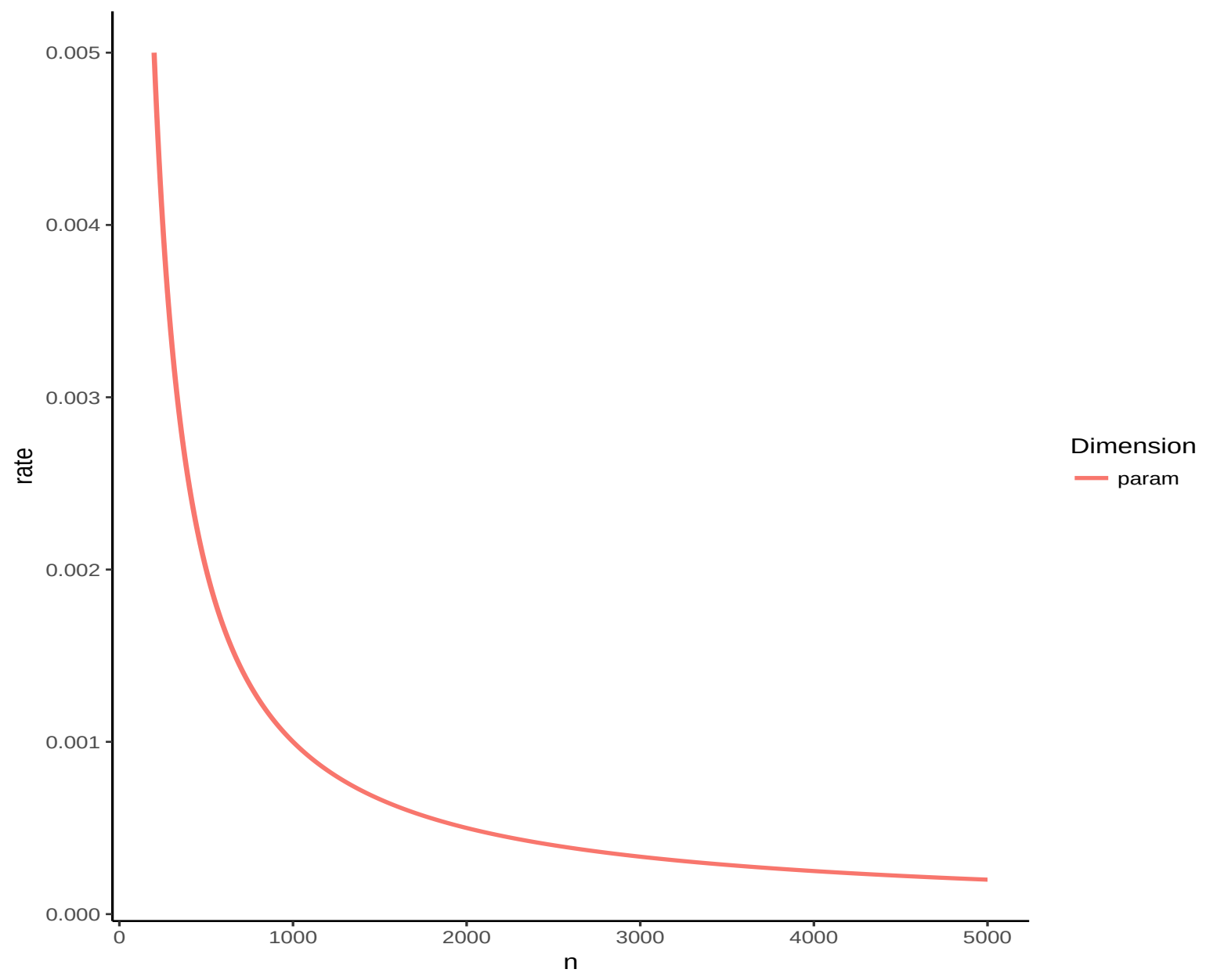
Consequence

- $d = 1$: rate $n^{-2/3}$, $d = 5$: rate $n^{-2/7}$.
- In practice, nonparametric estimates are not efficient in high dimensional spaces.

Curse of dimensionality (Illustration)



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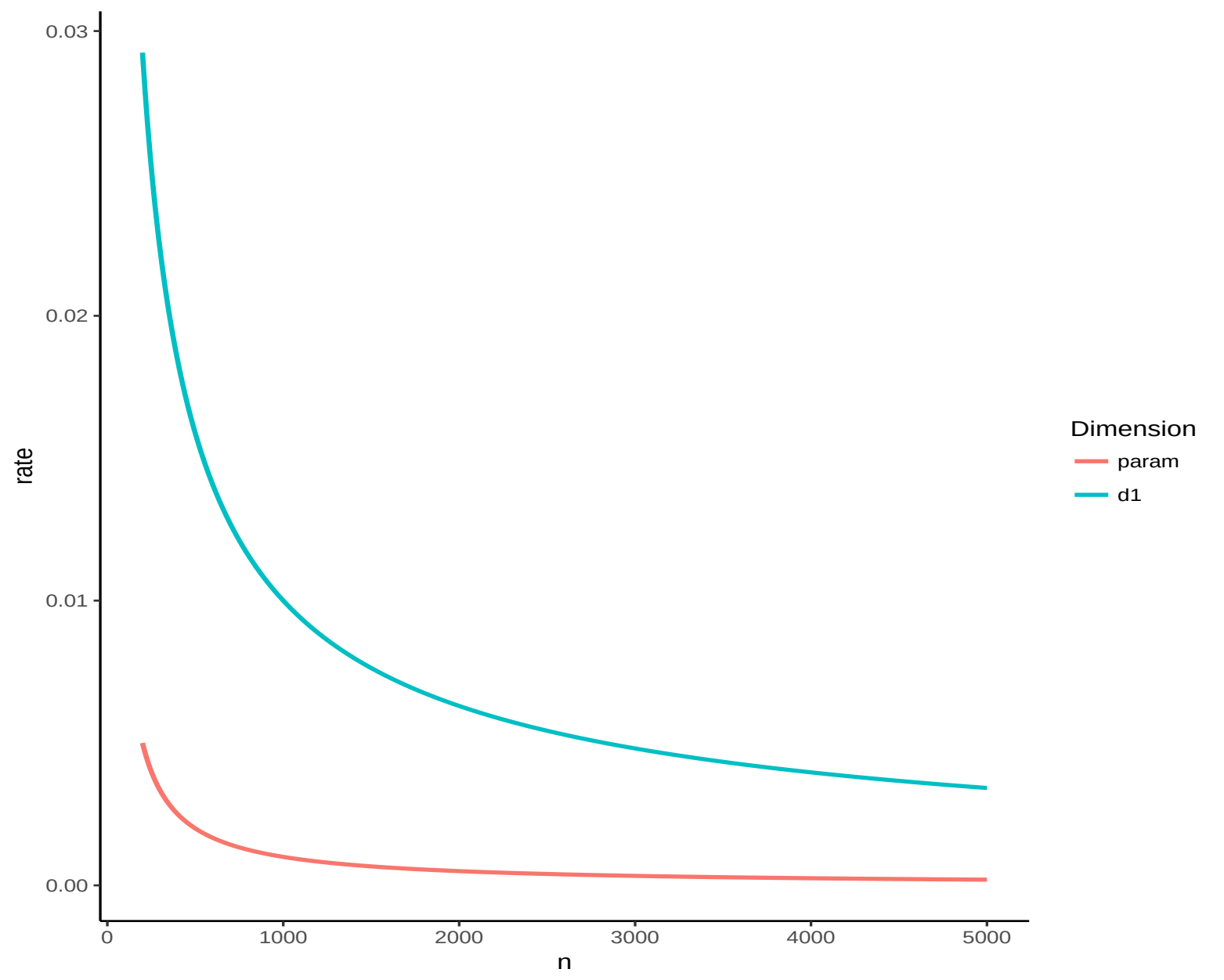

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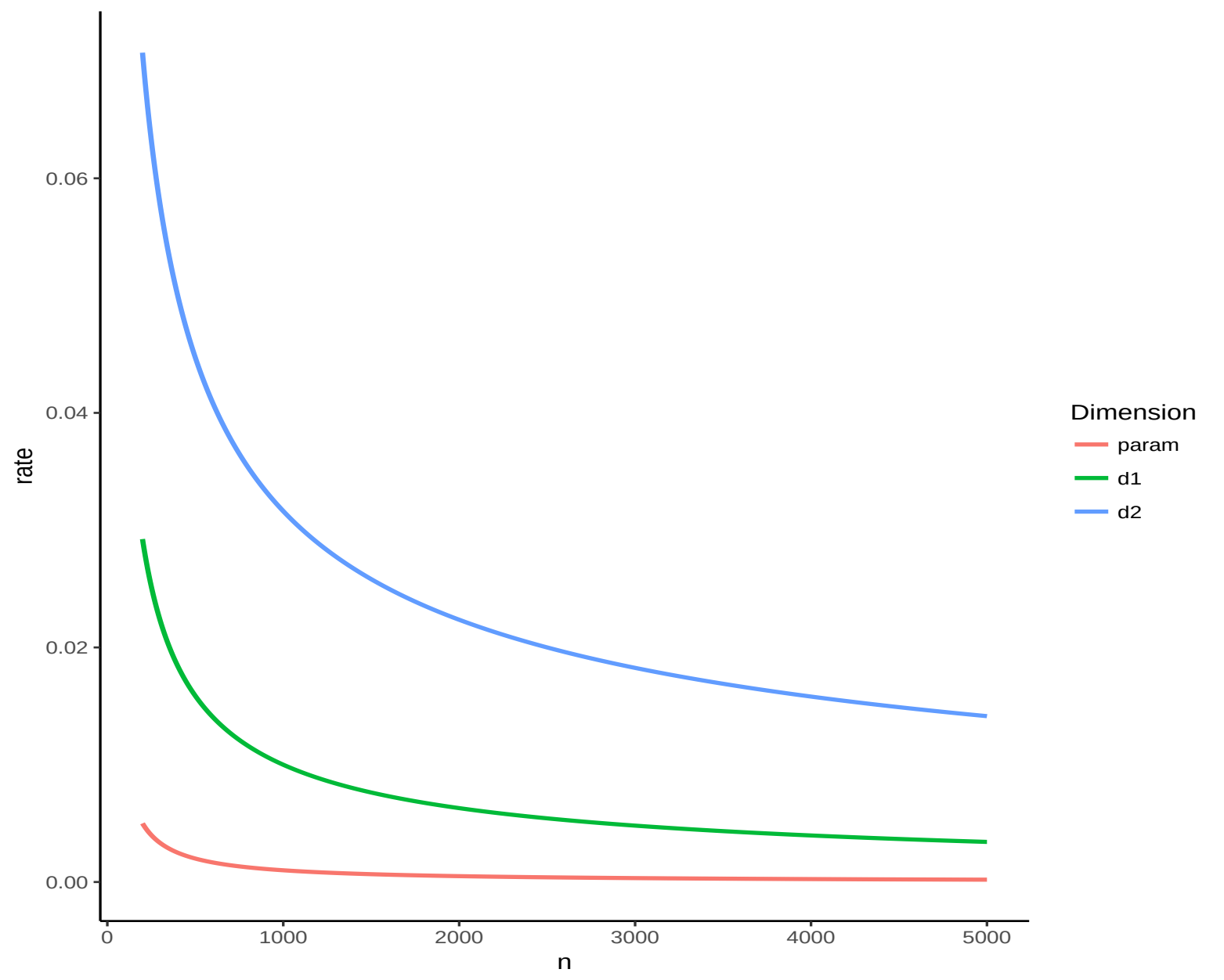

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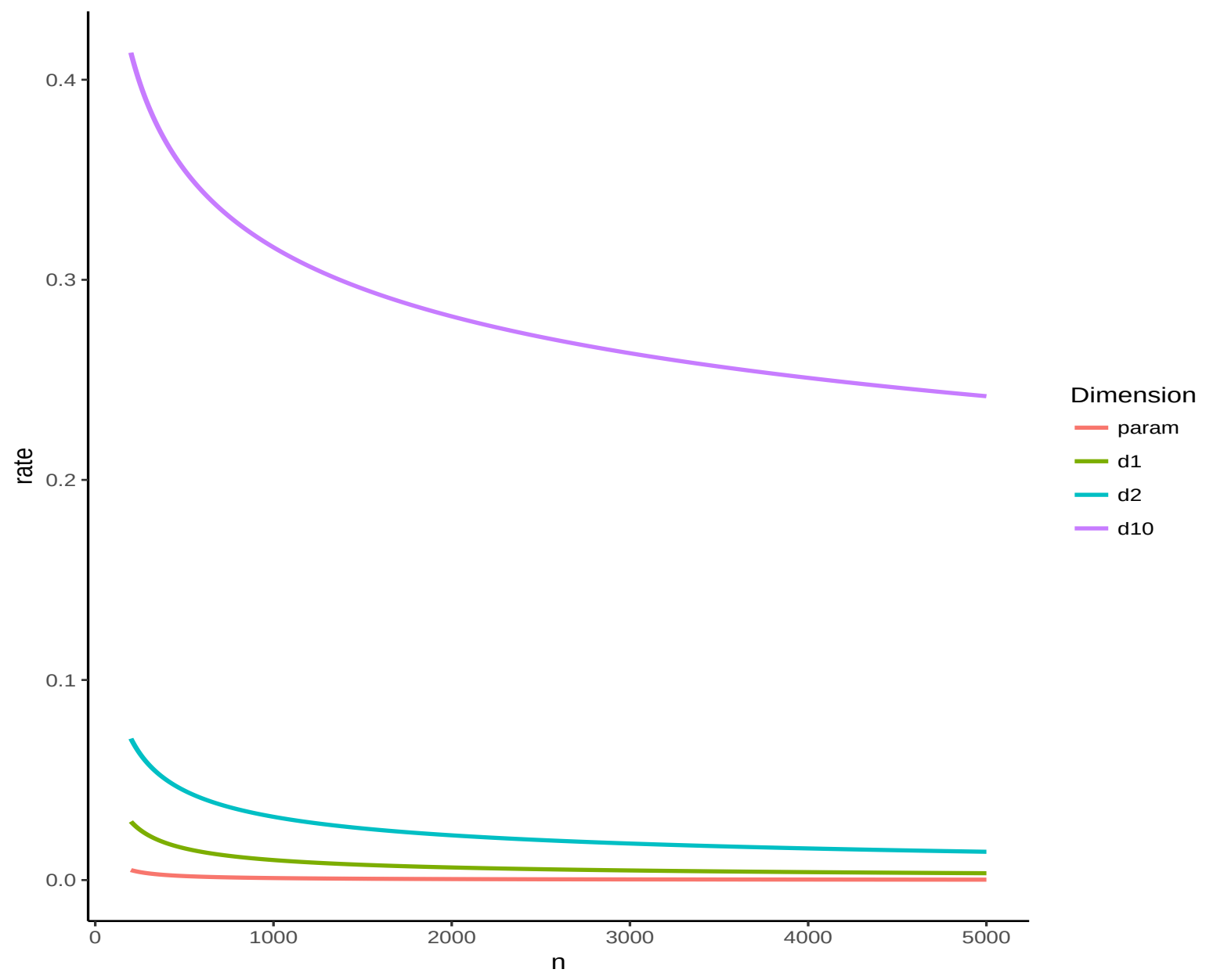

Outline

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Choosing parameters

- Most of the machines depends on parameters.

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Rules	Parameters
k-nn	k: number of neighbors
kernel	h: bandwidth
trees	depth
boosting	number of iterations
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Rules	Parameters
k-nn	k: number of neighbors
kernel	h: bandwidth
trees	depth
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- Selection of these parameters reveals crucial for the performances of the estimates.
- Goal:
  - define procedures which allow to automatically select these parameters;
  - establish theoretical guarantees for these procedures (GB lecture).

ERM strategy

Framework

- $\mathcal{F}$ a collection of machines.
- Risk for a machine f: $\mathcal{R}(f) = \mathbf{E}[\ell(Y, f(X))]$.
- Goal: select $\hat{f}$ in $\mathcal{F}$ such that

$$\mathcal{R}(\hat{f}) \approx \inf_{f \in \mathcal{F}} \mathcal{R}(f).$$

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$$\mathcal{R}(\hat{f}) \approx \inf_{f \in \mathcal{F}} \mathcal{R}(f).$$

ERM

- Estimate the risk of the machines in $\mathcal{F}$ (validation hold out, cross validation...) $\Longrightarrow \widehat{R}_n(f)$.
- Choose the machine $\hat{f}$ which minimizes the estimated risk $\widehat{R}_n(f)$.

Selecting k (k-nn rule)

- Data splitting:
  - A learning or train set $\mathcal{D}_m = \{(X_1, Y_1), \ldots, (X_m, Y_m)\}$;
  - A test set $\mathcal{D}_\ell = \{(X_{m+1}, Y_{m+1}), \ldots, (X_n, Y_n)\}$ with $m + \ell = n$.
- Candidates: $\mathcal{G}_m = \{g_k, 1 \leq k \leq m\} \to k$-nn rules using $\mathcal{D}_m$.
- Risk: $L(g) = \mathbf{P}(g(X) \neq Y)$.

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ERM Strategy

Choose $\widehat{g}_n$ which minmizes

$$\frac{1}{\ell} \sum_{i=m+1}^{n} \mathbf{1}_{g_k(X_i) \neq Y_i}.$$

Outline

- Classification and regression training.
- This package allows to select machines and to estimate their performances.
- More than 230 algorithms are available on caret: http://topepo.github.io/caret/index.html

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- This package allows to select machines and to estimate their performances.
- More than 230 algorithms are available on caret: http://topepo.github.io/caret/index.html
- We just have to specify:
  - the method (logistic, k-nn, trees, randomForest...)
  - a grid for the parameters to select parameters (number of NN...)
  - the risk (error probability, AUC, quadratic risk...)
  - how to estimate the risk (validation hold out, cross validation, bootstrap...)

Validation hold out i

```
> K_cand <- seq(1,500,by=20)
> library(caret)
> ctrl1 <- trainControl(method="LGOCV",number=1,index=list(1:1500))
> KK <- data.frame(k=K_cand)
> e1 <- train(Y~.,data=donnees,method="knn",trControl=ctrl1,tuneGrid=KK)
> e1
k-Nearest Neighbors

2000 samples
   2 predictor
   2 classes: '0', '1'

No pre-processing
Resampling: Repeated Train/Test Splits Estimated (1 reps, 75%)
Summary of sample sizes: 1500
Resampling results across tuning parameters:
  k    Accuracy  Kappa
```

Validation hold out ii

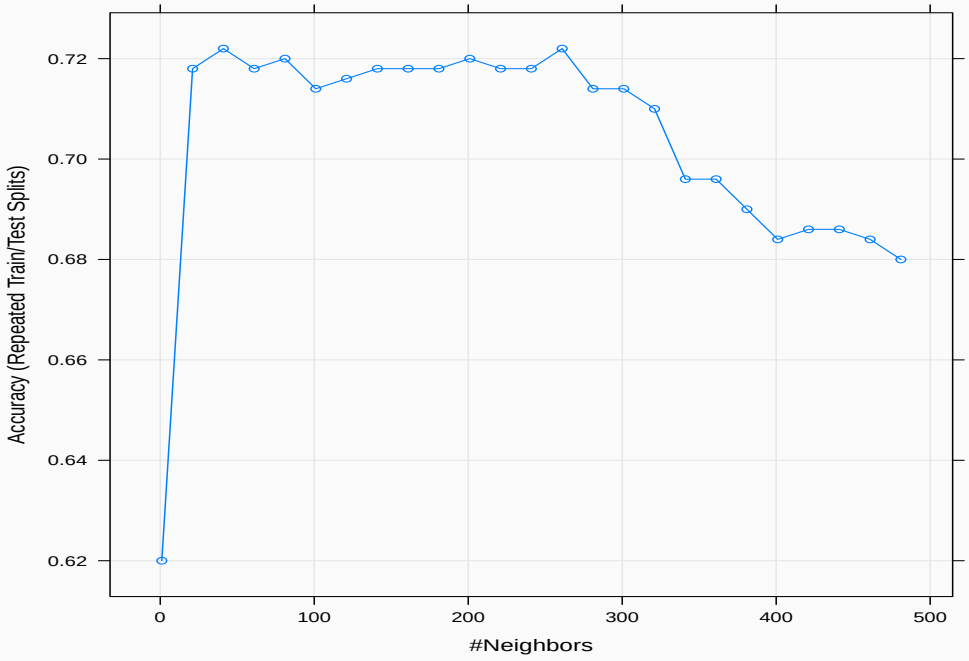
1	0.620	0.2382571
21	0.718	0.4342076
41	0.722	0.4418388
61	0.718	0.4344073
81	0.720	0.4383195
101	0.714	0.4263847
121	0.716	0.4304965
141	0.718	0.4348063
161	0.718	0.4348063
181	0.718	0.4348063
201	0.720	0.4387158
221	0.718	0.4350056
241	0.718	0.4350056
261	0.722	0.4428232
281	0.714	0.4267894
301	0.714	0.4269915
321	0.710	0.4183621
341	0.696	0.3893130

Validation hold out iii

```
  361  0.696     0.3893130
  381  0.690     0.3767090
  401  0.684     0.3645329
  421  0.686     0.3686666
  441  0.686     0.3679956
  461  0.684     0.3638574
  481  0.680     0.3558050

Accuracy was used to select the optimal model using  the largest value.
The final value used for the model was k = 261.
> plot(e1)
```

Validation hold out iv



Cross validation i

```
> library(doMC)
> registerDoMC(cores = 3)
> ctrl2 <- trainControl(method="cv",number=10)
> e2 <- train(Y~.,data=dapp,method="knn",trControl=ctrl2,tuneGrid=KK)
> e2
k-Nearest Neighbors

1500 samples
   2 predictor
   2 classes: '0', '1'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 1350, 1350, 1350, 1350, 1350, 1350, ...
Resampling results across tuning parameters:

  k    Accuracy   Kappa
```

Cross validation ii

1	0.6280000	0.2519051
21	0.7333333	0.4623213
41	0.7273333	0.4503384
61	0.7360000	0.4682891
81	0.7353333	0.4673827
101	0.7313333	0.4596395
121	0.7306667	0.4584747
141	0.7366667	0.4703653
161	0.7340000	0.4654675
181	0.7306667	0.4585136
201	0.7313333	0.4597224
221	0.7333333	0.4638243
241	0.7333333	0.4637789
261	0.7306667	0.4581189
281	0.7320000	0.4604955
301	0.7246667	0.4452185
321	0.7166667	0.4283226
341	0.7120000	0.4183438

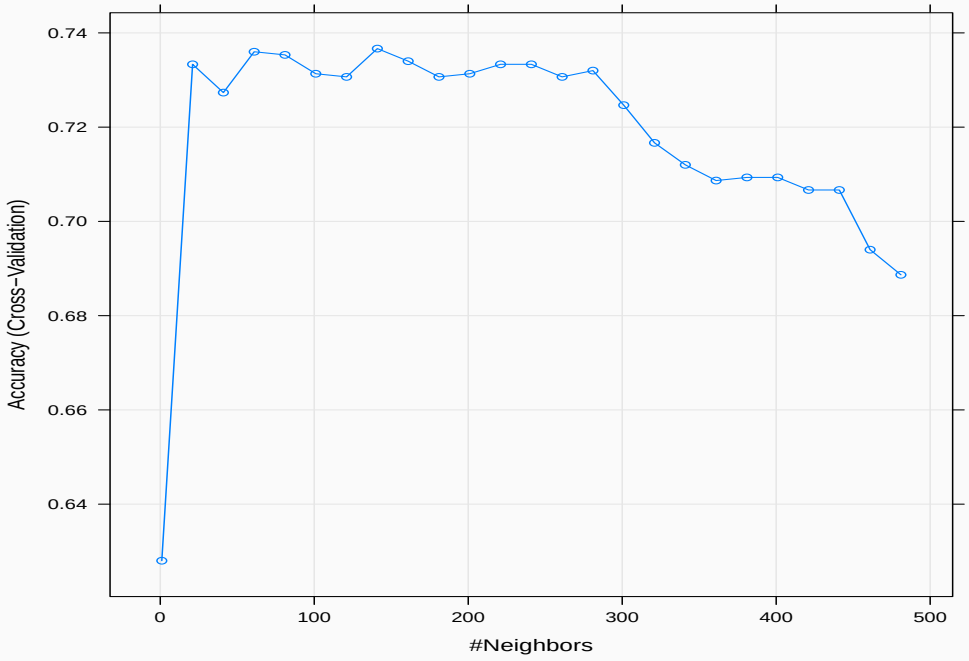
Cross validation iii

```
  361  0.7086667  0.4109784
  381  0.7093333  0.4121146
  401  0.7093333  0.4117108
  421  0.7066667  0.4057889
  441  0.7066667  0.4047529
  461  0.6940000  0.3782209
  481  0.6886667  0.3662798

Accuracy was used to select the optimal model using  the largest value.
The final value used for the model was k = 141.

> plot(e2)
```

Cross validation iv



Repeated cross-validation i

```
> ctrl3 <- trainControl(method="repeatedcv",repeats=5,number=10)
> e3 <- train(Y~.,data=dapp,method="knn",trControl=ctrl3,tuneGrid=KK)
> e3
k-Nearest Neighbors

1500 samples
   2 predictor
   2 classes: '0', '1'

No pre-processing
Resampling: Cross-Validated (10 fold, repeated 5 times)
Summary of sample sizes: 1350, 1350, 1350, 1350, 1350, 1350, ...
Resampling results across tuning parameters:

  k    Accuracy   Kappa
    1  0.6222667  0.2416680
   21  0.7352000  0.4661220
```

Repeated cross-validation ii

```
 41  0.7312000  0.4580125
 61  0.7310667  0.4580882
 81  0.7321333  0.4606022
101  0.7329333  0.4626718
121  0.7326667  0.4623496
141  0.7328000  0.4628236
161  0.7345333  0.4663240
181  0.7344000  0.4660110
201  0.7322667  0.4616271
221  0.7324000  0.4619926
241  0.7326667  0.4624912
261  0.7310667  0.4591799
281  0.7282667  0.4530797
301  0.7248000  0.4454653
321  0.7170667  0.4292033
341  0.7118667  0.4181330
361  0.7112000  0.4163210
381  0.7109333  0.4154893
```

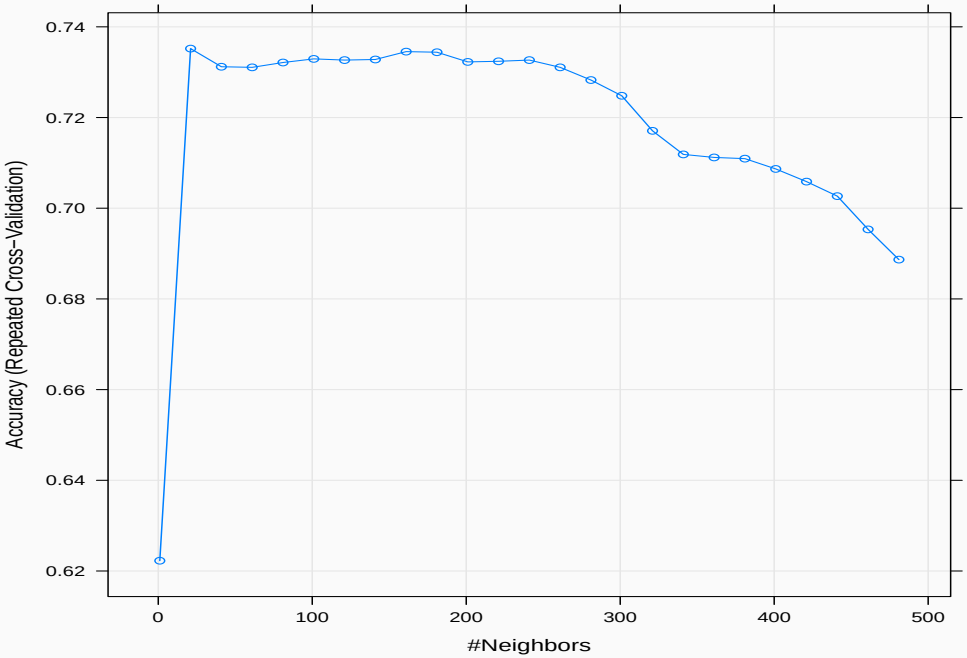
Repeated cross-validation iii

```
  401  0.7086667  0.4104291
  421  0.7058667  0.4043432
  441  0.7026667  0.3972028
  461  0.6953333  0.3813444
  481  0.6886667  0.3664347

Accuracy was used to select the optimal model using  the largest value.
The final value used for the model was k = 21.

> plot(e3)
```

Repeated cross-validation iv



Minimizing AUC i

```
> donnees1 <- donnees
> names(donnees1)[3] <- c("Class")
> levels(donnees1$Class) <- c("G0","G1")
> ctrl11 <- trainControl(method="LGOCV",number=1,index=list(1:1500),
                         classProbs=TRUE,summary=twoClassSummary)
> e4 <- train(Class~.,data=donnees1,method="knn",trControl=ctrl11,
                         metric="ROC",tuneGrid=KK)
> e4
k-Nearest Neighbors

2000 samples
   2 predictor
   2 classes: 'G0', 'G1'

No pre-processing
Resampling: Repeated Train/Test Splits Estimated (1 reps, 75%)
Summary of sample sizes: 1500
```

Minimizing AUC ii

```
Resampling results across tuning parameters:

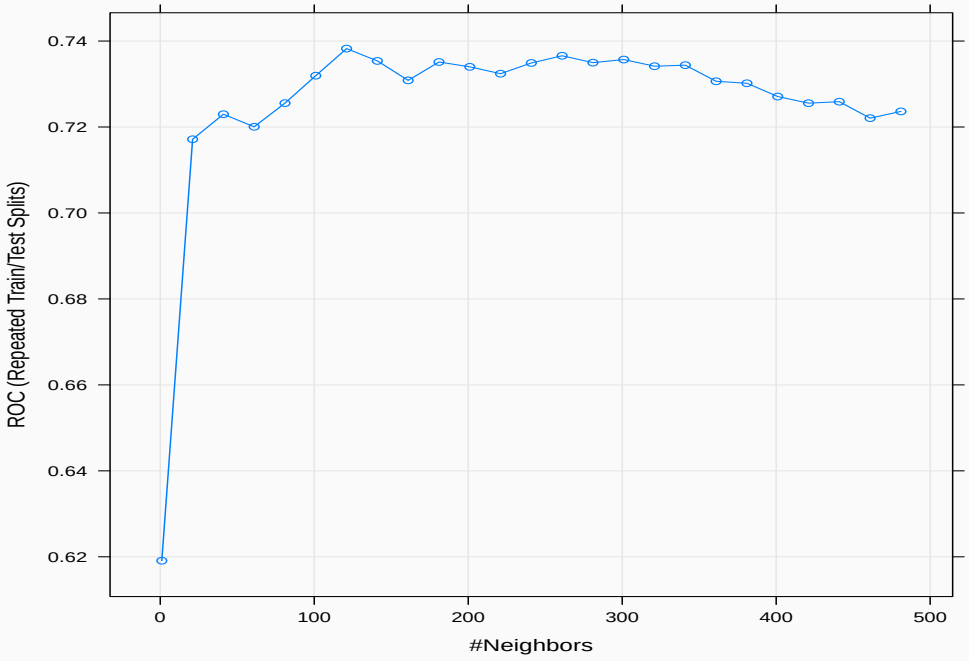
  k    ROC        Sens       Spec
    1  0.6190866  0.5983264  0.6398467
   21  0.7171484  0.6903766  0.7432950
   41  0.7229757  0.6861925  0.7547893
   61  0.7200500  0.6945607  0.7394636
   81  0.7255567  0.6945607  0.7432950
  101  0.7319450  0.6903766  0.7356322
  121  0.7382452  0.6945607  0.7356322
  141  0.7353757  0.7029289  0.7318008
  161  0.7308549  0.7029289  0.7318008
  181  0.7351272  0.7029289  0.7318008
  201  0.7340050  0.7029289  0.7356322
  221  0.7324099  0.7071130  0.7279693
  241  0.7349028  0.7071130  0.7279693
  261  0.7365780  0.7071130  0.7356322
  281  0.7349749  0.6987448  0.7279693
```

Minimizing AUC iii

```
  301  0.7356963  0.7029289  0.7241379
  321  0.7341493  0.6861925  0.7318008
  341  0.7343898  0.6527197  0.7356322
  361  0.7306385  0.6527197  0.7356322
  381  0.7301816  0.6359833  0.7394636
  401  0.7270957  0.6276151  0.7356322
  421  0.7255487  0.6317992  0.7356322
  441  0.7258933  0.6192469  0.7471264
  461  0.7220619  0.6150628  0.7471264
  481  0.7236330  0.6108787  0.7432950

ROC was used to select the optimal model using  the largest value.
The final value used for the model was k = 121.
> getTrainPerf(e4)
   TrainROC TrainSens TrainSpec method
1 0.7382452 0.6945607 0.7356322    knn
> plot(e4)
```

Minimizing AUC iv



Summary

- Parametric: strong assumption but fast rates $(1/n)$.
- Non parametric: less restrictive but slow rates plus curse of dimensionality $(1/n^{2/(d+2)})$.

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Summary

- Parametric: strong assumption but fast rates $(1/n)$.
- Non parametric: less restrictive but slow rates plus curse of dimensionality $(1/n^{2/(d+2)})$.
- ERM strategy: select (automatically) parameters which minimizes the estimated risk.
- Exercise 5, IML1.

Outline

References i

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Part III

Linear model: variable selection and et regularization

Outline

Framework

- $(X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d. observations with the same distribution as (X, Y) which takes values in $\mathcal{X} \times \mathcal{Y}$;
- In this part, we assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}$ or $\{-1, 1\}$.

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Linear and logistic models

1. If $\mathcal{Y} = \mathbb{R}$,

$$m(x) = \mathbf{E}[Y|X = x] = \beta_0 + \beta_1 x_1 + \ldots + \beta_d x_d = x^t \beta.$$

2. If $\mathcal{Y} = \{-1, 1\}$,

$$\operatorname{logit} p(x) = \beta_0 + \beta_1 x_1 + \ldots + \beta_d x_d = x^t \beta$$

where $p(x) = \mathbf{P}(Y = 1|X = x)$.

Some limits

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  1. prediction accuracy: LS and ML estimates can have large variance (especially when d is large) and thus poor prediction accuracy.

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  2. interpretation: when d is large, we don't know what are the most important variables.

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  1. prediction accuracy: LS and ML estimates can have large variance (especially when d is large) and thus poor prediction accuracy.
  2. interpretation: when d is large, we don't know what are the most important variables.

Goals

- Since we have more and more data, these drawbacks are occurring more and more often.
- We need to develop new automatic procedures to select important variables.

An example

- We generate observations $(x_i, y_i), i = 1, \ldots, 500$ according to

$$Y = 1X_1 + 0X_2 + \ldots + 0X_{q+1} + \varepsilon$$

where $X_2, X_{q+1}, \ldots, \varepsilon$ are i.i.d. with law $\mathcal{N}(0, 1)$.

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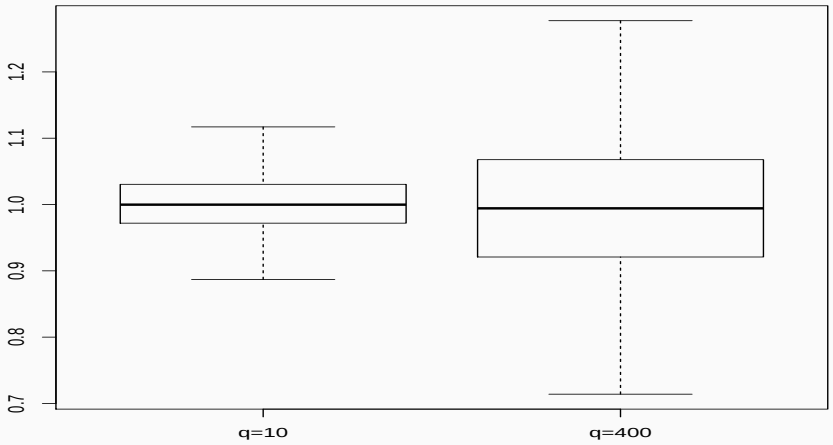
- We compute the LS estimator of β_1 for 1000 replications. We draw boxplot of these estimators for $q = 10$ and $q = 400$.



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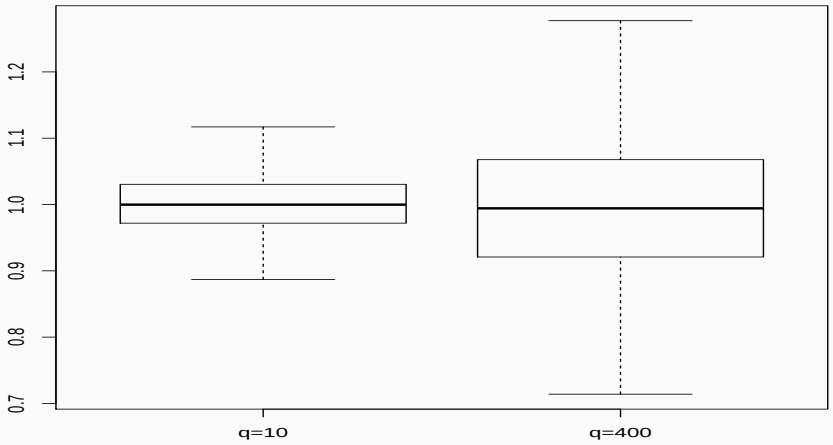
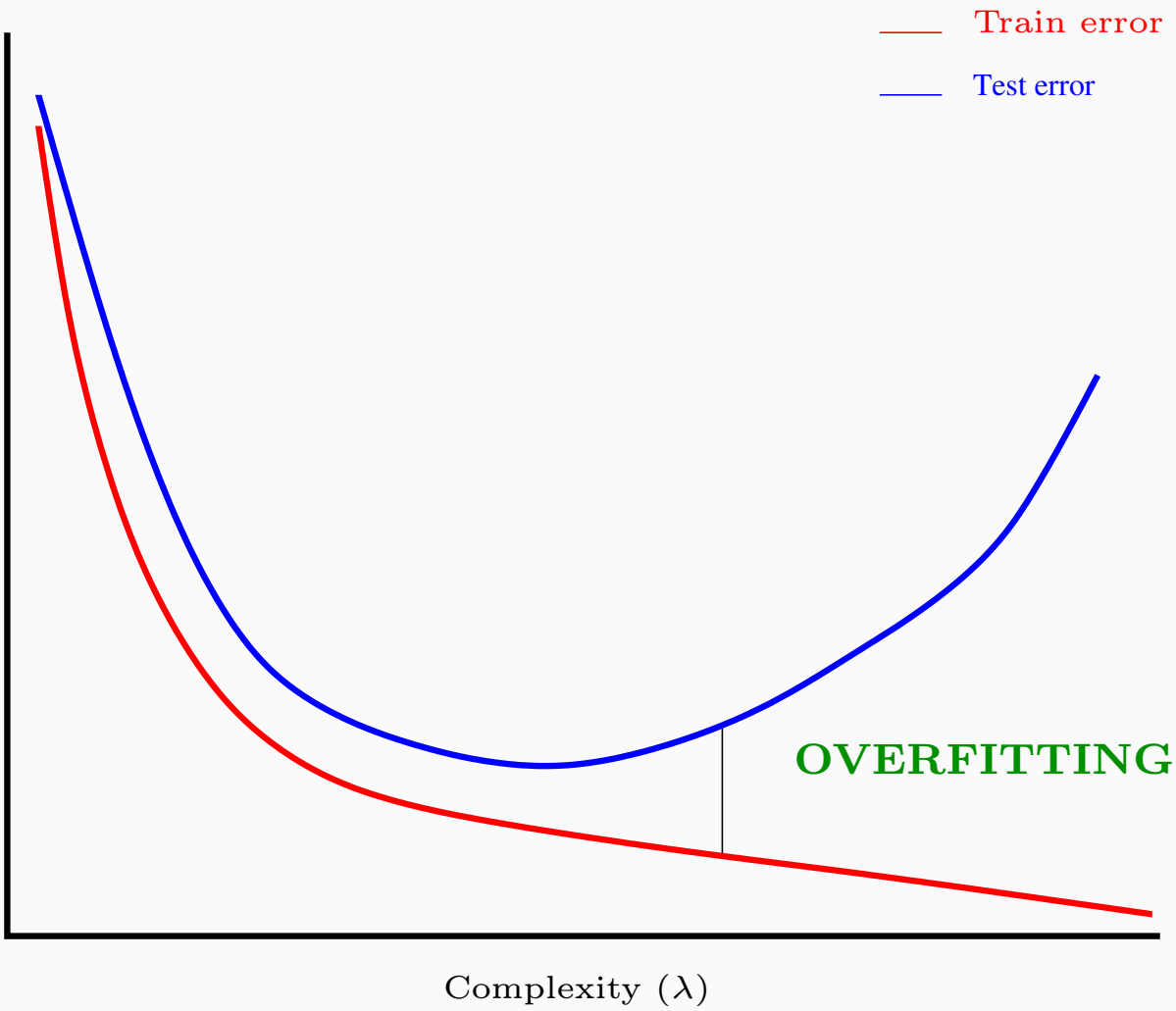


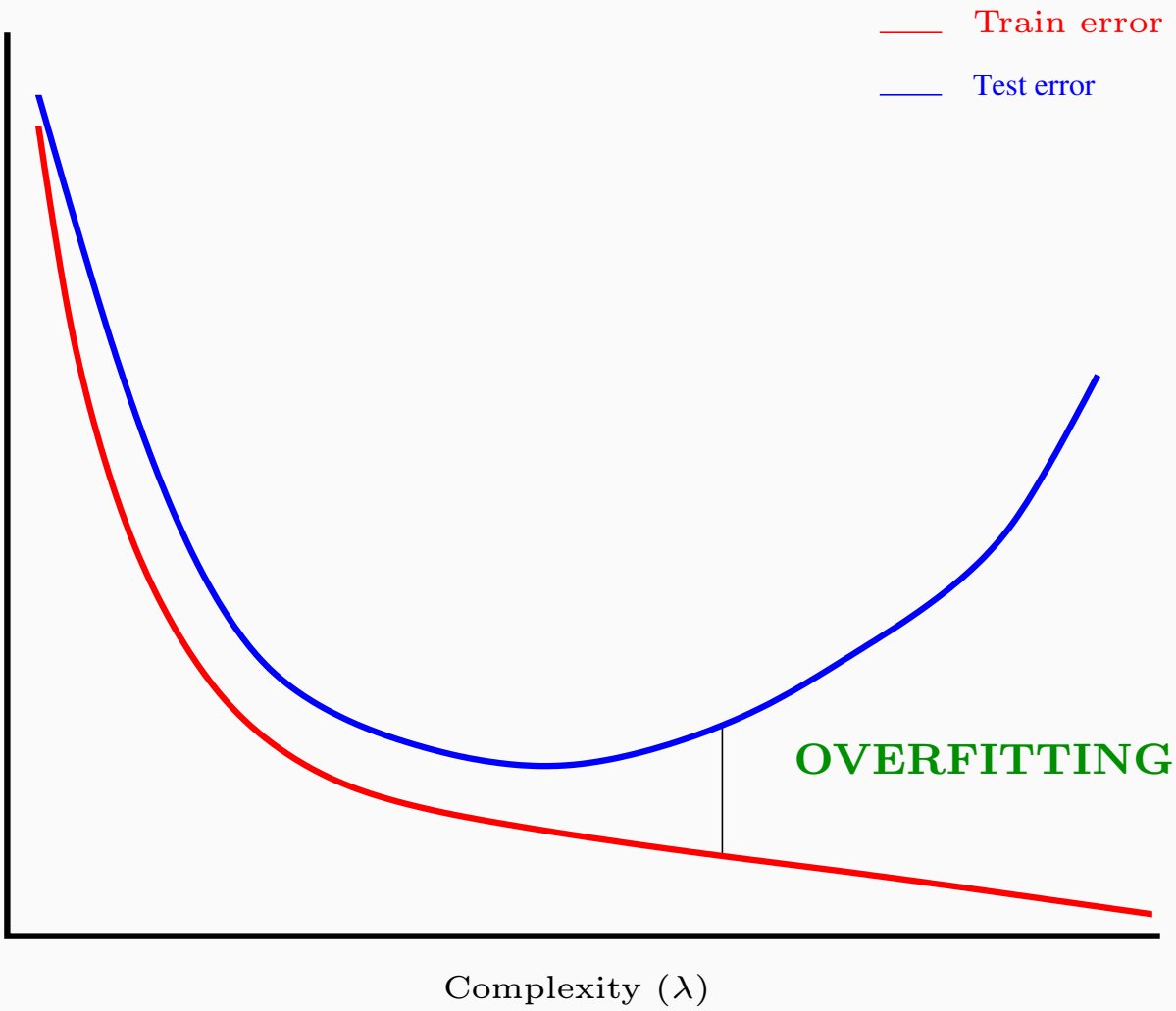
Conclusion

Large variance (thus loss of accuracy) when the number of unnecessary variables increases.

Size of the model



Size of the model



Conclusion

The size of the model governs the bias/variance trade-off.

Outline

Best subset selection

- $(X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d. with the same law as (X, Y) which takes values in $\mathbb{R}^d \times \mathbb{R}$;
- d input variables $\Longrightarrow$

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The idea

1. Fit the 2^d models;
2. Choose the one which optimizes a given criterion.

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The idea

1. Fit the 2^d models;
2. Choose the one which optimizes a given criterion.

Algorithm : best subset selection

1. for $k = 0, \ldots, d$:
   1.1 Fit the $\binom{d}{k}$ linear models with k variables;
   1.2 Choose the model with the higher R^2. Denote $\mathcal{M}_k$ this model.
2. Select, among $\mathcal{M}_0, \mathcal{M}_1, \ldots, \mathcal{M}_d$, the best model according to a given criterion.

Some criteria

- AIC: Akaike Information Criterion

$$-2\mathcal{L}_n(\hat{\beta}) + 2d.$$

- BIC: Bayesian Information Criterion

$$-2\mathcal{L}_n(\hat{\beta}) + \log(n)d.$$

- Adjusted R^2:

$$R_a^2 = 1 - \frac{n-1}{n-d+1}(1-R^2) \quad \text{where} \quad R^2 = \frac{SSR}{SST} = \frac{\|\hat{\mathbb{Y}} - \bar{\mathbb{Y}}\mathbf{1}\|^2}{\|\mathbb{Y} - \bar{\mathbb{Y}}\mathbf{1}\|^2}.$$

- Mallows's C_p:

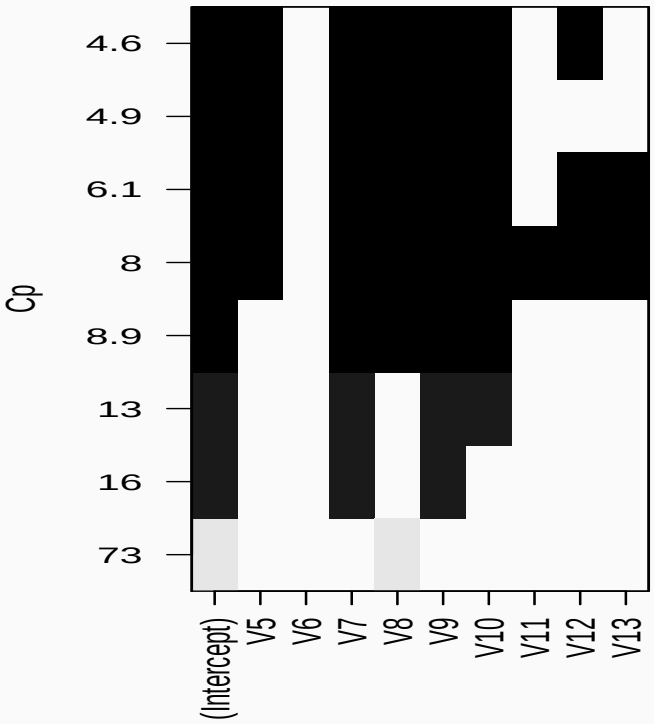
$$C_p = \frac{1}{n}\left(\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 + 2d\hat{\sigma}^2\right).$$

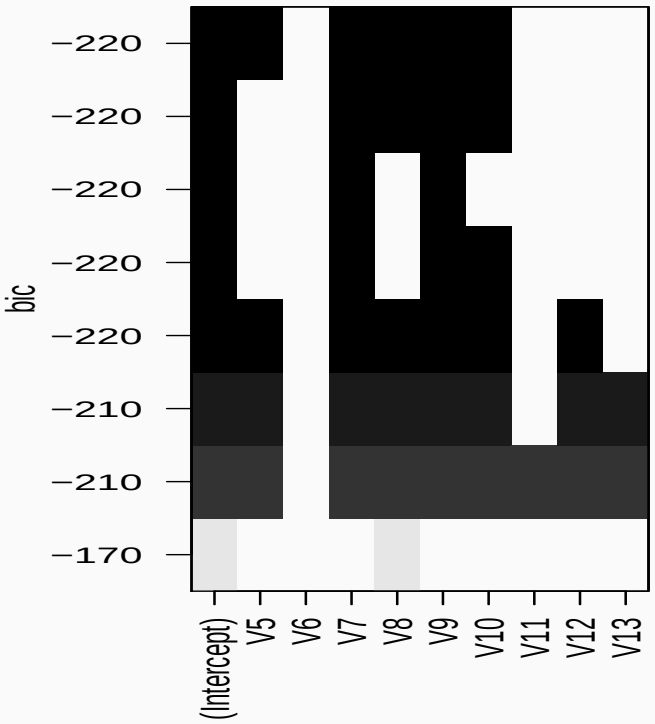
R user

- regsubsets from leaps package allows to make best subset selection.

```
> library(leaps)
> reg.fit <- regsubsets(V4~V5+V6+V7+V8+V9+V10+V11+V12+V13,data=Ozone)
> summary(reg.fit)
1 subsets of each size up to 8
Selection Algorithm: exhaustive
         V5  V6  V7  V8  V9  V10 V11 V12 V13
1  ( 1 ) " " " " " " "*" " " " " " " " " " "
2  ( 1 ) " " " " "*" " " "*" " " " " " " " "
3  ( 1 ) " " " " "*" " " "*" "*" " " " " " "
4  ( 1 ) " " " " "*" "*" "*" "*" " " " " " "
5  ( 1 ) "*" " " "*" "*" "*" "*" " " " " " "
6  ( 1 ) "*" " " "*" "*" "*" "*" " " "*" " "
7  ( 1 ) "*" " " "*" "*" "*" "*" " " "*" "*"
8  ( 1 ) "*" " " "*" "*" "*" "*" "*" "*" "*"
```

```
> plot(reg.fit,scale="Cp")
> plot(reg.fit,scale="bic")
```





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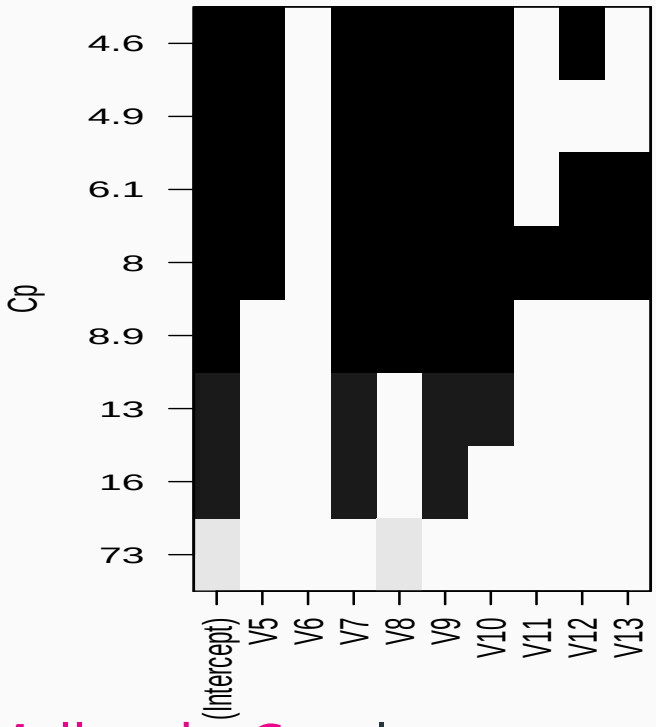

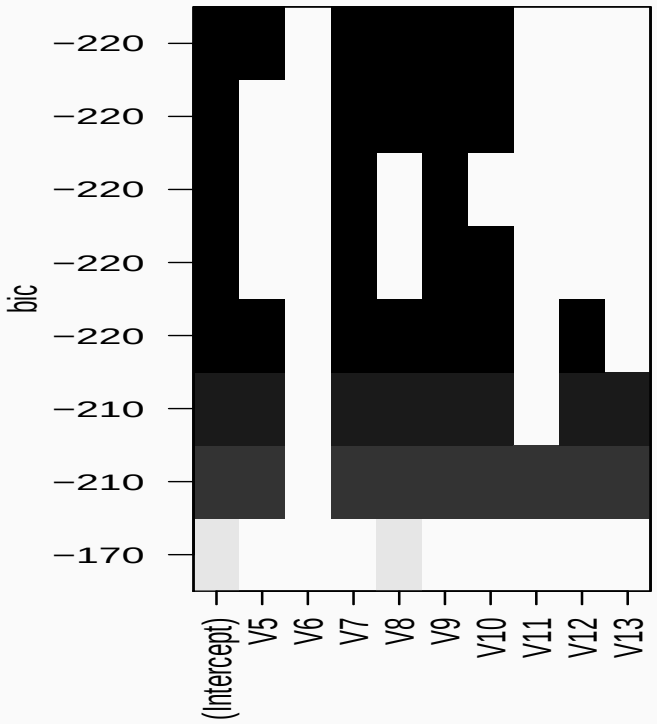

- Mallows's C_p selects:

$$Y = \beta_0 + \beta_1 V_5 + \beta_2 V_7 + \beta_3 V_8 + \beta_4 V_9 + \beta_5 V_{10} + \beta_6 V_{12} + \varepsilon.$$

- BIC selects:

$$Y = \beta_0 + \beta_1 V_5 + \beta_2 V_7 + \beta_3 V_8 + \beta_4 V_9 + \beta_5 V_{10} + \varepsilon.$$

Stepwise selection

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- Drawback: it becomes infeasible (too long computational time) when d is large ($d \geq 40$).
- When d is large, we can seek a good path through all possible subsets.
- Stepwise selection procedures define recursive models by adding or deleting one variable at each step.

Forward stepwise selection

1. Let $\mathcal{M}_0$ the null model (only the intercept);
2. for $k = 0, \ldots, d-1$:
   2.1 Define the $d-k$ models by adding one variable in $\mathcal{M}_k$;
   2.2 Choose, among those $d-k$ models, the one which maximizes the R^2. Denote $\mathcal{M}_{k+1}$ this model.
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Backward stepwise selection

1. Let $\mathcal{M}_d$ the full model (d variables);
2. For $k = d, \ldots, 1$:
   2.1 Define the k models by deleting one variable in $\mathcal{M}_k$;
   2.2 Choose, among those k models, the one which maximizes R^2. Denote $\mathcal{M}_{k-1}$ this model.
3. Select, among $\mathcal{M}_0, \ldots, \mathcal{M}_d$, the best model according to a given criterion.

R user

- We just have to add the argument method="forward" or method="backward" in regsubsets to make subset selection.

```
> reg.fit.for <- regsubsets(V4~V5+V6+V7+V8+V9+V10+V11+V12+V13,data=Ozone,
    method="forward")
> reg.fit.back <- regsubsets(V4~V5+V6+V7+V8+V9+V10+V11+V12+V13,data=Ozone,
    method="backward")
```

```
> summary(reg.fit.for)

         V5  V6  V7  V8  V9  V10 V11 V12 V13
1  ( 1 ) " " " " " " "*" " " " " " " " " " "
2  ( 1 ) " " " " "*" "*" " " " " " " " " " "
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7  ( 1 ) "*" " " "*" "*" "*" "*" " " "*" "*"
8  ( 1 ) "*" " " "*" "*" "*" "*" "*" "*" "*"
```

```
> summary(reg.fit.back)

         V5  V6  V7  V8  V9  V10 V11 V12 V13
1  ( 1 ) " " " " " " " " " " "*" " " " " " "
2  ( 1 ) " " " " "*" " " "*" " " " " " " " "
3  ( 1 ) " " " " "*" " " "*" "*" " " " " " "
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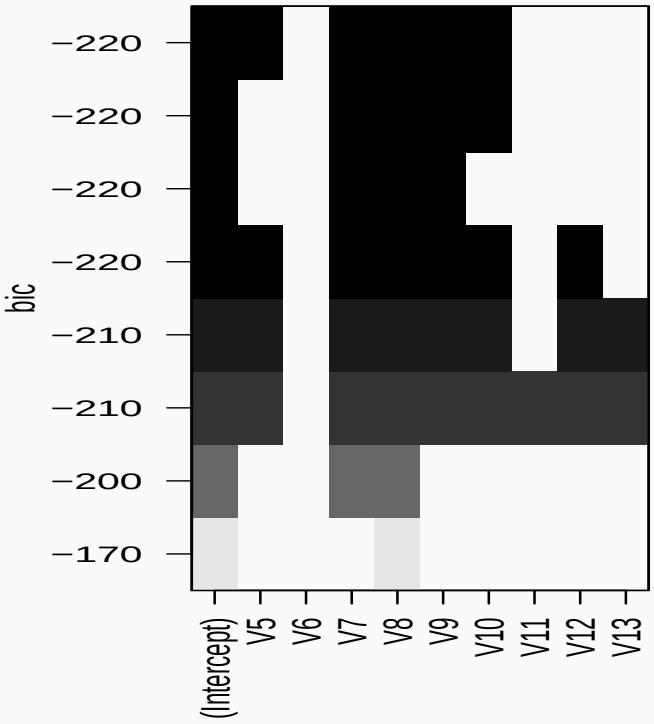
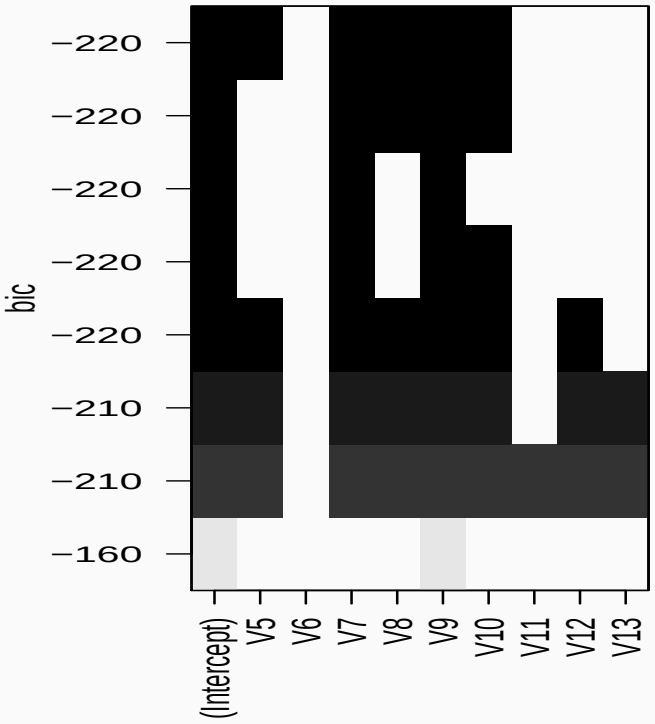
```

```
> plot(reg.fit.for,scale="bic")
> plot(reg.fit.back,scale="bic")
```





Remark

For this example, forward and backward selection provide the same model (it's not always the case).

Binary classification

- Best subset and stepwise selection have been proposed for regression ($\mathcal{Y} = \mathbb{R}$).

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- Exercise 1-2, IML2.

Outline

- For large values of d, least square estimates in the linear model

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- How? By imposing a constraint on the size of the coefficients:

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- Which norm for the constraint?
- How should we select t?
  - t small $\Longrightarrow$ strong constraint ($\hat{\beta}_j \approx 0$) ;
  - t large $\Longrightarrow$ small constraint ($\hat{\beta}_j \approx \hat{\beta}_{j,LS}$).

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Definition

1. Ridge estimates $\hat{\beta}^R$ minimize

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2. or equivalently by imposing a penalty on the size of the coefficients

$$\hat{\beta}^R = \underset{\beta}{\operatorname{argmin}}\left\{\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{d} x_{ij}\beta_j\right)^2 + \lambda\sum_{j=1}^{d}\beta_j^2\right\}. \tag{3}$$

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- (2) are (3) the same in the sense that there is a one-to-one correspondence between t and λ.
- Ridge estimate depends on t (or λ) : $\hat{\beta}^R = \hat{\beta}^R(t) = \hat{\beta}^R(\lambda)$.
- Input variables are generally standardized to make the variables at the same scale (it is automatic in classical softwares).

An example

- The problem: explain the level of prostate specific antigen by a number (8) of clinical measures.
- $n = 100$ data available at https://web.stanford.edu/~hastie/ElemStatLearn/

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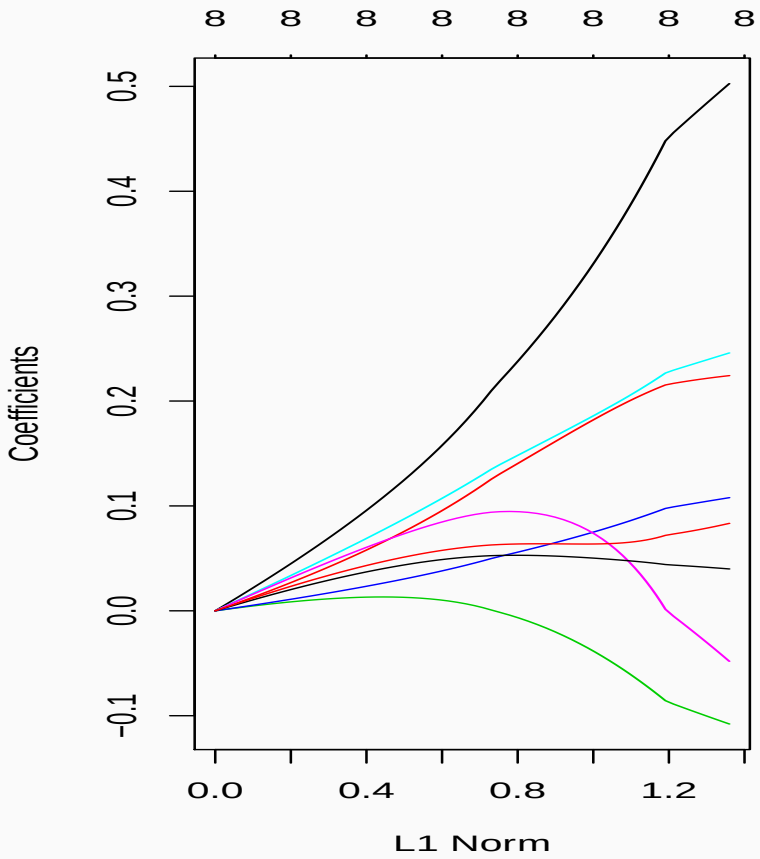
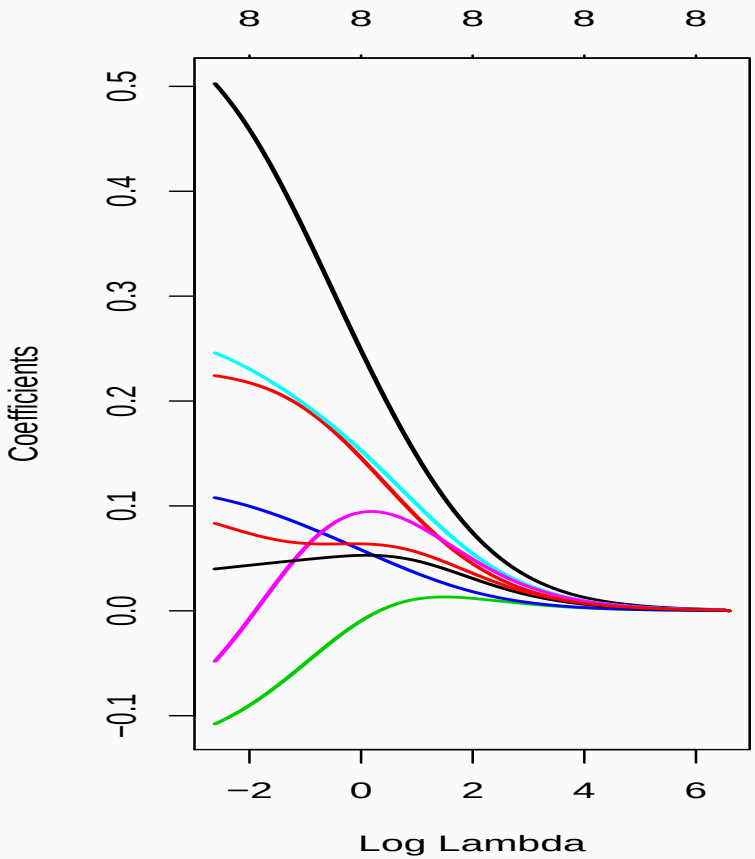
- The problem: explain the level of prostate specific antigen by a number (8) of clinical measures.
- $n = 100$ data available at `https://web.stanford.edu/~hastie/ElemStatLearn/`
- Package glmnet allows to make ridge regression on R.

UseR

```
> reg.ridge <- glmnet(prostate.data2[,2:9],prostate.data2[,10],alpha=0)
> plot(reg.ridge,label=TRUE)
> plot(reg.ridge,xvar="lambda",label=TRUE,lwd=2)
```





Some properties of ridge estimates

Proposition

1. *Solution of* (3) *is given by*

$$\hat{\beta}^R = \hat{\beta}^R(\lambda) = (\mathbb{X}^t\mathbb{X} + \lambda\mathbb{I})^{-1}\mathbb{X}^t\mathbb{Y}.$$

2. *It follows that*

$$\textit{bias}\,(\hat{\beta}^R) = -\lambda(\mathbb{X}^t\mathbb{X} + \lambda\mathbb{I})^{-1}\beta$$

and

$$\mathbf{V}(\hat{\beta}^R) = \sigma^2(\mathbb{X}^t\mathbb{X} + \lambda\mathbb{I})^{-1}\mathbb{X}^t\mathbb{X}(\mathbb{X}^t\mathbb{X} + \lambda\mathbb{I})^{-1}.$$

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Remarks

- For $\lambda = 0$, we obtain LS estimates.
- $\lambda \nearrow \implies$ bias $\nearrow$ and variance $\searrow$ and conversely as $\lambda \searrow$.

Choice of λ

- This choice of λ reveals crucial for the performance: if $\lambda \approx 0$ then $\hat{\beta}^R \approx \hat{\beta}^{MCO}$, if λ "large" then $\hat{\beta}^R \approx 0$.

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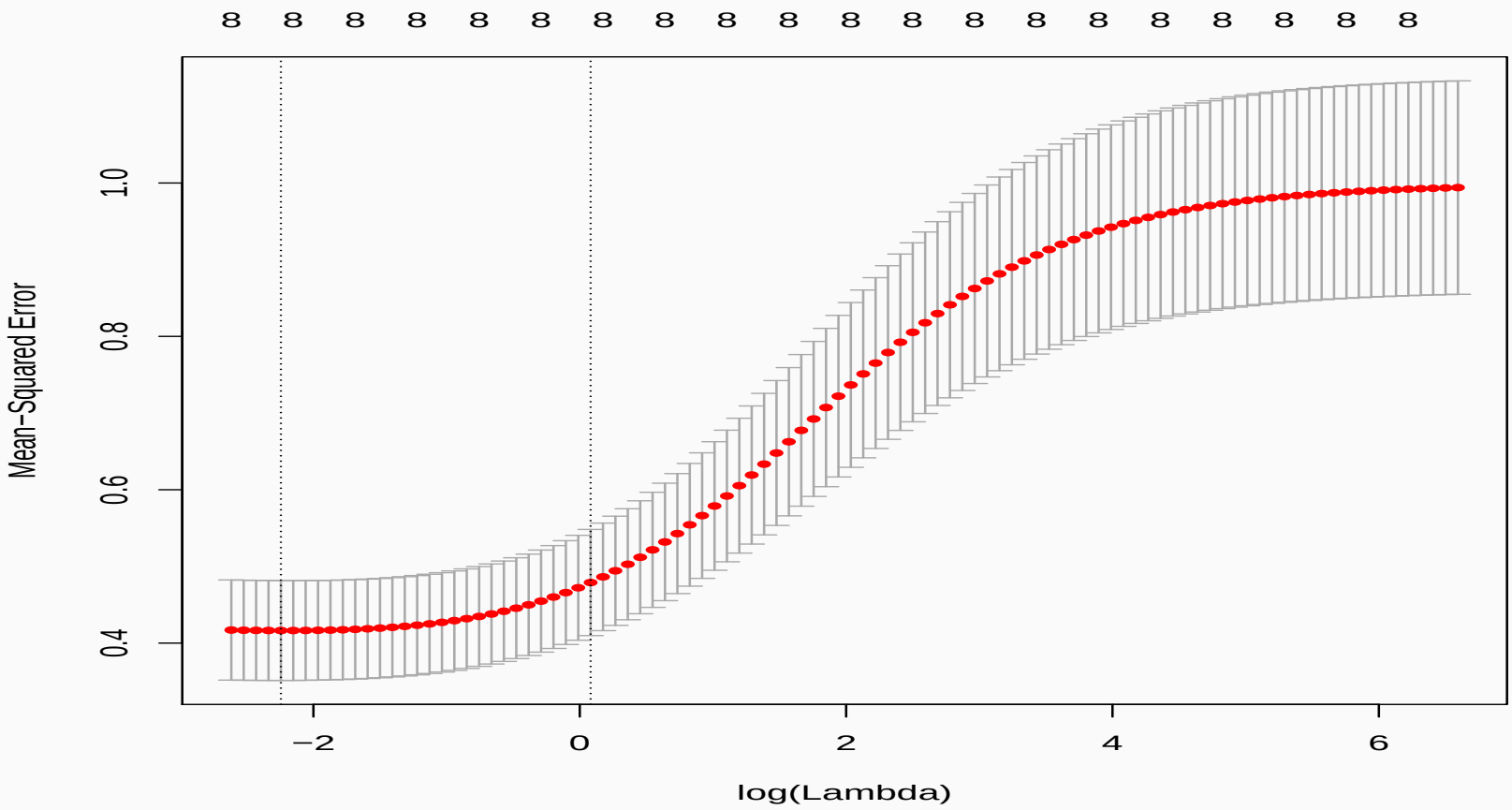
- Example: cv.glmnet selects the value of λ which minimizes the quadratic risk:

$$\mathbf{E}[(Y - X^t \hat{\beta}^R(\lambda))^2]$$

estimated by cross validation.

```
> reg.cvridge <- cv.glmnet(prostate.data2[,2:9],prostate.data2[,10],alpha=0)
> bestlam <- reg.cvridge$lambda.min
> bestlam
[1] 0.1060069
> plot(reg.cvridge)
```



Outline

- Lasso regression shrinks the regression coefficients by constraining the L_1 norm of the parameters.

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Definition [Tibshirani, 1996]

1. Lasso estimates $\hat{\beta}^L$ minimize

$$\sum_{i=1}^{n}\left(Y_i - \beta_0 - \sum_{j=1}^{d} X_{ij}\beta_j\right)^2 \quad \text{subject to} \quad \sum_{j=1}^{d}|\beta_j| \leq t \tag{4}$$

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- If $\mathbb{X}$ is an orthonormal input matrix, we have an explicit solution for ridge and lasso.

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Proposition

If $\mathbb{X}$ is orthonormal, then

$$\hat{\beta}_j^R = \frac{\hat{\beta}_j}{1+\lambda} \quad \text{and} \quad \hat{\beta}_j^L = \begin{cases} \text{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda) & \text{if } |\hat{\beta}_j| \geq \lambda \\ 0 & \text{otherwise.} \end{cases}$$

where $\hat{\beta}_j$ is the LS of β_j.

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Comments

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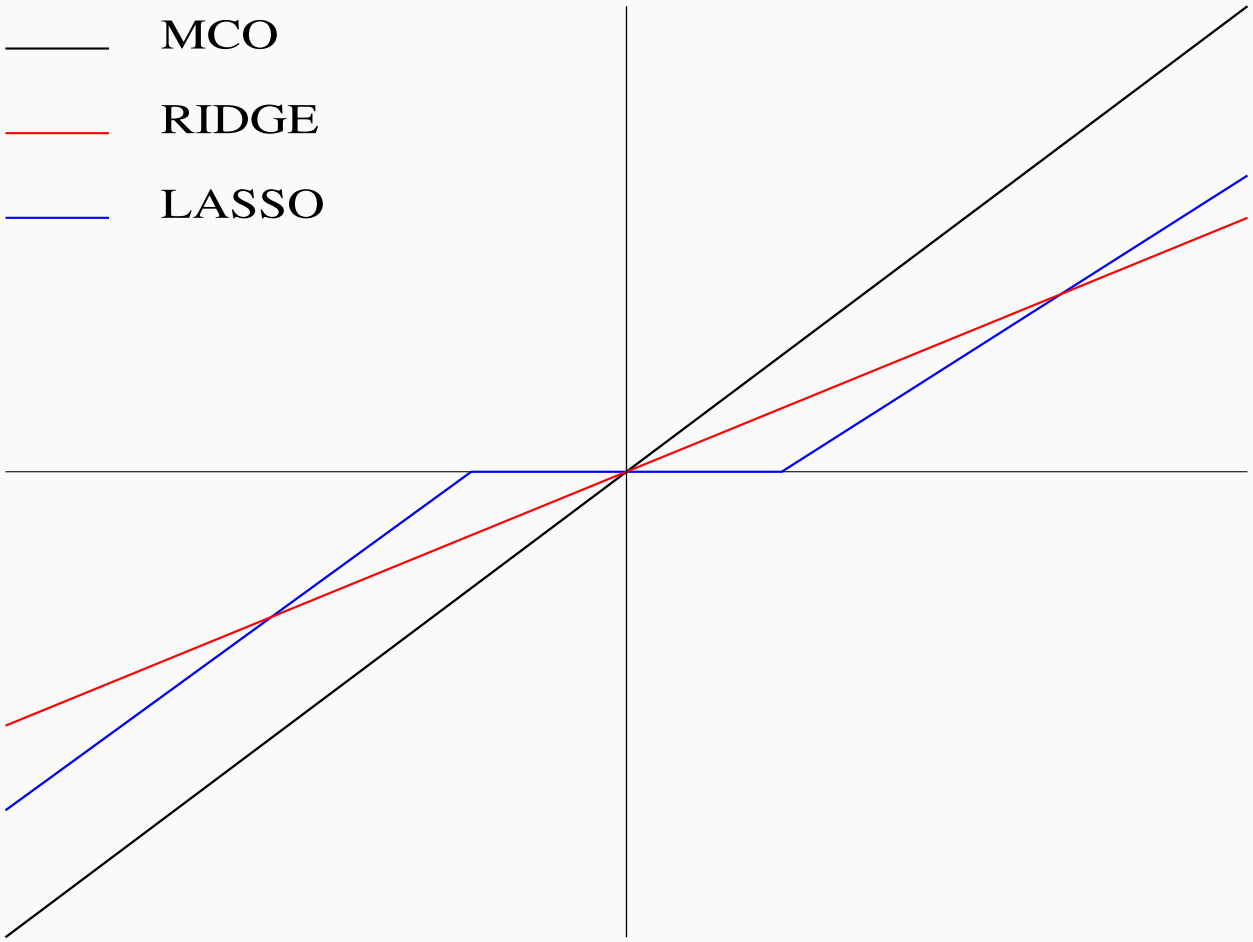
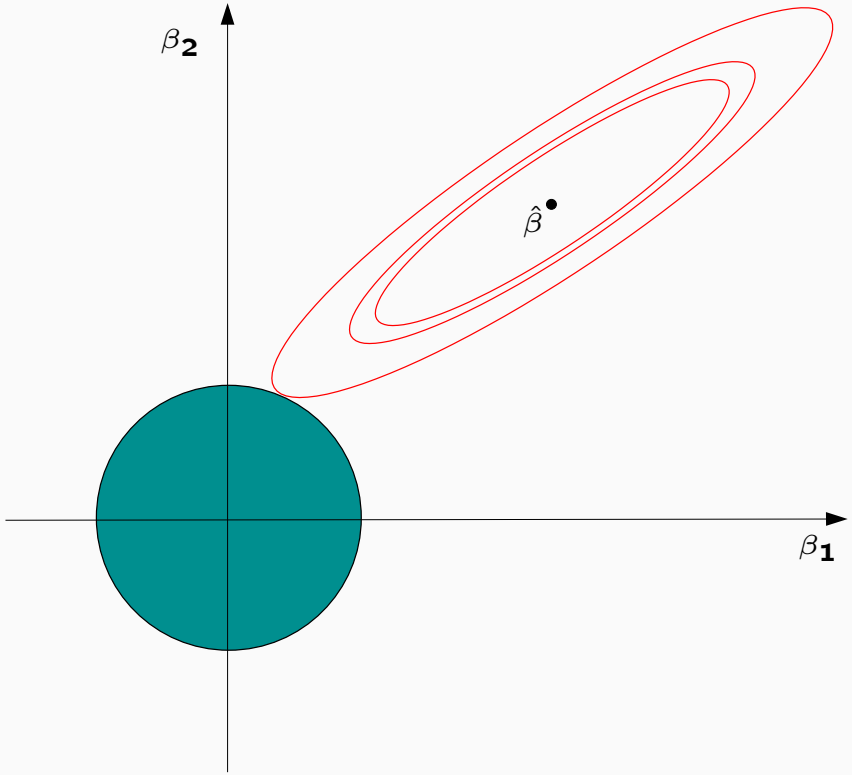
Comments

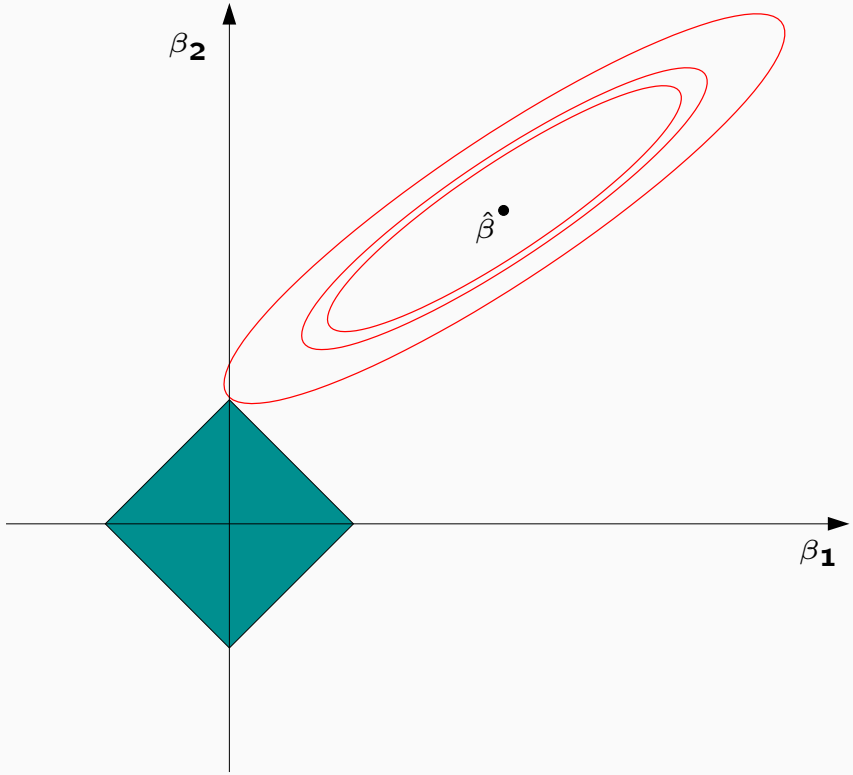
- Ridge does a proportional shrinkage;
- Lasso translates each coefficient by a factor λ, truncating at 0 (when it is small).

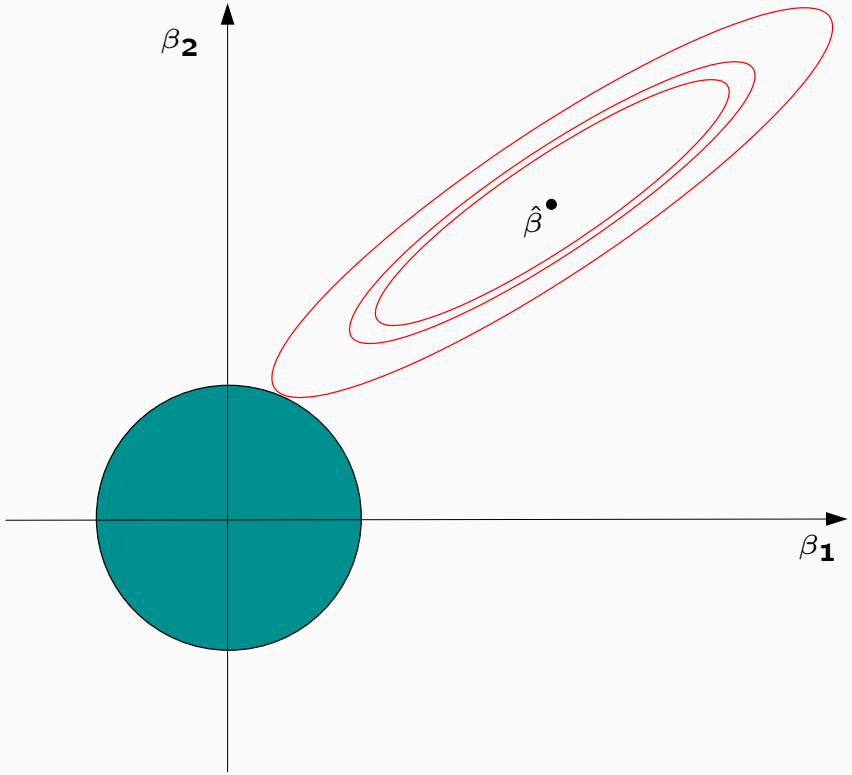


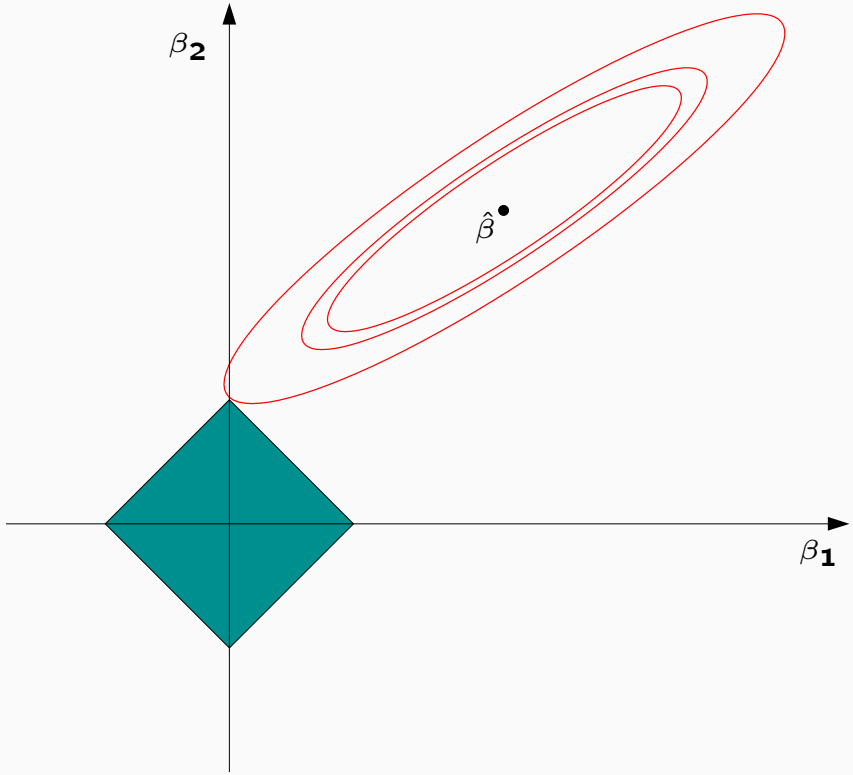
Conclusion

Lasso put small coefficients to 0 $\Longrightarrow$ variables with small coefficients are excluded from the model.


β_2
$\hat{\beta}$
β_1


β_2
$\hat{\beta}$
β_1





Relationship between ridge and lasso

Both methods find the first point where the elliptical contours hit the constraint region:

1. L_2 for ridge and L_1 norm for lasso.
2. The diamonds (L_1) has corner $\Longrightarrow$ the constraint region is often hit at a corner.

Some remarks

- As for ridge:
  - input variables $X_1, \ldots, X_d$ are generally standardized before the analysis.

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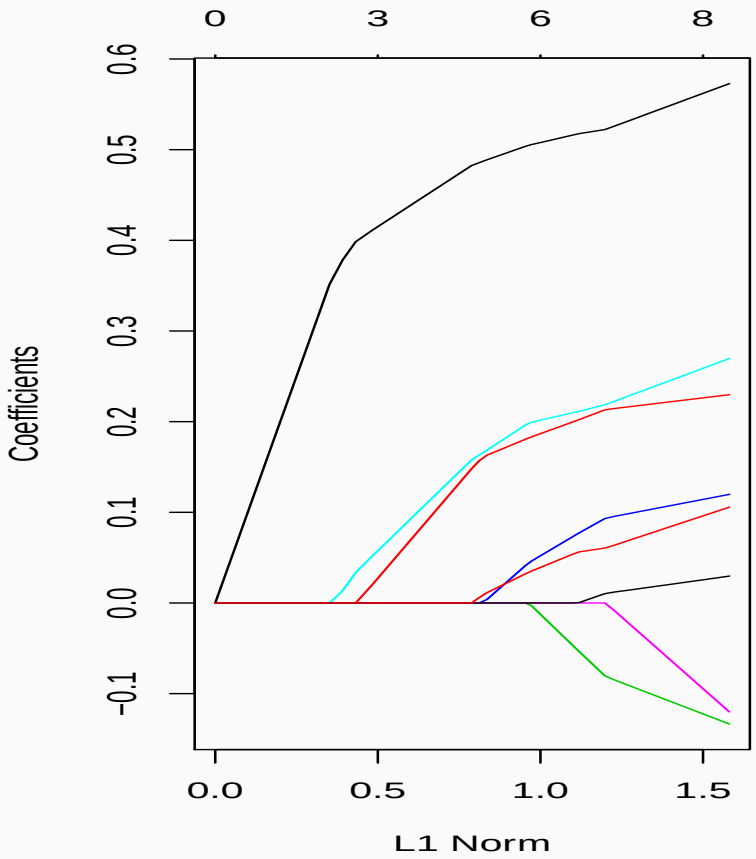
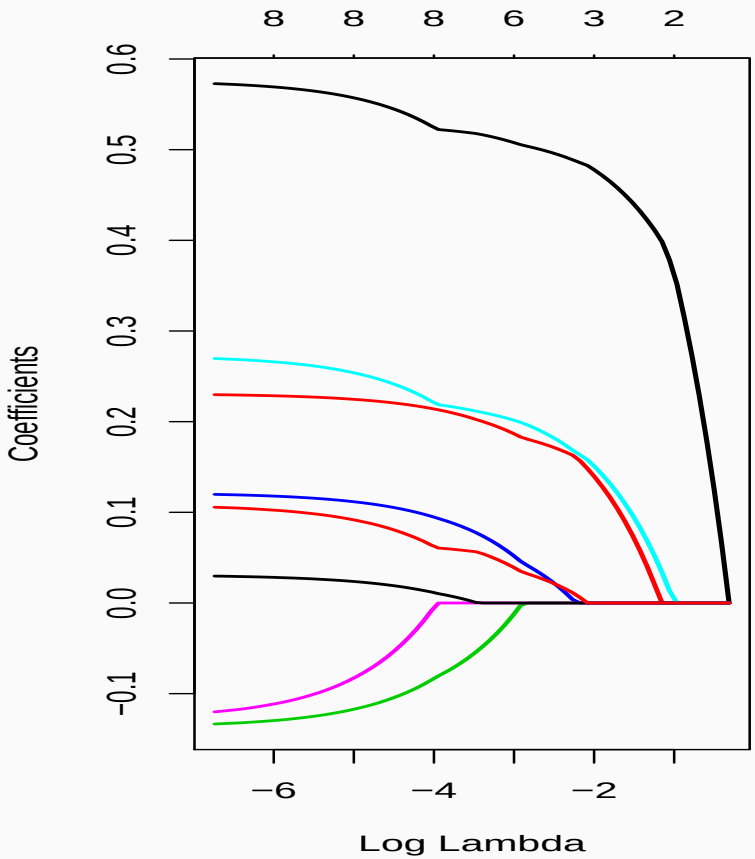
  - $\lambda \nearrow \Longrightarrow$ bias $\nearrow$ and variance $\searrow$ and reciprocally as $\lambda \searrow$.
  - Choice of λ reveals crucial (minimization of an estimated criterion).
- BUT, unlike ridge: $\lambda \nearrow \Longrightarrow$ some estimated parameters equal 0 for lasso ([Bühlmann and van de Geer, 2011]).

UseR

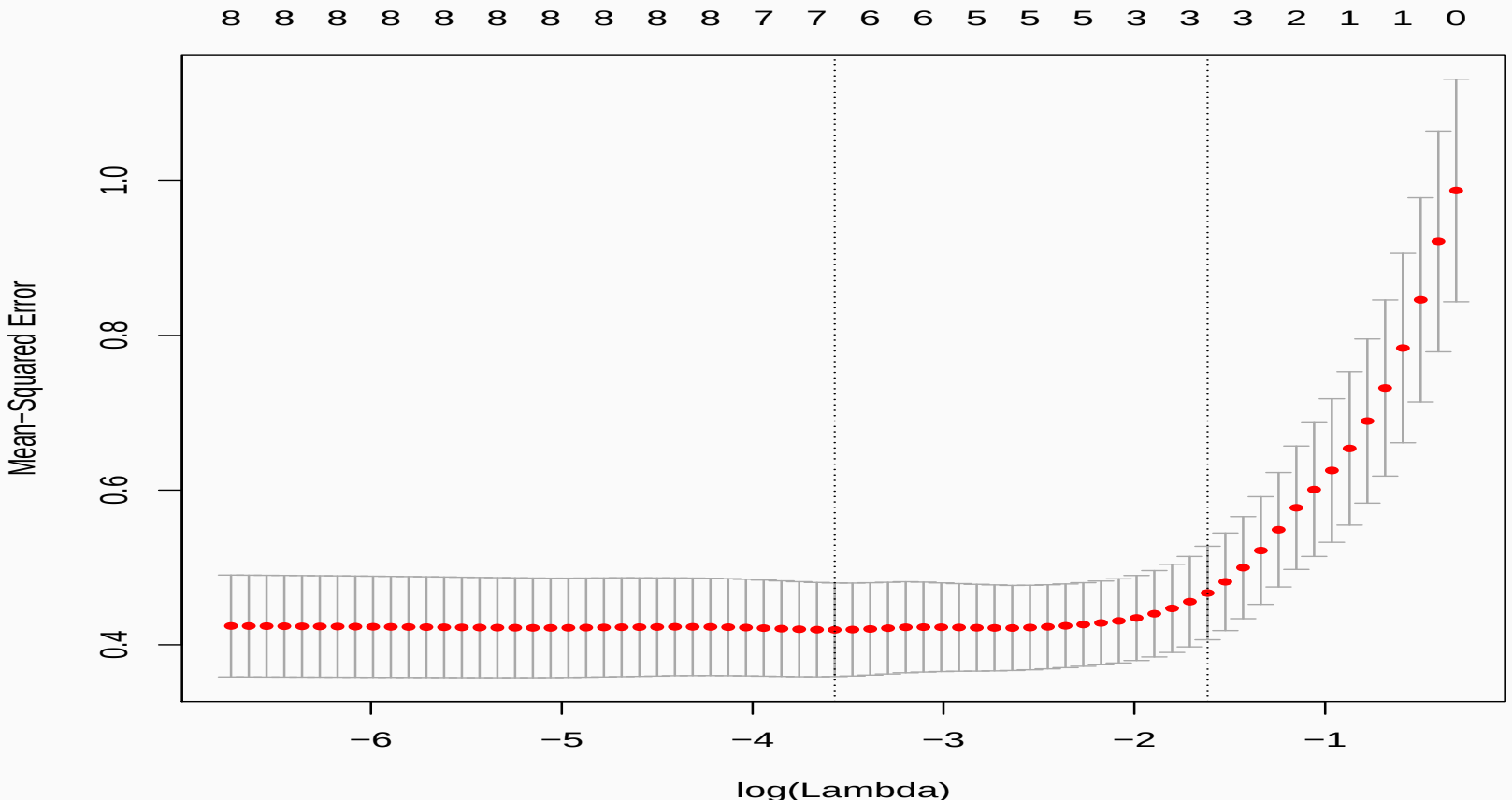
```
> reg.lasso <- glmnet(prostate.data2[,2:9],prostate.data2[,10],alpha=1)
> plot(reg.lasso,label=TRUE)
> plot(reg.lasso,xvar="lambda",label=TRUE,lwd=2)
```





Choice of λ

```
> reg.cvlasso <- cv.glmnet(prostate.data2[,2:9],prostate.data2[,10],alpha=1)
> bestlam <- reg.cvlasso$lambda.min
> bestlam
[1] 0.02815637
> plot(reg.cvlasso)
```



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- It is not difficult to adjust these methods to the logistic model $\mathcal{Y} = \{-1, 1\}$.
- Penalty terms are the same.
- Only change: least square criterion is replaced by likelihood.

Lasso and Ridge for logistic regression

Definition

Let $\tilde{y}_i = (y_i + 1)/2$ ($\tilde{y}_i = 0$ or 1).

- Ridge estimates for logistic regression are defined by

$$\hat{\beta}^R = \underset{\beta}{\operatorname{argmin}} \left\{ -\sum_{i=1}^{n} (\tilde{y}_i x_i^t \beta - \log(1 + \exp(x_i^t \beta))) + \lambda \sum_{j=1}^{d} \beta_j^2 \right\}.$$

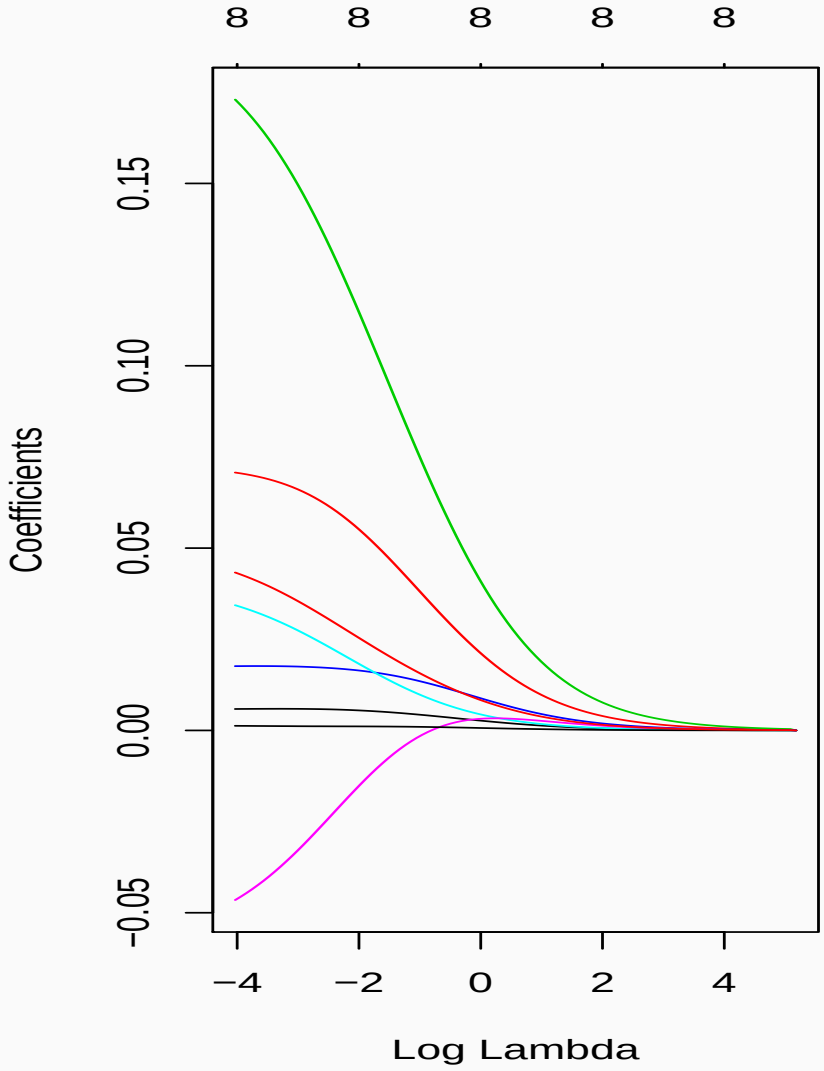
- Lasso estimates for logistic regression are defined by

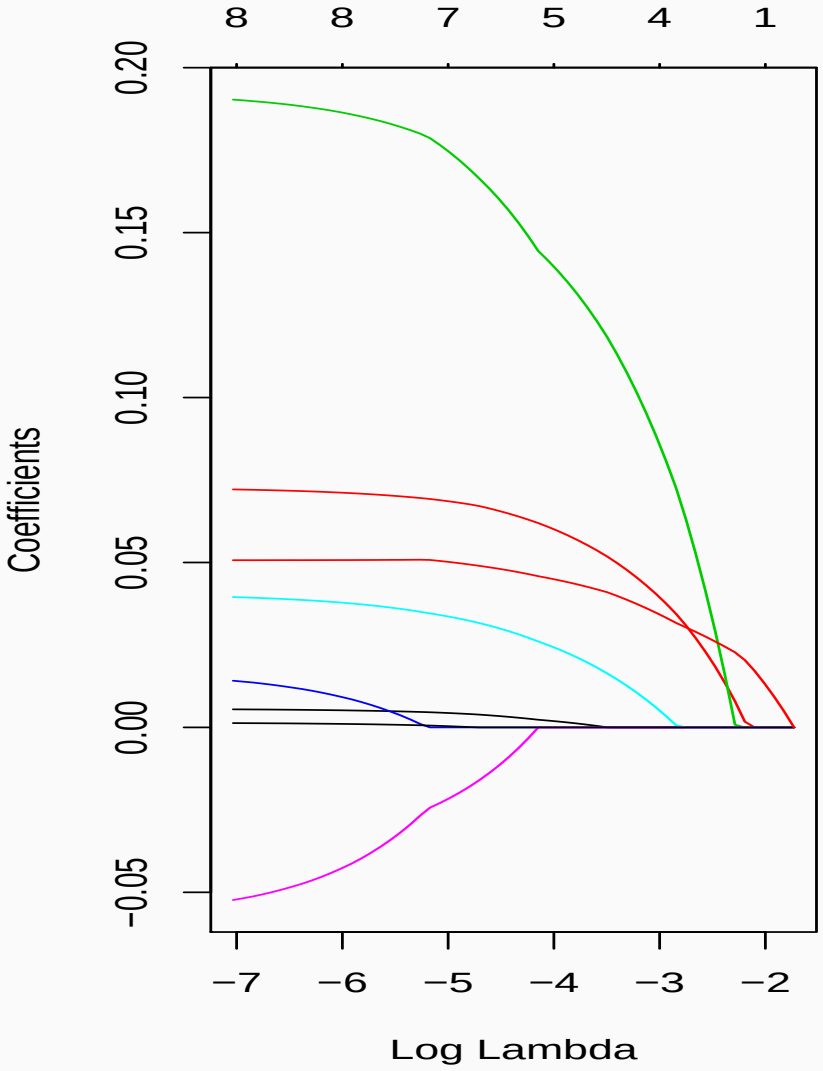
$$\hat{\beta}^L = \underset{\beta}{\operatorname{argmin}} \left\{ -\sum_{i=1}^{n} (\tilde{y}_i x_i^t \beta - \log(1 + \exp(x_i^t \beta))) + \lambda \sum_{j=1}^{d} |\beta_j| \right\}.$$

UseR

- To make ridge or lasso for logistic regression, we just have to add family=binomial in glmnet function.
- It is the only change (coefficient paths, choice of λ are the same...).

```
> colnames(donnees)
[1] "sbp"       "tobacco"   "ldl"       "adiposity" "typea"     "obesity"
[7] "alcohol"   "age"       "chd"
> log.ridge <- glmnet(donnees[,1:8],donnees[,9],family="binomial",alpha=0)
> log.lasso <- glmnet(donnees[,1:8],donnees[,9],family="binomial",alpha=1)
> plot(log.ridge,xvar="lambda")
> plot(log.lasso,xvar="lambda")
```


8 8 8 8 8
Coefficients
0.15
0.10
0.05
0.00
−0.05
−4 −2 0 2 4
Log Lambda


8 8 7 5 4 1
Coefficients
0.20
0.15
0.10
0.05
0.00
−0.05
−7 −6 −5 −4 −3 −2
Log Lambda

Elastic net

- [Zou and Hastie, 2005] have proposed to combine ridge and lasso with the following penalty term (called elastic net penalty)

$$\lambda \sum_{j=1}^{d} ((1-\alpha)\beta_j^2 + \alpha|\beta_j|)$$

where $\alpha \in [0, 1]$.

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  - $\alpha = 0 \Longrightarrow$ Ridge.
  - This parameter corresponds (obviously) to the alpha parameter in glmnet function.
- Advantage: more flexible since elastic net includes ridge and lasso.
- Drawback: we have to select both α and λ (you can use caret to do that).

Summary

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  - high correlations between inputs;
  - high dimension (large number of inputs).
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- Exercise 3-4, IML2.

Outline

Références i

Bühlmann, P. and van de Geer, S. (2011).
Statistics for high-dimensional data.
Springer.

Hastie, T., Tibshirani, R., and Friedman, J. (2009).
The Elements of Statistical Learning: Data Mining, Inference, and Prediction.
Springer, second edition.

Tibshirani, R. (1996).
Regression shrinkage and selection via the lasso.
Journal of the Royal Statistical Society, Series B, 58:267–288.

Références ii

Zou, H. and Hastie, T. (2005).
Regularization and variable selection via the elastic net.
Journal of the Royal Statistical Society, Series B, 67:301–320.

Part IV

Trees

Outline

Presentation

- Tree algorithms are statistical learning algorithms for both regression and supervised classification.
- Popular method, not (too) difficult to understand, visualization tool.

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Presentation

- Tree algorithms are statistical learning algorithms for both regression and supervised classification.
- Popular method, not (too) difficult to understand, visualization tool.
- Tree algorithms are not generally the most performant algorithms... but a lot of efficient algorithms are defined from trees (random forest, gradient tree boosting...).
- There are different ways to build trees.
- We focus on the CART algorithm [Breiman et al., 1984] which is the most widely used algorithm to define trees.

Outline

Notations

- The problem: explain output Y by p inputs $X_1, \ldots, X_p$.

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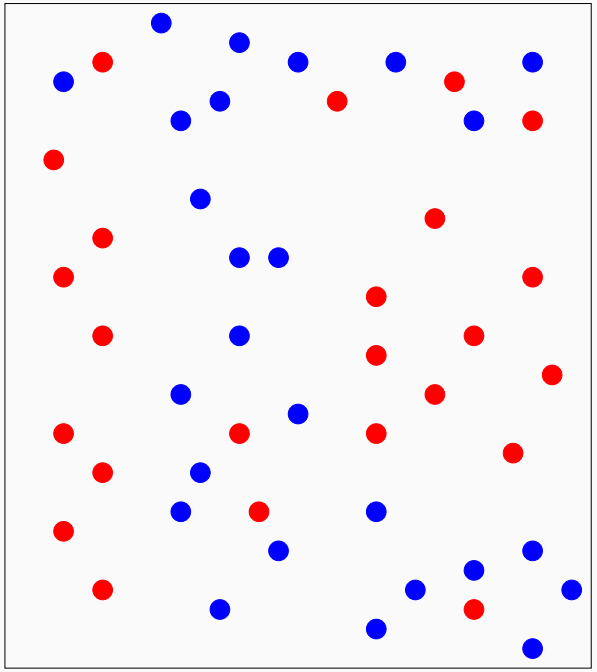
- Y might be categorical (binary or not) or continuous and $X_1, \ldots, X_p$ categorical or continous.
- For simplicity (to make figures), we first assume that Y is binary (-1 ou 1) and that $p = 2$ (2 inputs X_1 and X_2 continuous).

Data visualization

- n observations $(X_1, Y_1), \ldots, (X_n, Y_n)$ where $X_i \in \mathbb{R}^2$ and $Y_i \in \{-1, 1\}$.



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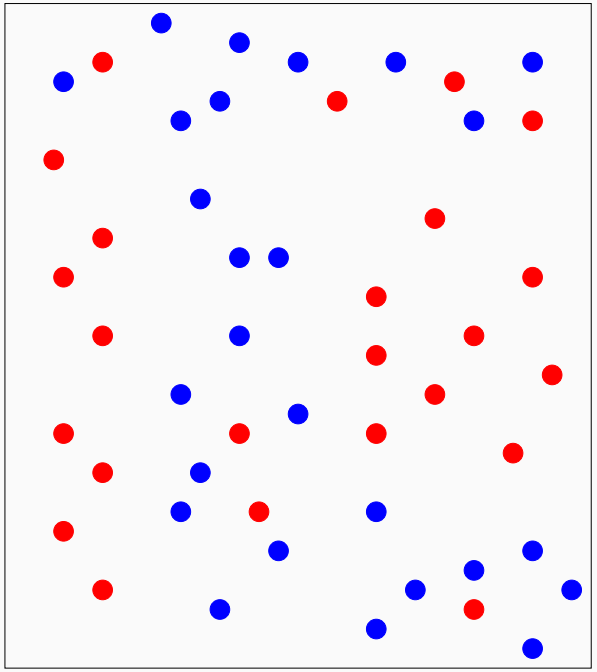
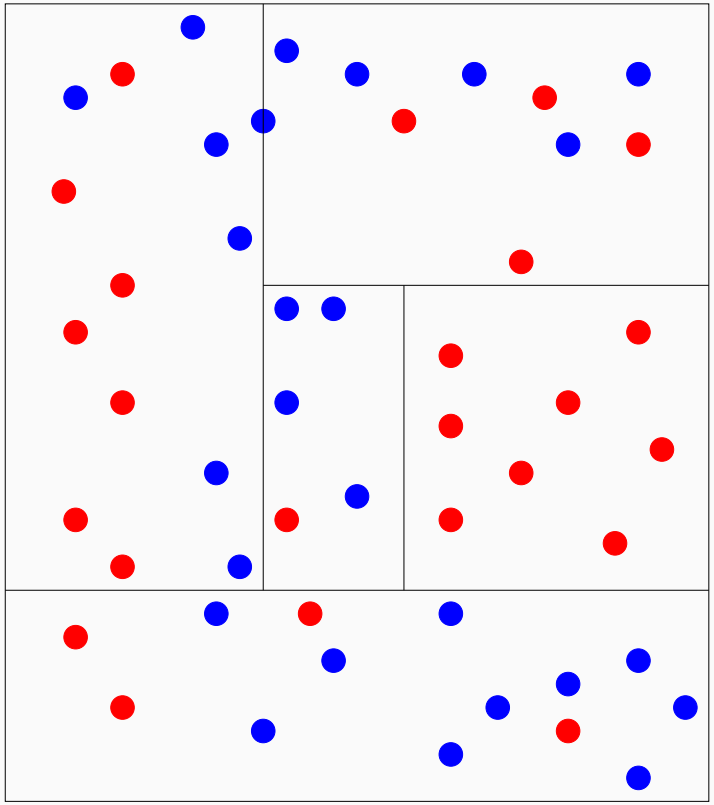


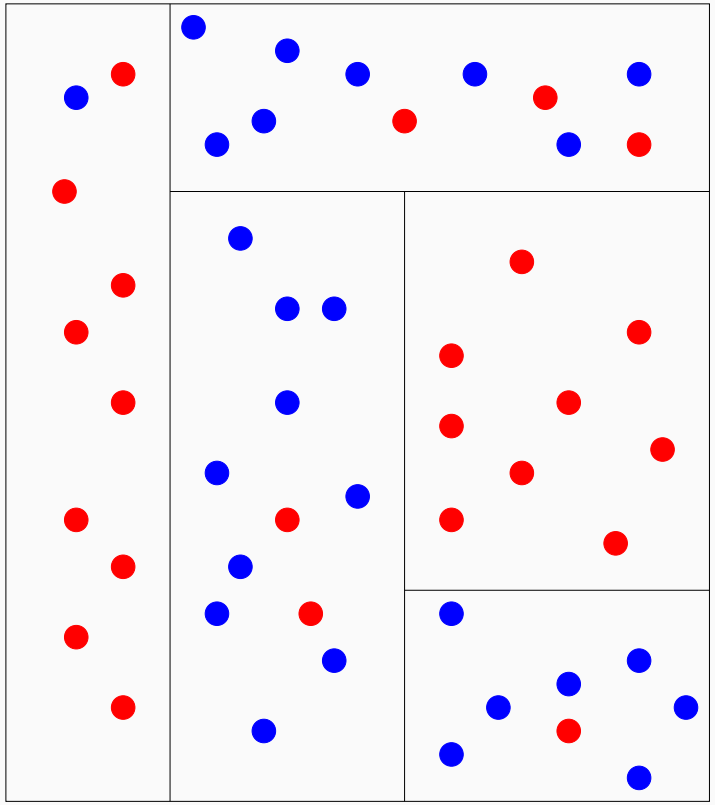
Tree partitions

Find a partition of the feature space into a set of rectangles which divides points according to their color.

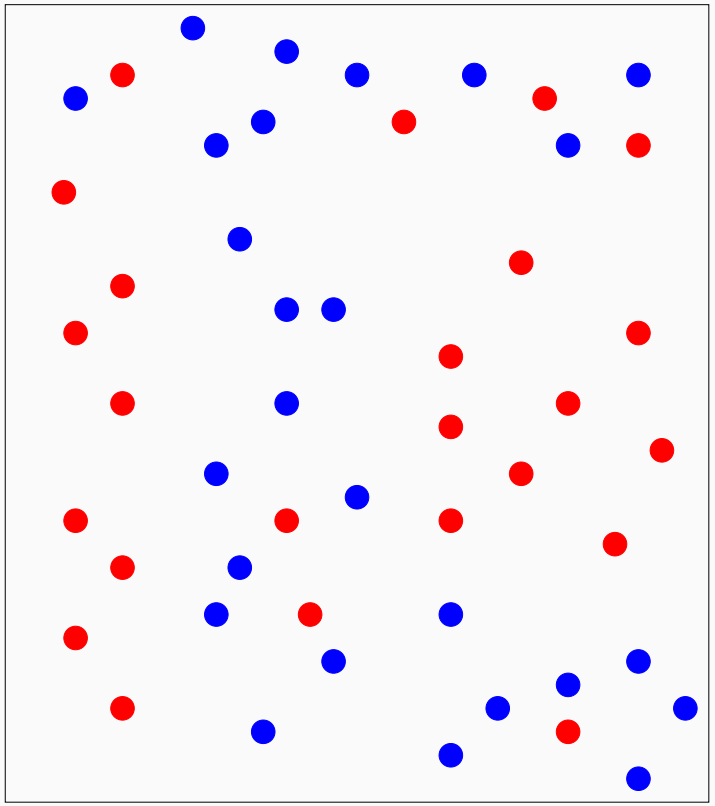
Binary partitions

- CART algorithm restricts attention to recursive binary partitions.
- 2 examples:





- At each step, the method splits the data into two regions according to a split variable and a split point.



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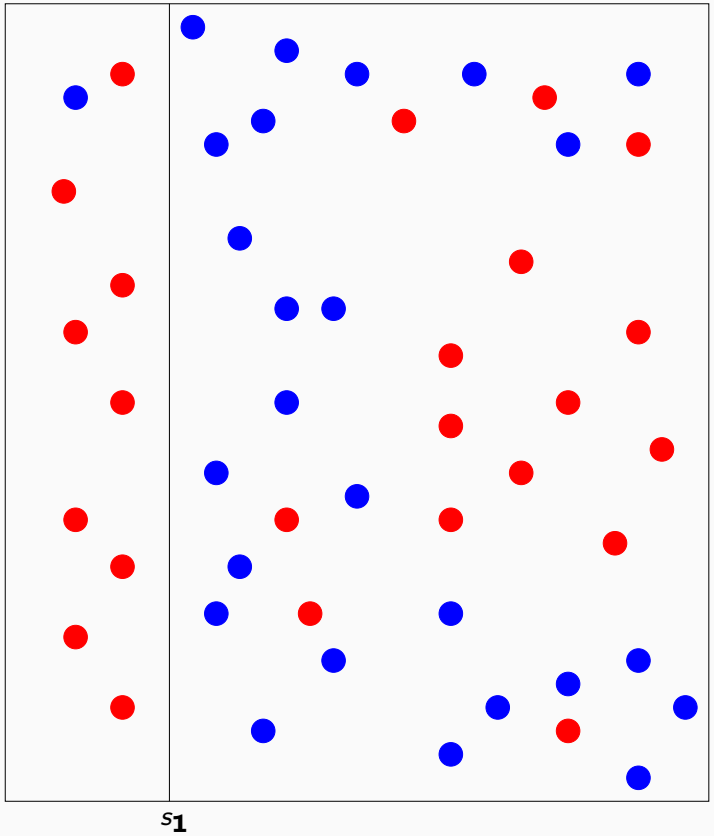

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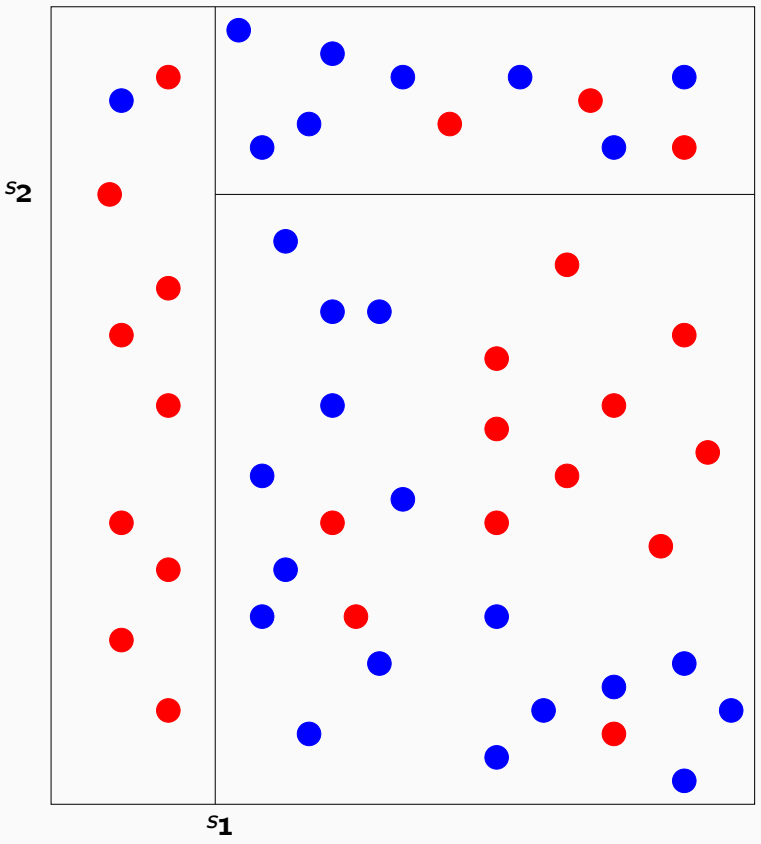

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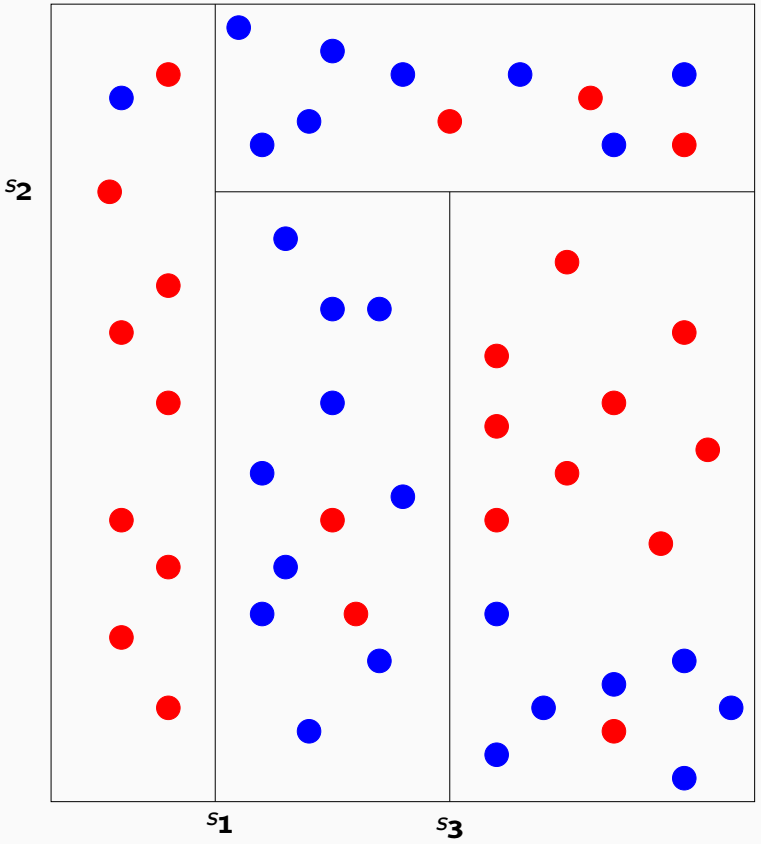

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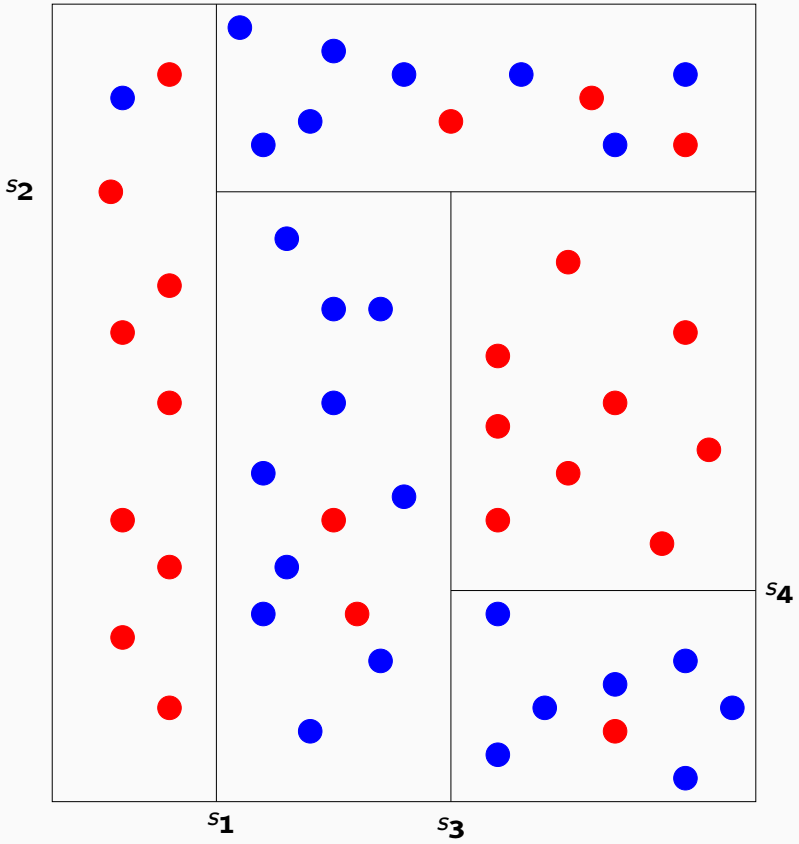
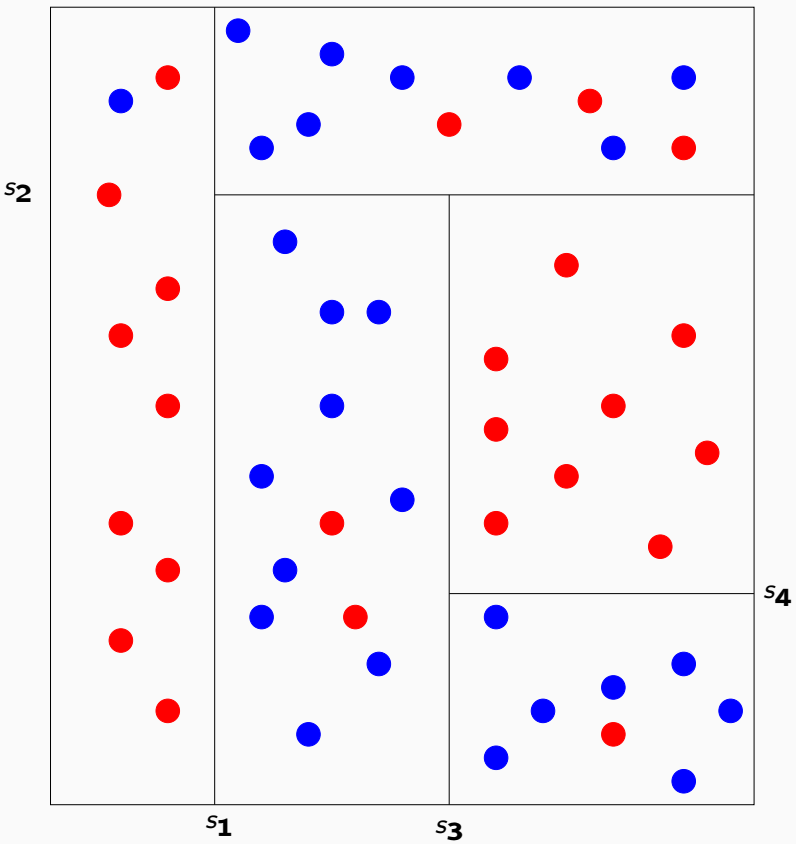
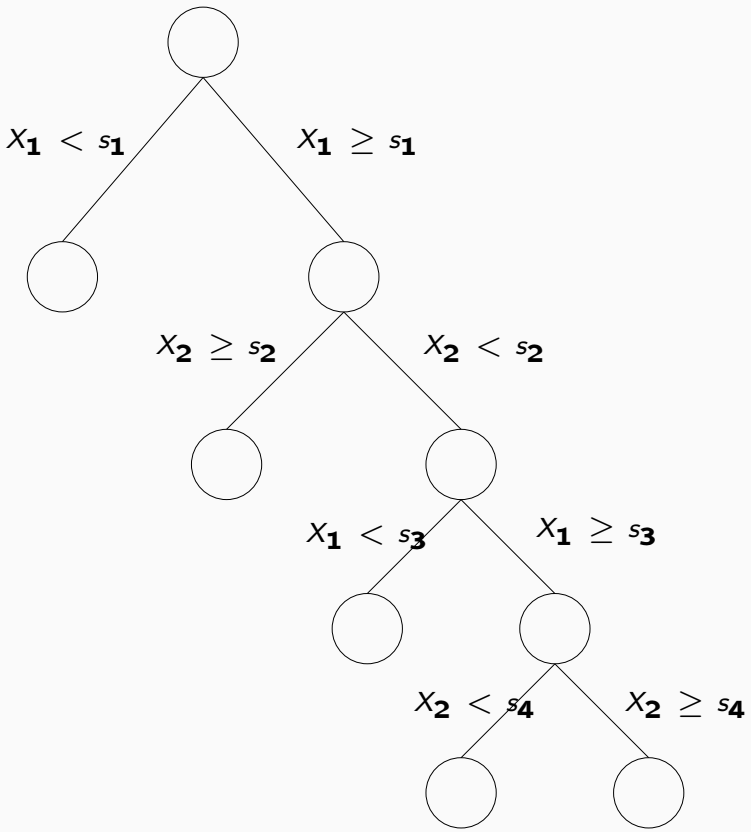


A tree partition





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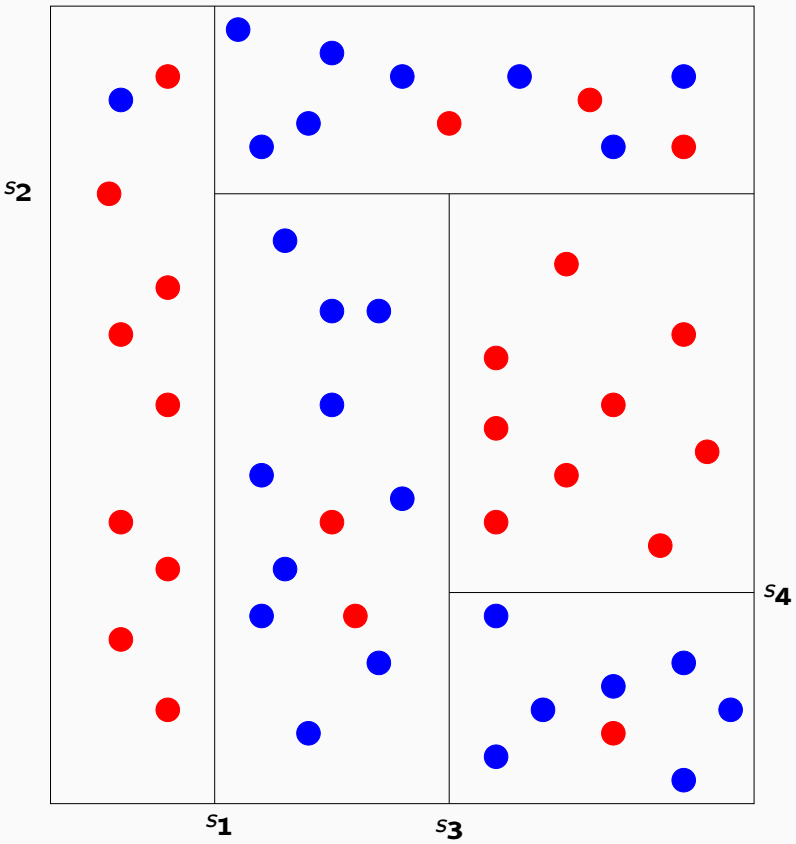

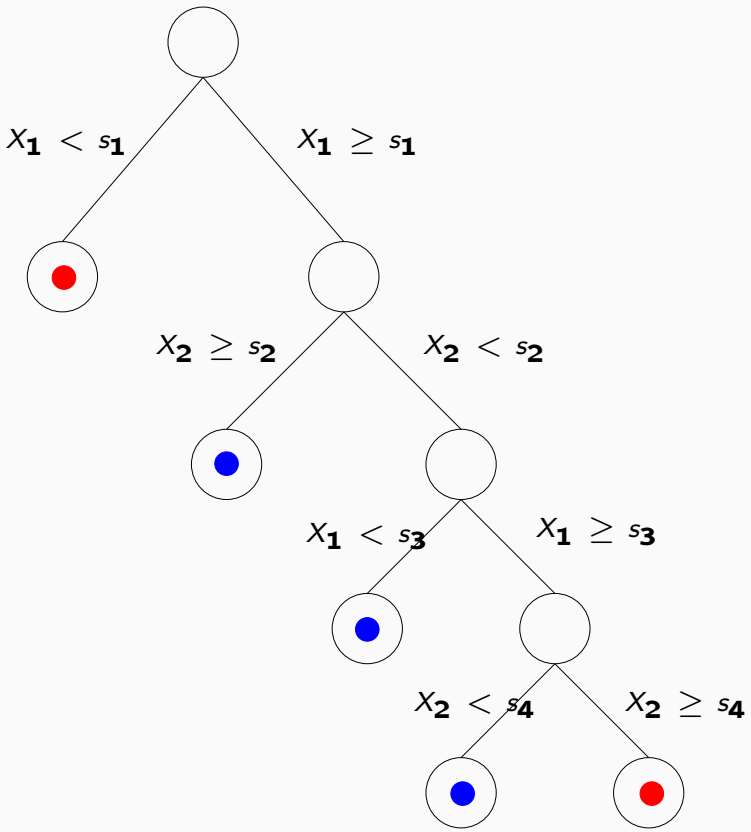

Classification rule

At the end, we do a majority vote in each cell of the partition (in each rectangle).

Definitions

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- Each elements of the partition are called terminal nodes.
- $\mathbb{R}^p$ (the first node) is the root node.
- Each split (each question) defines two child nodes, the left and right child nodes.

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- Each split (each question) defines two child nodes, the left and right child nodes.

Question

- Tree process is recursive: we just have to know how to split a node.
- How to define a good split (or find a good question)?

Outline

Question

How to choose a split?

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How to choose a split?

- At each step, we have to find (j, s) which split a node $\mathcal{N}$ into two children nodes

$$\mathcal{N}_1(j,s) = \{X \in \mathcal{N} | X_j \leq s\} \quad \text{and} \quad \mathcal{N}_2(j,s) = \{X \in \mathcal{N} | X_j > s\}.$$

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- (j, s) is selected by minimizing a criterion which measures the impurity of the two children nodes.

Impurity

- Impurity of a node should be
  1. small when the node is homogeneous: values of Y are closed to each other in the node.
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The idea

For a given impurity measure $\mathcal{I}$, we choose the split (j, s) which minimizes

$$\mathbf{P}(\mathcal{N}_1)\mathcal{I}(\mathcal{N}_1(j,s)) + \mathbf{P}(\mathcal{N}_2)\mathcal{I}(\mathcal{N}_2(j,s))$$

where $\mathbf{P}(\mathcal{N}_k)$ stands for the proportion of observations in $\mathcal{N}_k, k = 1, 2$

Outline

- In regression (Y continuous), we usually use the variance to measure the impurity in the node

$$\mathcal{I}(\mathcal{N}) = \frac{1}{|\mathcal{N}|} \sum_{i:X_i \in \mathcal{N}} (Y_i - \bar{Y}_{\mathcal{N}})^2,$$

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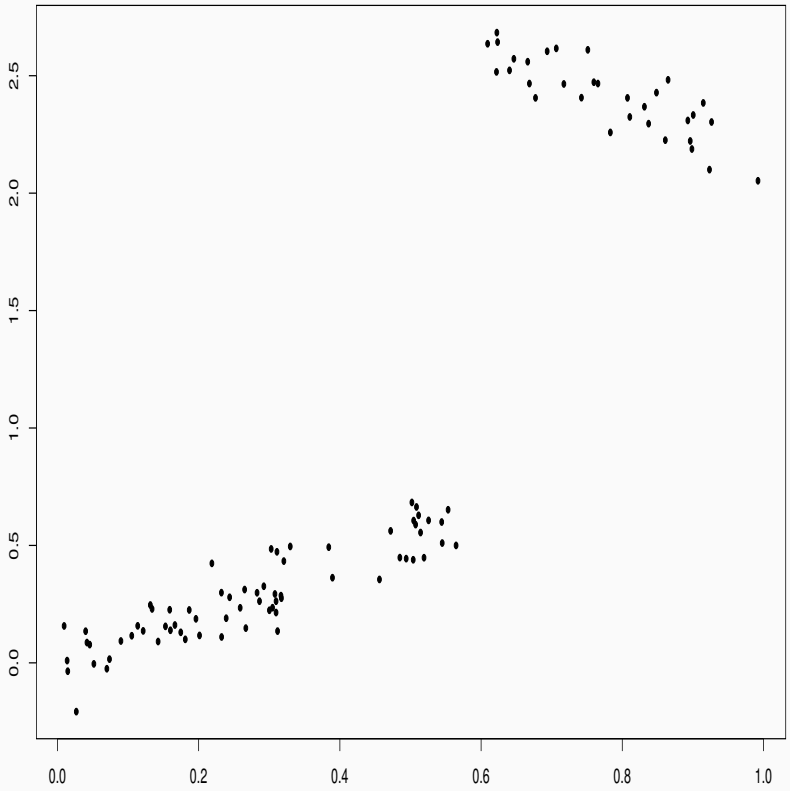
Split for regression

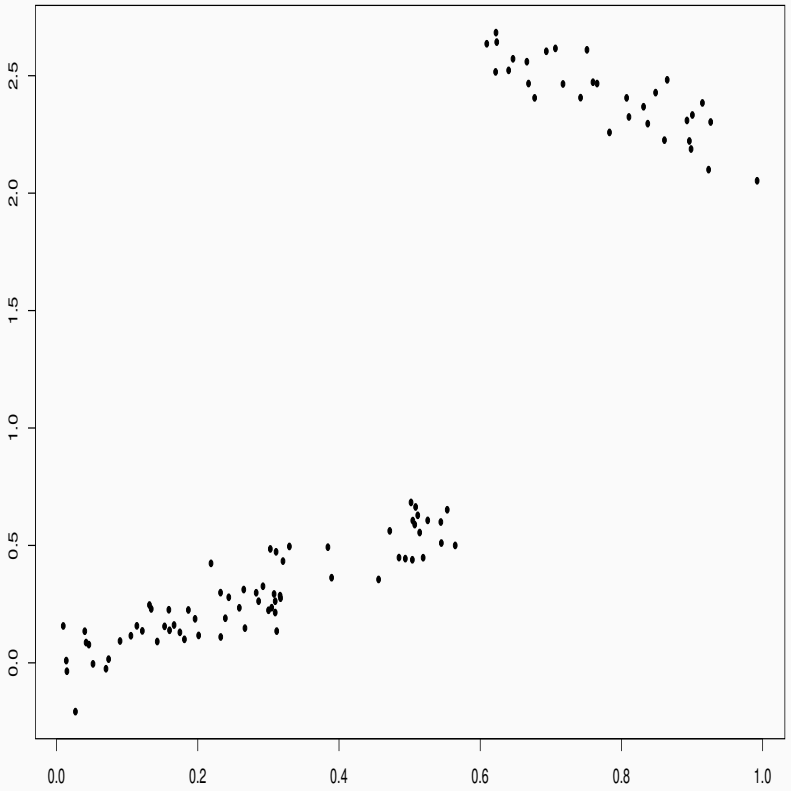
At each step, we choose (j, s) which minimizes

$$\sum_{X_i \in \mathcal{N}_1(j,s)} (Y_i - \bar{Y}_1)^2 + \sum_{X_i \in \mathcal{N}_2(j,s)} (Y_i - \bar{Y}_2)^2$$

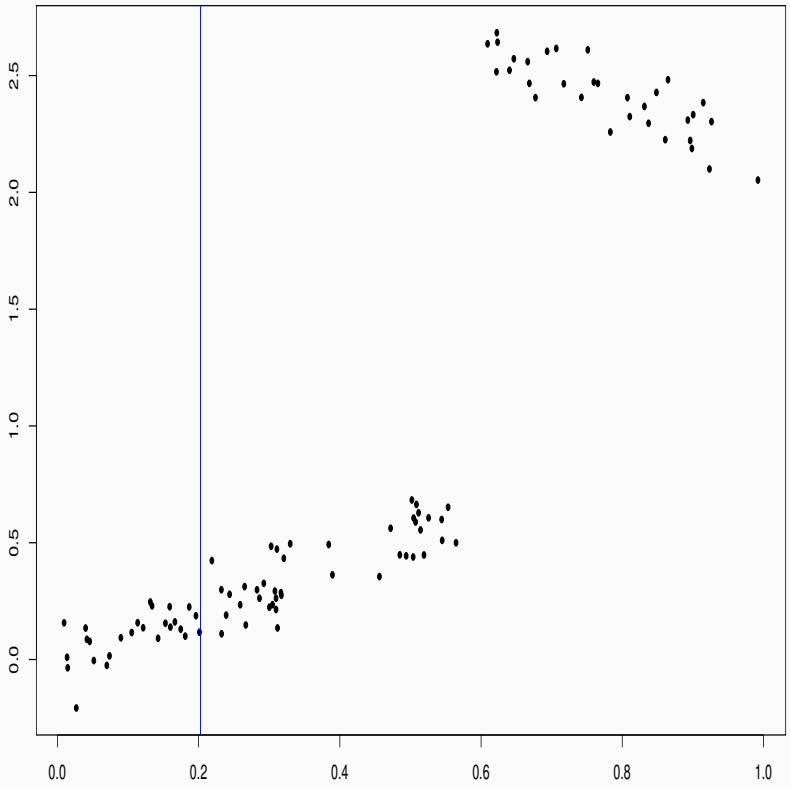
where $\bar{Y}_k = \frac{1}{|\mathcal{N}_k(j,s)|} \sum_{X_i \in \mathcal{N}_k(j,s)} Y_i$, $k = 1, 2$.

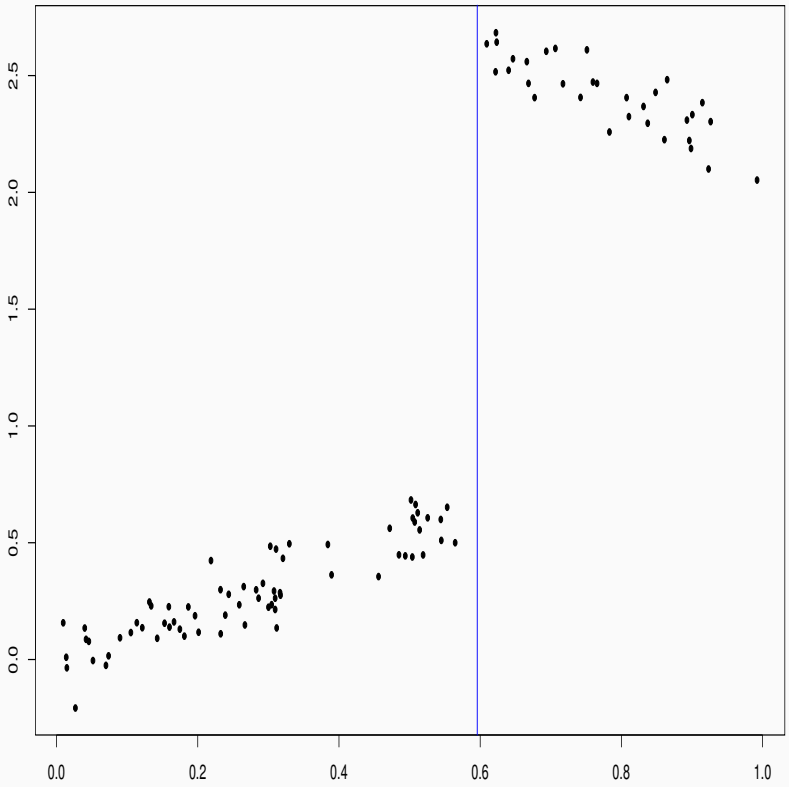
Example



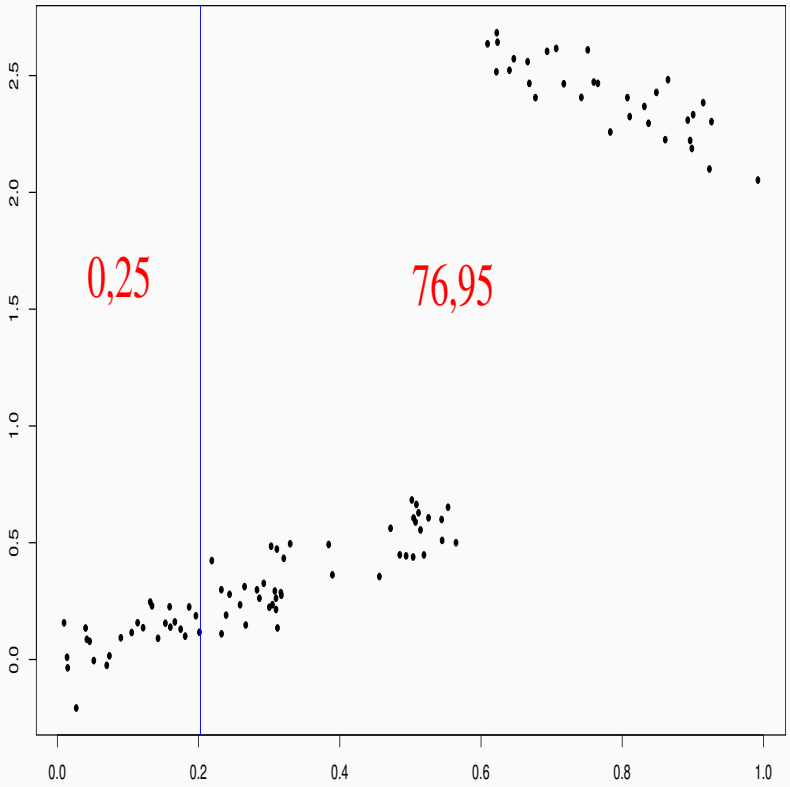


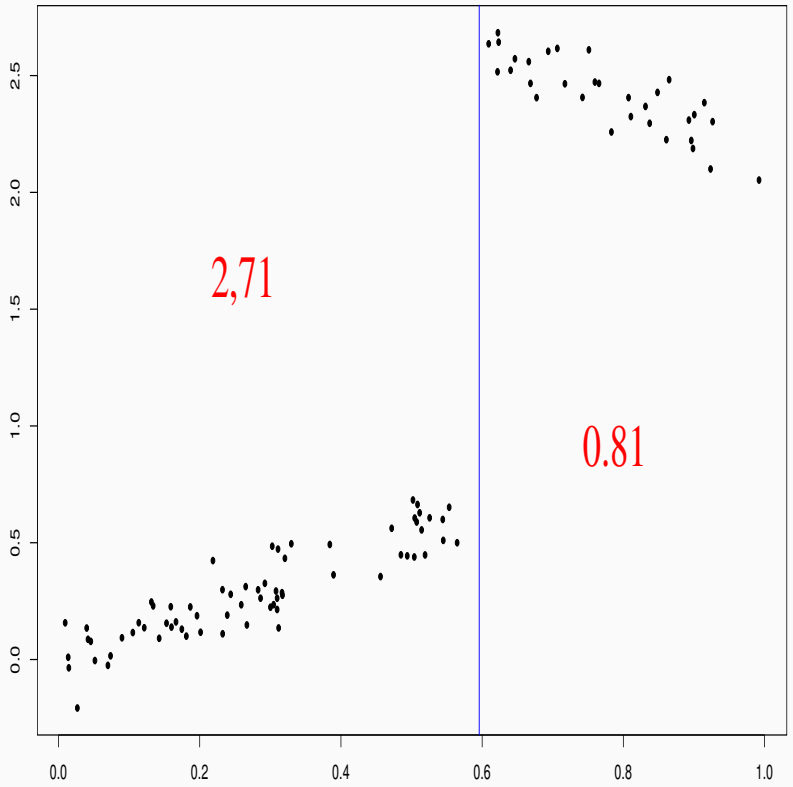
Example



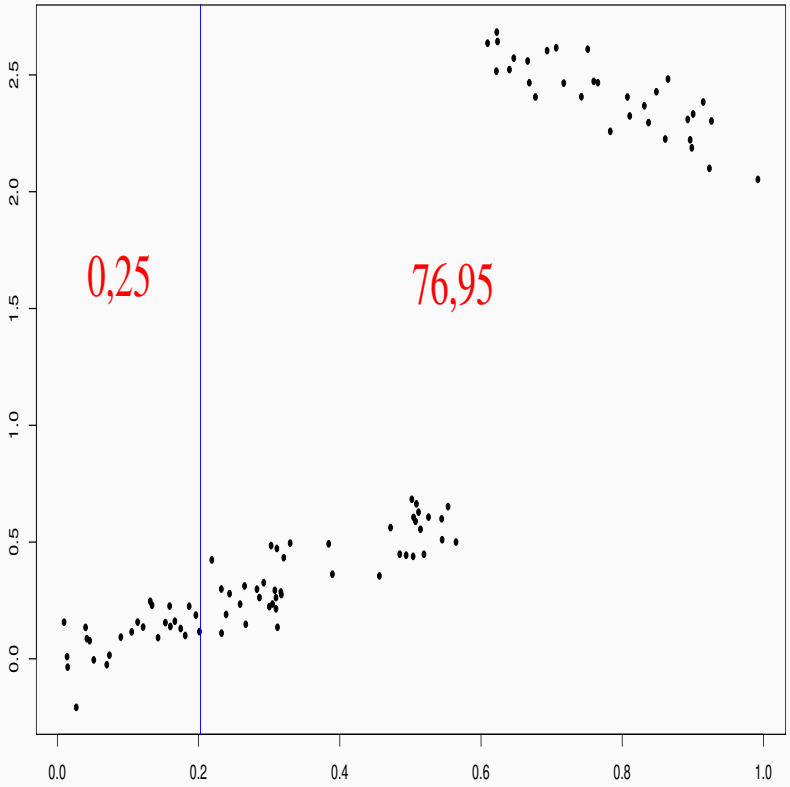


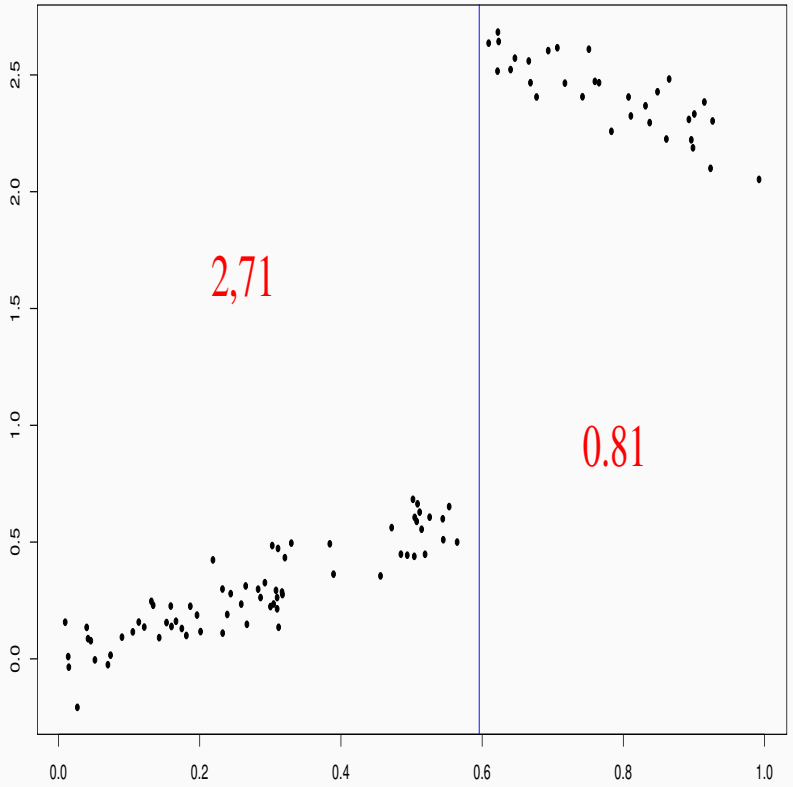
Example


0,25
76,95
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.2
0.4
0.6
0.8
1.0


2,71
0.81
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.2
0.4
0.6
0.8
1.0

Example





Conclusion

We choose the right split.

Outline

- $Y_i, i = 1, \ldots, n$ take values in $\{1, \ldots, K\}$.

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Definition

Impurity of $\mathcal{N}$ is defined by

$$\mathcal{I}(\mathcal{N}) = \sum_{j=1}^{K} f(p_j(\mathcal{N}))$$

where

- $p_j(\mathcal{N})$ stands for the proportion of class j in $\mathcal{N}$.
- f is a concave function $[0, 1] \to \mathbb{R}^+$ such that $f(0) = f(1) = 0$.

Examples of functions f

- If $\mathcal{N}$ is pur, we expect that $\mathcal{I}(\mathcal{N}) = 0$

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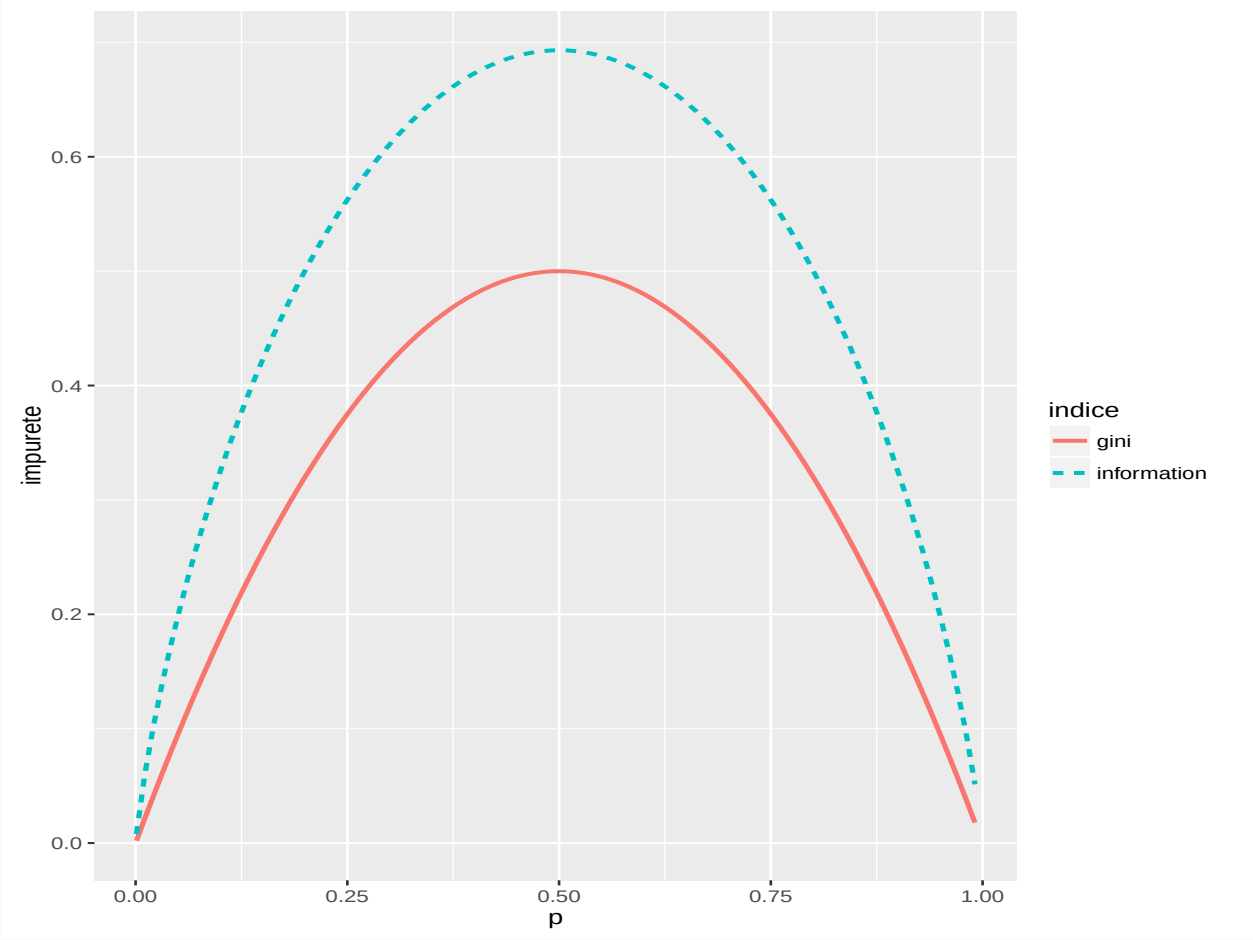
Binary case

We have

1. $\mathcal{I}(\mathcal{N}) = 2p(1-p)$ for Gini
2. $\mathcal{I}(\mathcal{N}) = -p\log p - (1-p)\log(1-p)$ for Information

where p stands for the proportion of 1 (or -1) in $\mathcal{N}$.


0.6
0.4
0.2
0.0
impurete
0.00
0.25
0.50
0.75
1.00
p
indice
gini
information

Split for supervised classification

- Recall that for a given node $\mathcal{N}$ and (j, s), the two child nodes are defined by

$$\mathcal{N}_1(j, s) = \{X \in \mathcal{N} | X_j \leq s\} \quad \text{and} \quad \mathcal{N}_2(j, s) = \{X \in \mathcal{N} | X_j > s\}.$$

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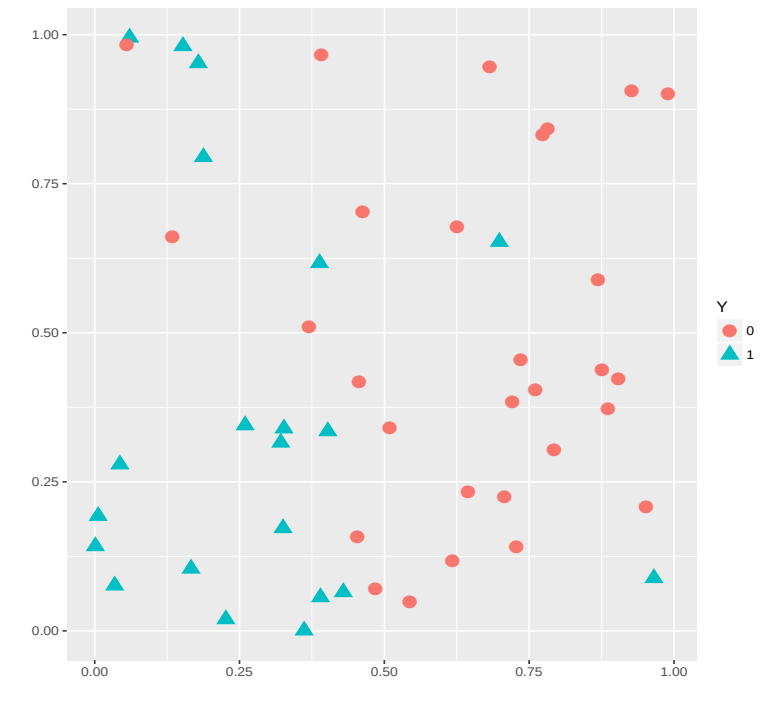
Choice of (j, s)

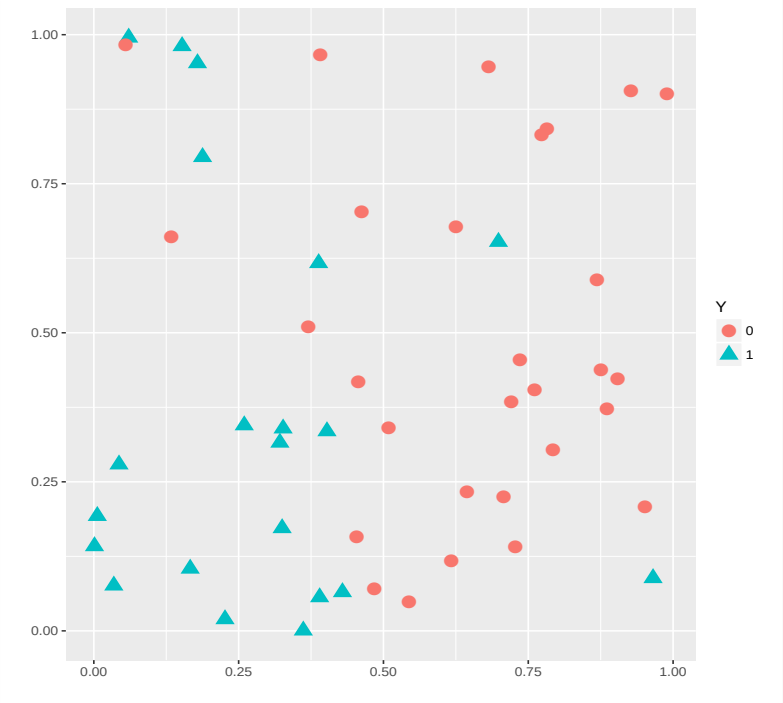
For a given impurity measure $\mathcal{I}$, we choose (j, s) wich minimizes:

$$\mathbf{P}(\mathcal{N}_1)\mathcal{I}(\mathcal{N}_1(j,s)) + \mathbf{P}(\mathcal{N}_2)\mathcal{I}(\mathcal{N}_2(j,s)).$$

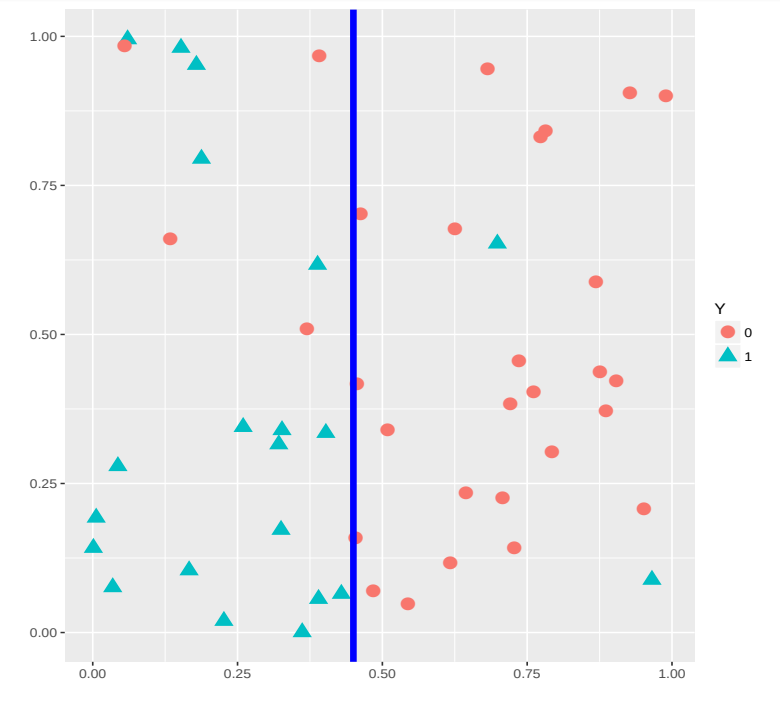
Example

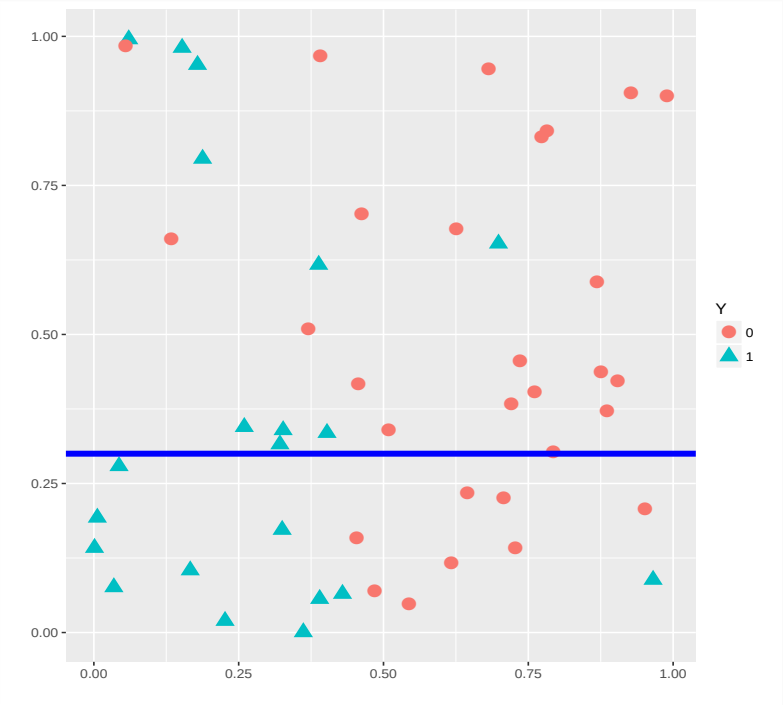
$$\mathcal{I}(\mathcal{N}) = 0.4872$$



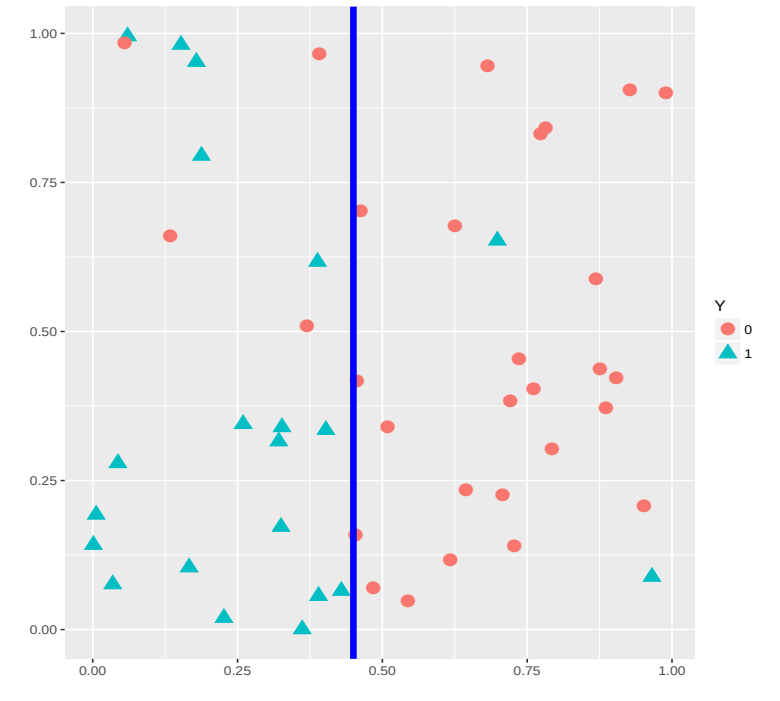


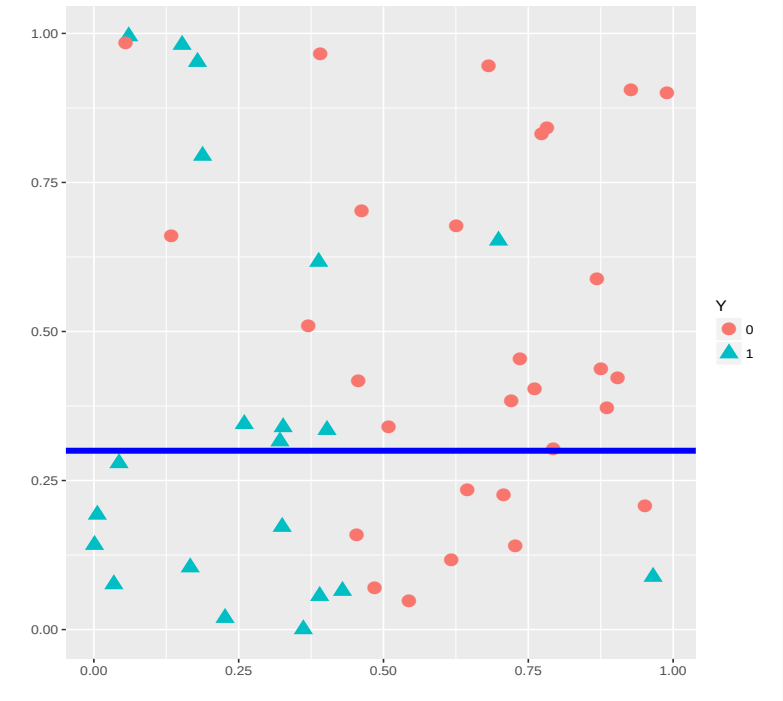
Example


1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
Y
0
1


1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
Y
0
1

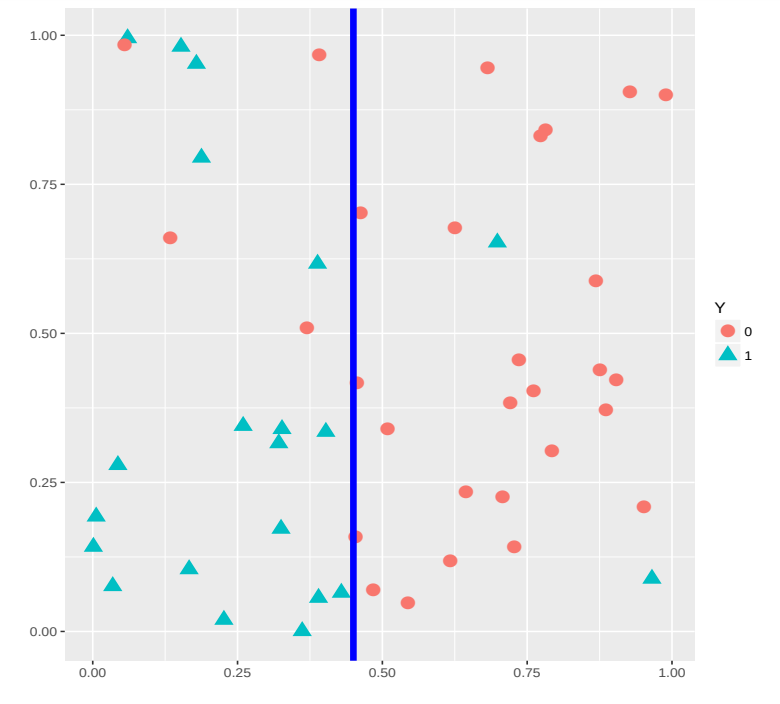
Example

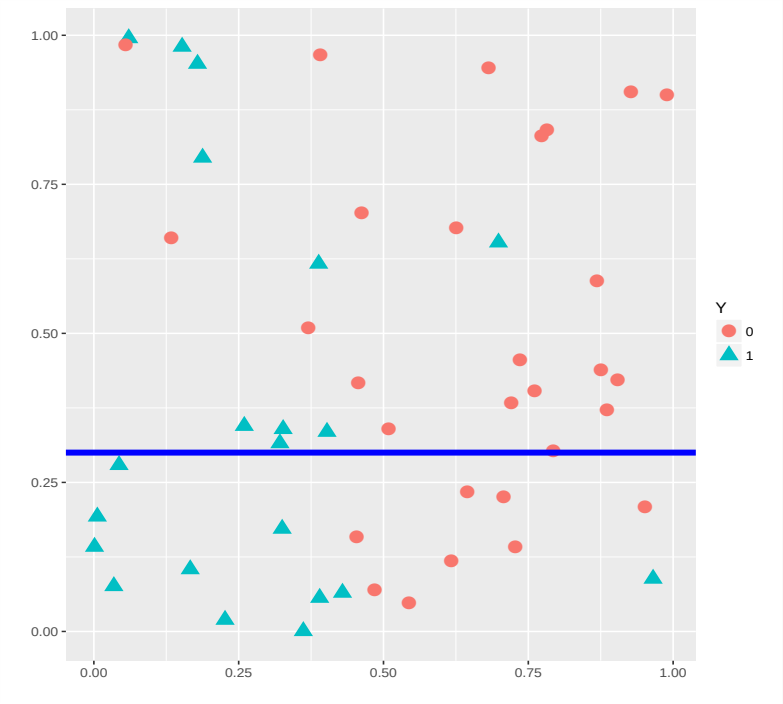




	$\mathcal{I}(\mathcal{N}_1)$	$\mathcal{I}(\mathcal{N}_2)$	Crit.
Left	0.287	0.137	0.2061
Right	0.488	0.437	0.4562

Example





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Left	0.287	0.137	0.2061
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Conclusion

We select the left split. (Exercise 1,2,3-IML3.)

Outline

Questions

- How to select an efficient tree?

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- Do we choose the maximum or deeper tree? (split the nodes until one observation by node).

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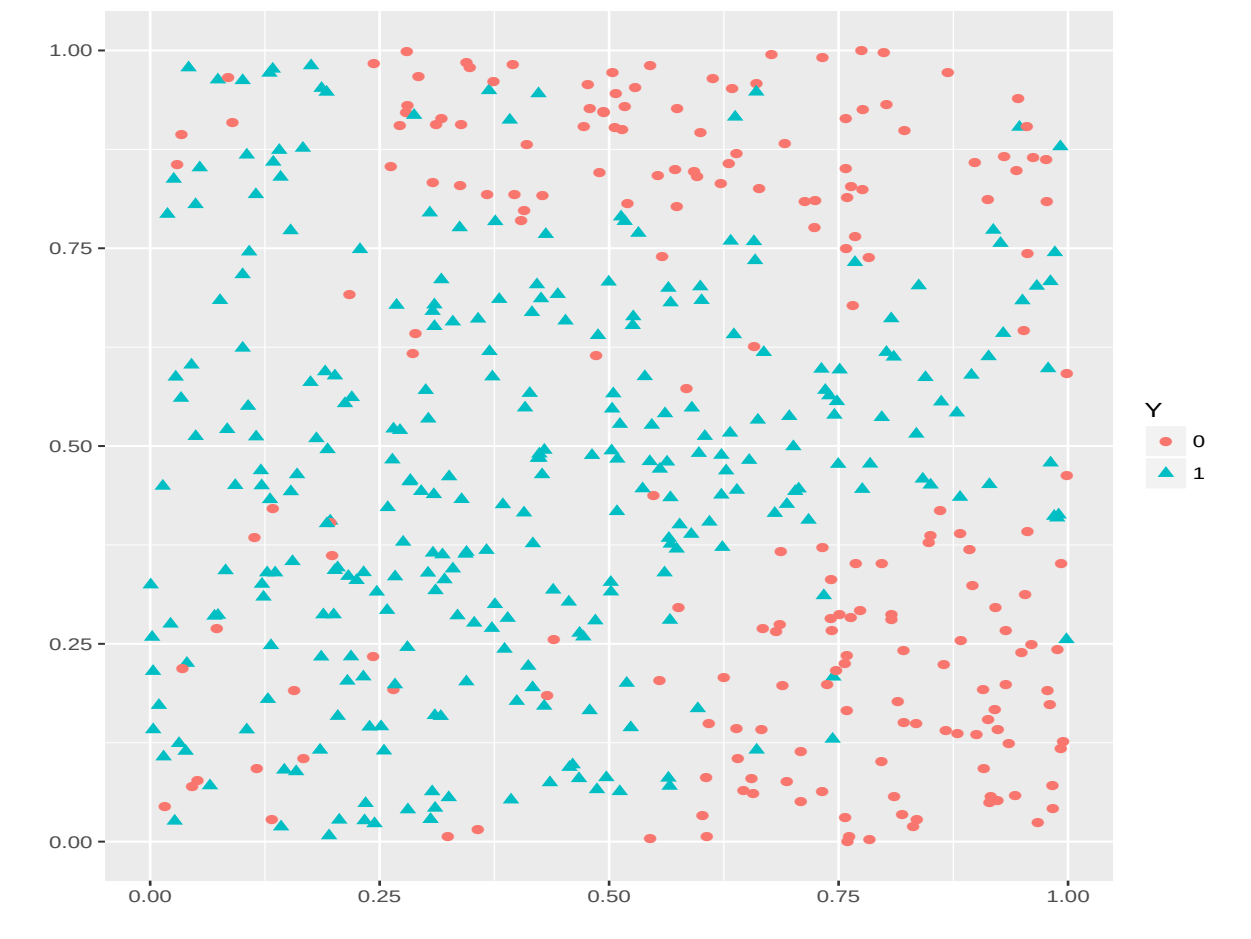
- How to select an efficient tree?
- Do we choose the maximum or deeper tree? (split the nodes until one observation by node).
- Grow a large tree and then prune this tree (select a subtree of this large tree)?

An example for binary classification



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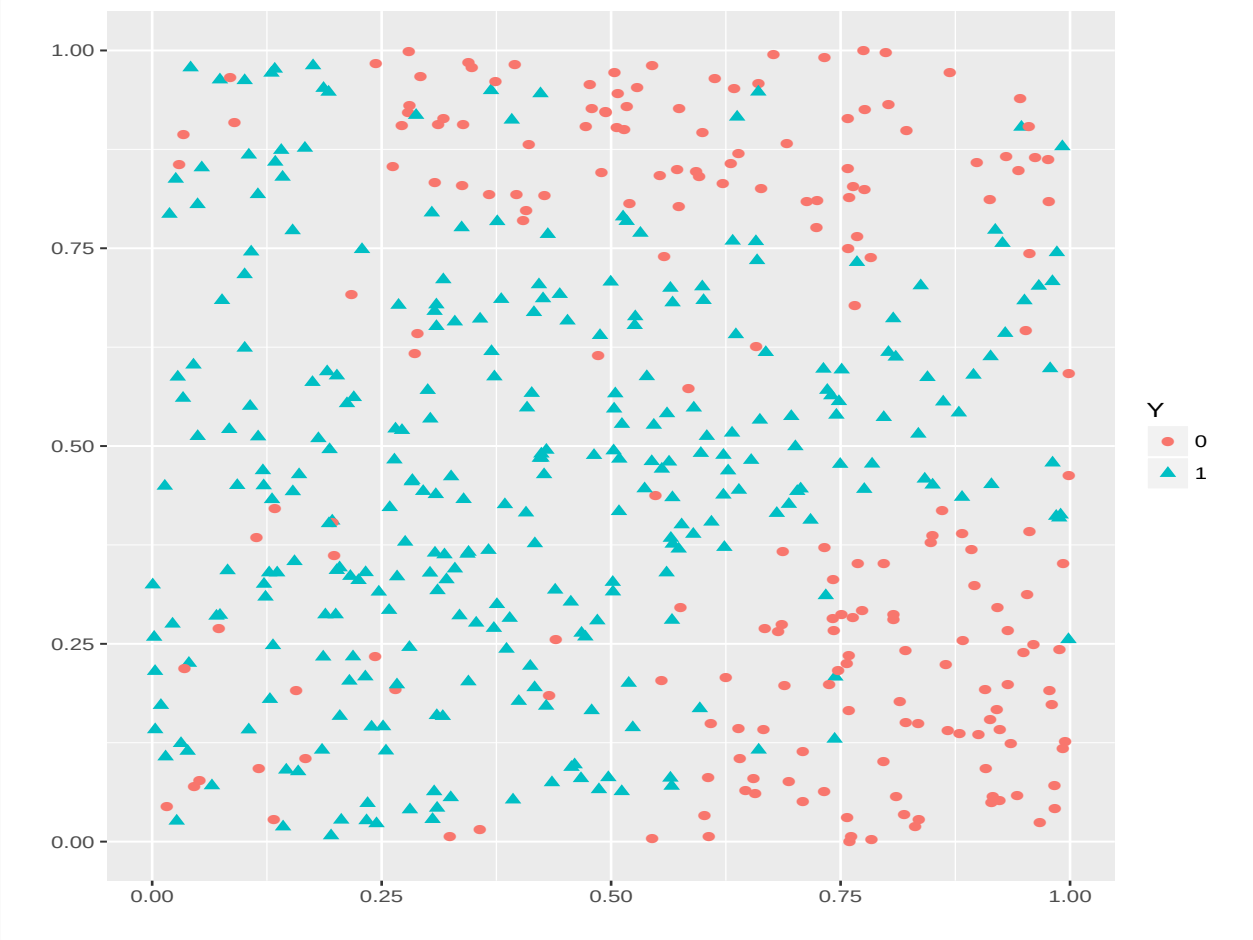
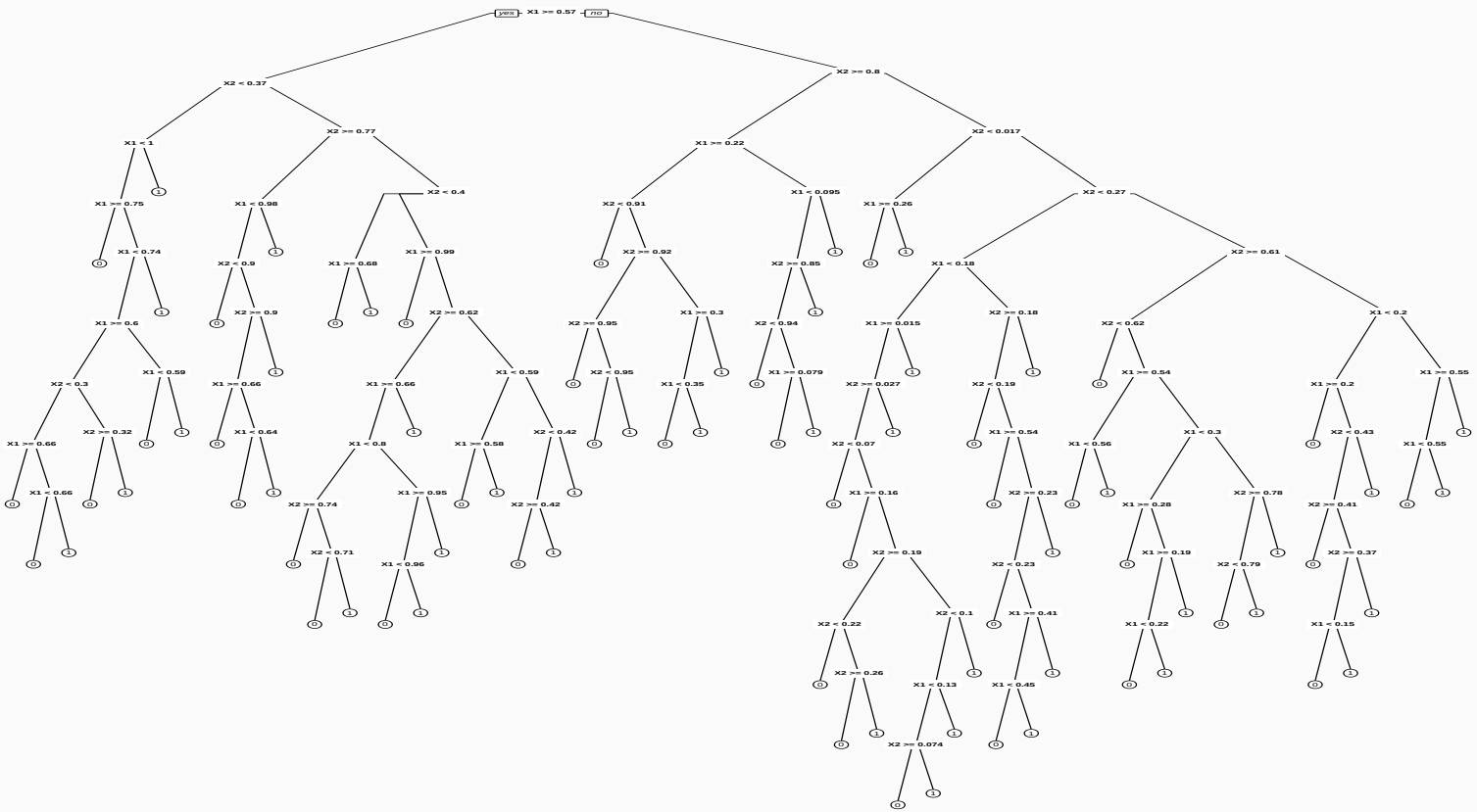


Optimal tree?

Intuitively, we are tempted to choose 5 or 6 terminal nodes.

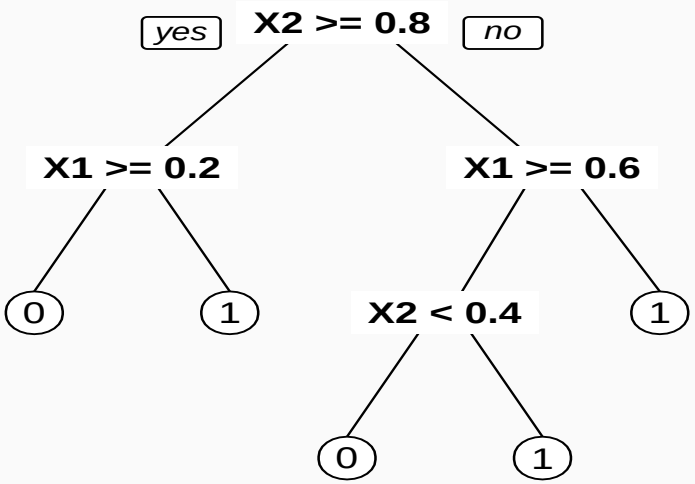
"Deeper" tree

```
> library(rpart)
> library(rpart.plot)
> tree1 <- rpart(Y~.,data=my_data,cp=0.0001,minsplit=2)
> prp(tree1)
```



A smaller tree

```
> tree2 <- rpart(Y~.,data=my_data)
> prp(tree2)
```



Comparison

- We estimate the misclassification error of these two trees on a test set.

```
> prev1 <- predict(tree1,newdata=dtest,type="class")
> prev2 <- predict(tree2,newdata=dtest,type="class")
> round(mean(prev1!=dtest$Y),3)
[1] 0.157
> round(mean(prev2!=dtest$Y),3)
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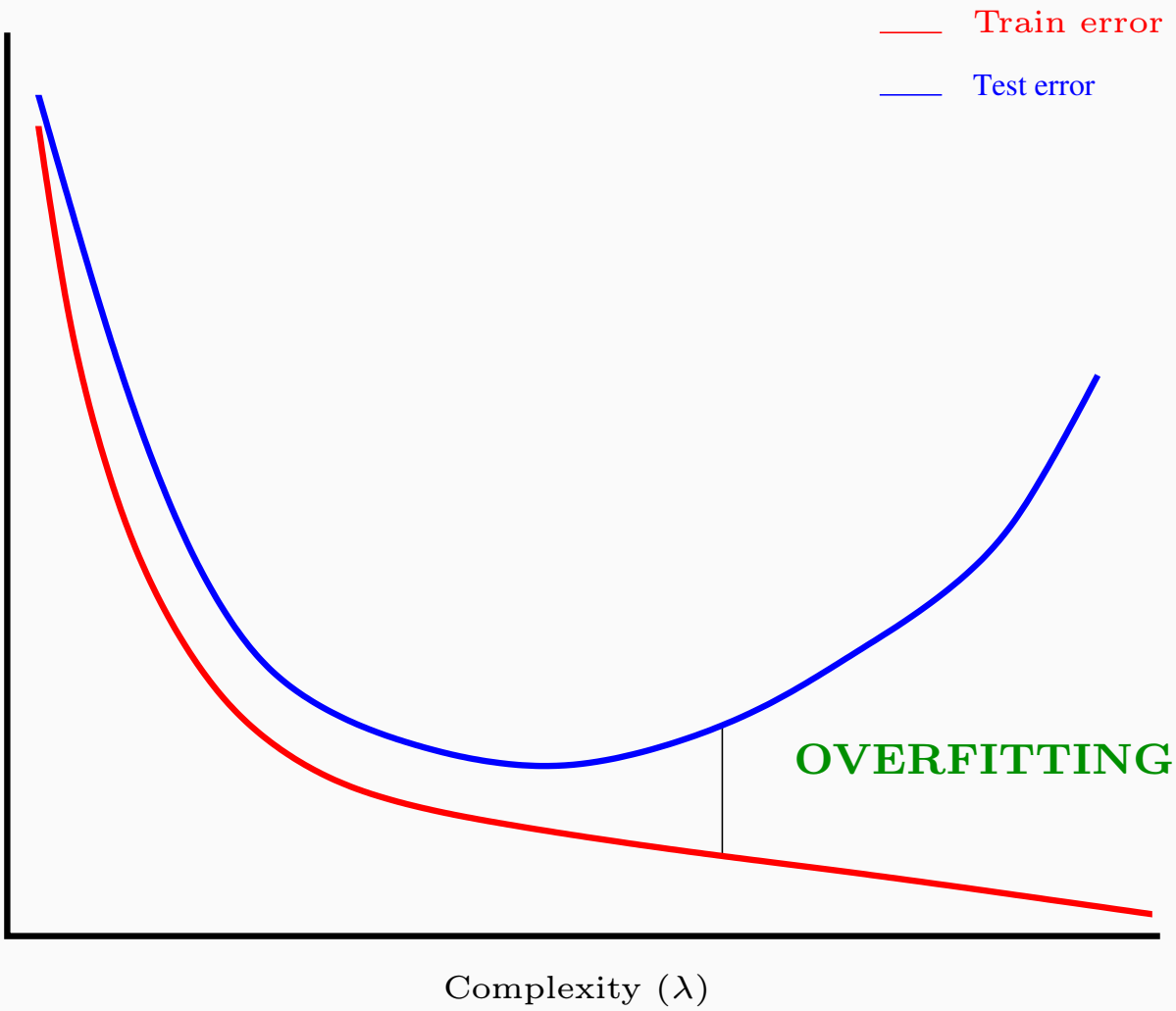
```

Conclusion

- Performance is not always improved by the size of the tree.
- Tree size is a tuning parameter which governs the model's complexity. We have to select this parameter.

Overfitting



Remark

Complexity is governed by the depth (or size) of the tree.

Bias and variance

Depth controls the tradeoff bias/variance :

1. Small tree $\Longrightarrow$ steady (robust) tree $\Longrightarrow$ small variance... but... large bias.
2. Large tree $\Longrightarrow$ unsteady tree $\Longrightarrow$ small bias... but... large variance (overfitting).

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2. Large tree $\Longrightarrow$ unsteady tree $\Longrightarrow$ small bias... but... large variance (overfitting).

Pruning [Breiman et al., 1984]

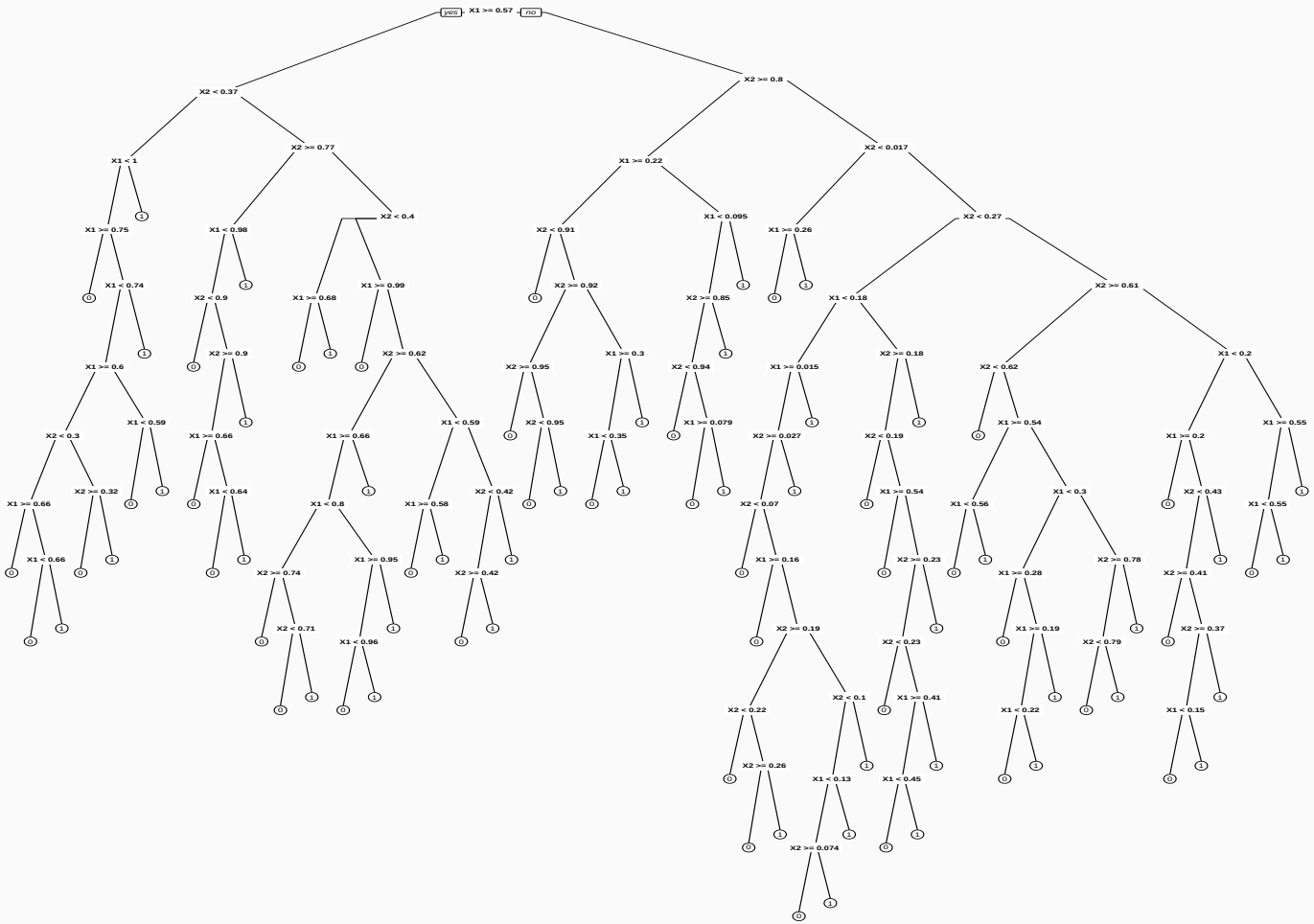
Instead of stopping the splitting process, we

1. grow a large tree (very deep tree) $\mathcal{T}_{max}$;
2. then select a sequence of nested subtrees:

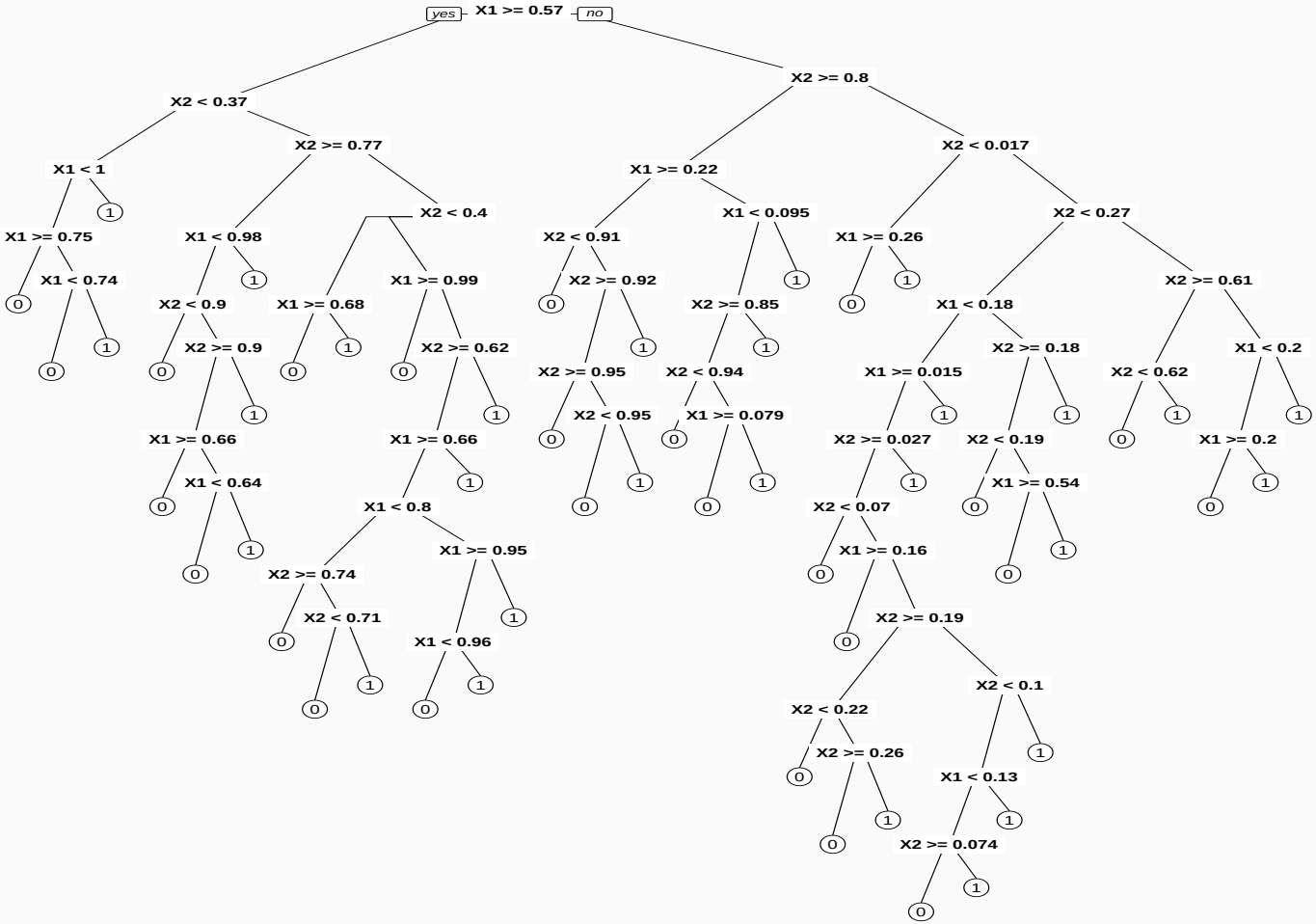
$$\mathcal{T}_{max} = \mathcal{T}_0 \supset \mathcal{T}_1 \supset \ldots \supset \mathcal{T}_K.$$

3. finally select one subtree in this sequence.

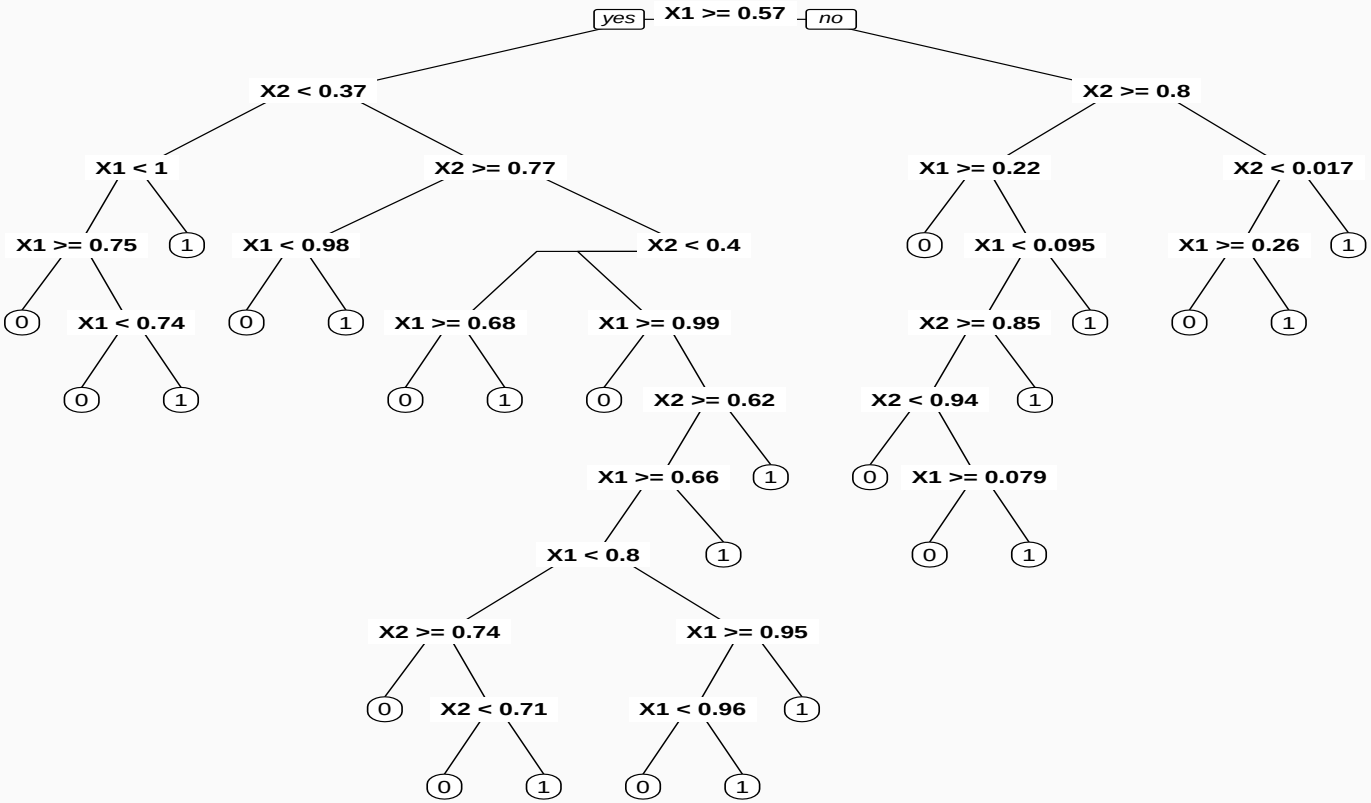
Nested trees



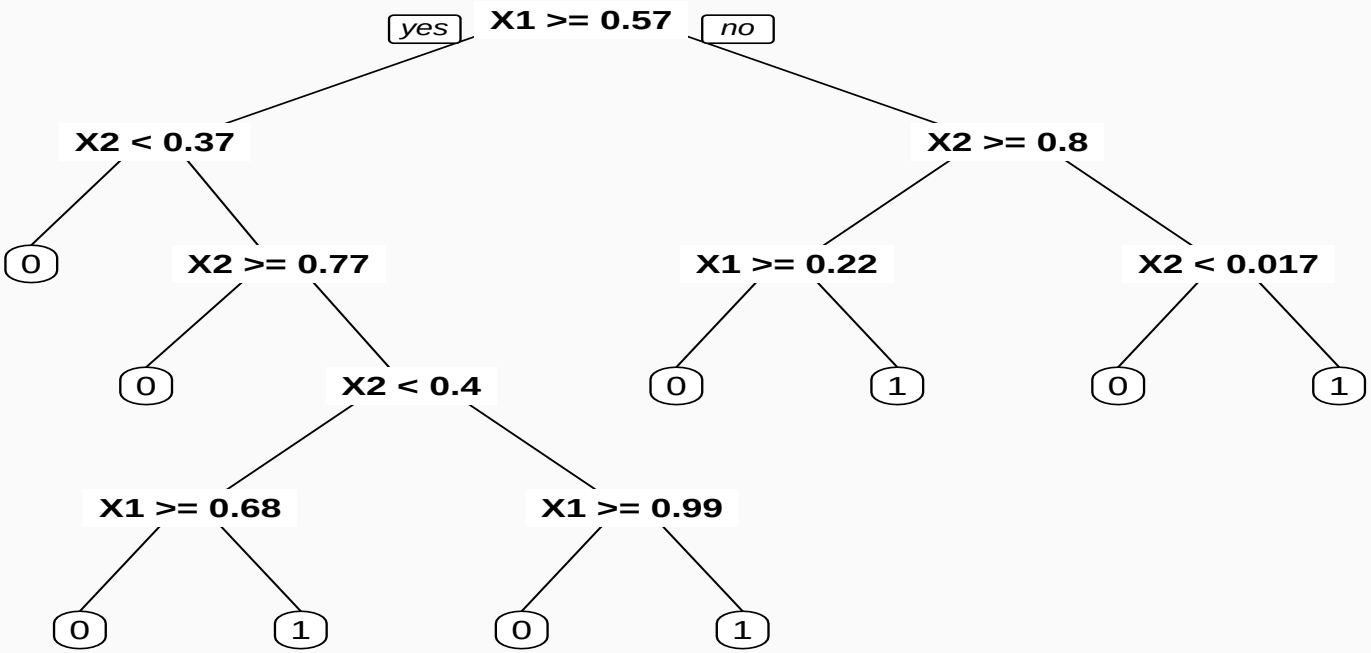
Nested trees



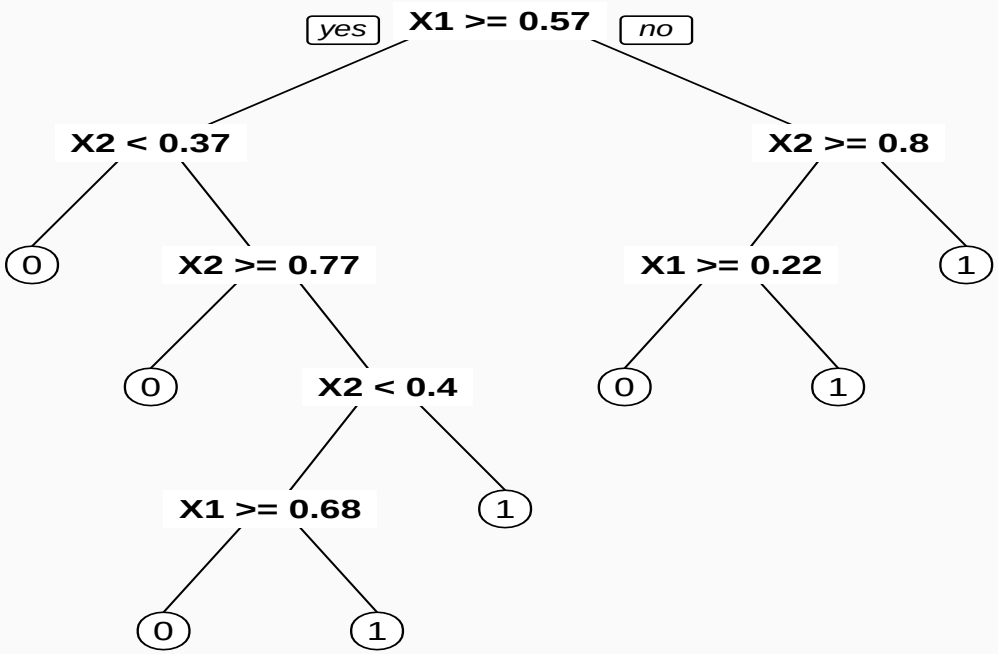
Nested trees



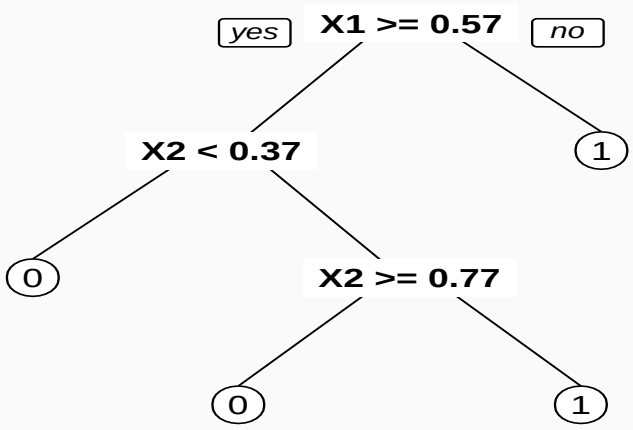
Nested trees



Nested trees



Nested trees



Nested trees

Construction of the sequence

- Let T be a tree with $|T|$ terminal nodes $\mathcal{N}_1, \ldots, \mathcal{N}_{|T|}$.
- Define $R(\mathcal{N})$ the risk (error) in node $\mathcal{N}$:
  - Regression:
$$R(\mathcal{N}) = \frac{1}{|\mathcal{N}|} \sum_{i:X_i \in \mathcal{N}} (Y_i - \bar{Y}_{\mathcal{N}})^2.$$
  - Classification:
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Definition

For $\alpha > 0$,
$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m R(\mathcal{N}_m) + \alpha |T|$$
is the cost complexity criterion of T.

The idea

- $C_\alpha(T)$ measures both the fitting and the complexity of the tree.
- The idea is to find the subtree T_α which minimizes $C_\alpha(T)$ for a safe choice of α.

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Remark

- $\alpha = 0 \Longrightarrow T_\alpha = T_0 = T_{max}$.
- $\alpha = +\infty \Longrightarrow T_\alpha = T_{+\infty} =$tree without split.
- α is called the complexity parameter.

Theorem [Breiman et al., 1984]

The exists a finite sequence $\alpha_0 = 0 < \alpha_1 < \ldots < \alpha_M$ with $M < |T_{max}|$ and a sequence of nested trees

$$T_{max} = T_0 \supset T_1 \supset \ldots \supset T_M$$

such thah $\forall \alpha \in [\alpha_m, \alpha_{m+1}[$

$$T_m = \operatorname*{argmin}_T C_\alpha(T).$$

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$$T_m = \underset{T}{\operatorname{argmin}}\, C_\alpha(T).$$

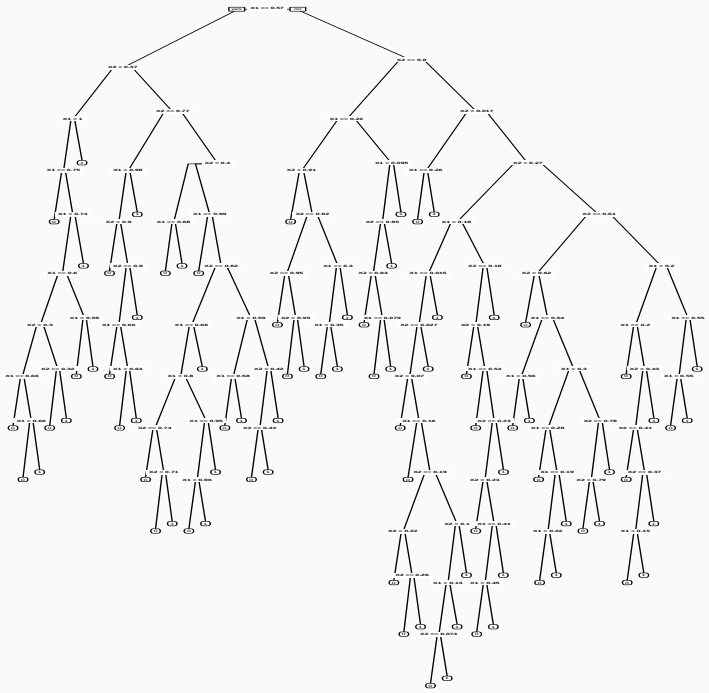
Important consequence

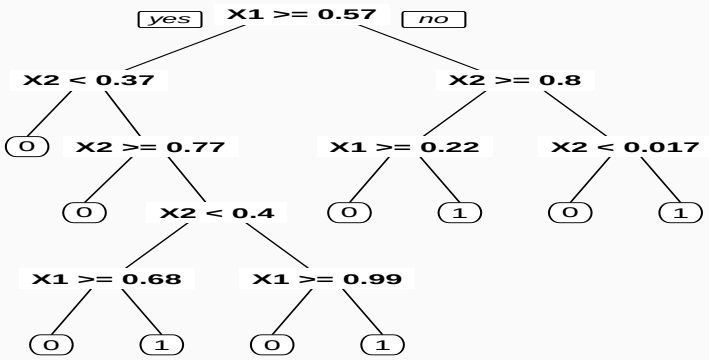
- We now are faced with a finite sequence of nested trees.
- We have to choose one tree in this sequence (or one value of α).

Example

```
> printcp(tree)
Classification tree:
rpart(formula = Y ~ ., data = my_data, cp = 1e-04, minsplit = 2)
Variables actually used in tree construction:
[1] X1 X2
Root node error: 204/500 = 0.408
n= 500
          CP nsplit rel error  xerror     xstd
1  0.2941176      0  1.000000 1.00000 0.053870
2  0.1225490      1  0.705882 0.71569 0.049838
3  0.0931373      3  0.460784 0.49020 0.043844
4  0.0637255      4  0.367647 0.43627 0.041928
5  0.0122549      5  0.303922 0.34314 0.038034
6  0.0098039      7  0.279412 0.34314 0.038034
7  0.0049020      9  0.259804 0.36275 0.038923
8  0.0040107     25  0.181373 0.34804 0.038260
9  0.0036765     41  0.112745 0.39216 0.040184
10 0.0032680     49  0.083333 0.40196 0.040586
11 0.0024510     52  0.073529 0.41176 0.040980
12 0.0001000     82  0.000000 0.43137 0.041742
```

```
> arbre1 <- prune(tree,cp=0.005)
> prp(tree)
> prp(tree1)
```





Remark

We have to select one tree in the sequence

$$T_{max} = T_0 \supset T_1 \supset \ldots \supset T_M.$$

The final tree

Risk estimation

We choose the final tree by minimizing a risk $\mathcal{R}(T_m) = \mathbf{E}[\ell(Y, T_m(X)]$ (as usual). For instance,

1. quadratic risk $\mathbf{E}[(Y - T_m(X))^2]$ in regression ;
2. misclassification error $\mathbf{P}(Y \neq T_m(X))$ in supervised classification.

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This risk is unknown and is generally estimated by cross validation.

Select the optimal tree

The approach consists in

1. estimating the risk for each subtree.
2. selecting the subtree which minimizes the estimated risk.

- Estimations of $\mathcal{R}(m)$ are in the column xerror of the function printcp:

```
          CP nsplit rel error  xerror     xstd
1  0.2941176      0  1.000000 1.00000 0.053870
2  0.1225490      1  0.705882 0.71569 0.049838
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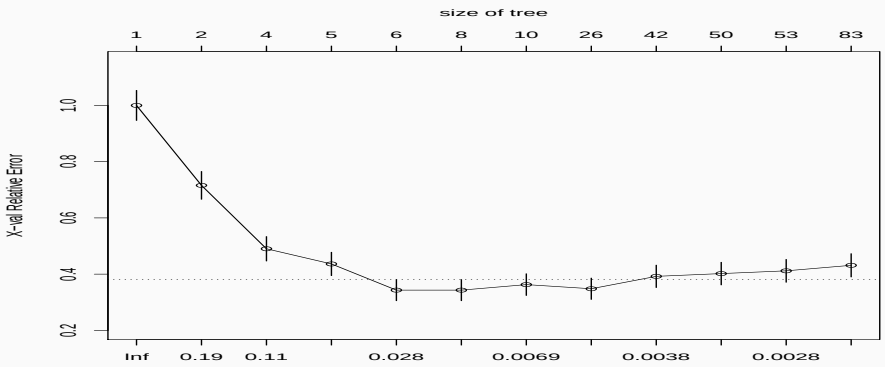
7  0.0049020      9  0.259804 0.36275 0.038923
```

- We can look at the estimated error for each subtree with plotcp

```
> plotcp(tree3)
```

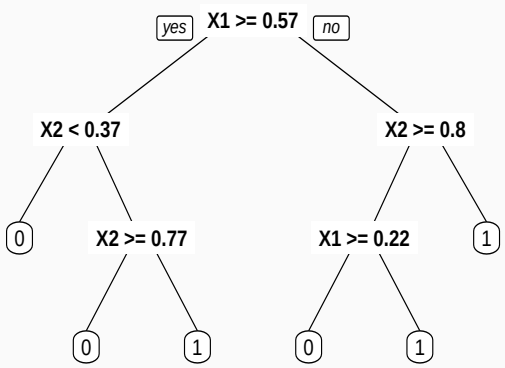


Conclusion

We choose the tree with 5 splits.

Visualisation of the final tree

```
> alpha_opt <- arbre$cptable[which.min(tree$cptable[,"xerror"]),"CP"]
> tree_final <- prune(tree,cp=alpha_opt)
> prp(tree_final)
```



Classification rule and score for a tree

- Final tree $\mathcal{T}$ consists of a partition of $\mathbb{R}^p$ into $|\mathcal{T}|$ terminal nodes $\mathcal{N}_1, \ldots, \mathcal{N}_{|\mathcal{T}|}$.

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$$\hat{g}(x) = \begin{cases} 1 & \text{if } \sum_{i:X_i \in \mathcal{N}(x)} \mathbf{1}_{Y_i=1} \geq \sum_{i:X_i \in \mathcal{N}(x)} \mathbf{1}_{Y_i=0} \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathcal{N}(x)$ stands for the terminal node which contains x.

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- Score:

$$\hat{S}(x) = \hat{\mathsf{P}}(Y = 1 | X = x) = \frac{1}{n} \sum_{i:X_i \in \mathcal{N}(x)} \mathbf{1}_{Y_i=1}.$$

Predict function

- predict function (or predict.rpart) allows to estimate the label or the score of a new observation:

```
> x_new <- data.frame(X1=0.5,X2=0.85)
> predict(arbre_final,newdata=x_new)
    0   1
1 0.9 0.1
> predict(arbre_final,newdata=x_new,type="class")
1
0
Levels: 0 1
```

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- We can interpret the model (plot the tree) if the tree is not too large.

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- One drawback: due to the recursive process, the algorithm is not stable, affected by small perturbations of the sample.
- This drawback will become an advantage for bootstrap aggregating $\Longrightarrow$ random forest.
- Exercise 4-IML3.

Outline

References i

Breiman, L., Friedman, J., Olshen, R., and Stone, C. (1984).
Classification and regression trees.
Wadsworth & Brooks.

Part V

Bagging and random forests

Outline

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The idea

- Instead of fitting one "sophisticated" machine, fit a lot of simple machines and aggregate them.
- Example:

$$\widehat{m}(x) = \frac{1}{B} \sum_{k=1}^{B} \widehat{m}_k(x)$$

where $\widehat{m}_1(x), \ldots, \widehat{m}_B(x)$ are simple machines.

Questions

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- How many machines?

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$$\widehat{m}(x) = \frac{1}{B} \sum_{k=1}^{B} \widehat{m}_k(x) = \widehat{m}_1(x)$$

  $\Longrightarrow$ aggregation is useless.
- Solution: run the same algorithm on different datasets.

Bootstrap sample

- We have at hand one dataset $\mathcal{D}_n = (X_1, Y_1), \ldots, (X_n, Y_n)$.

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Bootstrap

- Define new datasets by randomly draw dataset with replacement from the training data.

Bootstrap: example

- The sample:

1	2	3	4	5	6	7	8	9	10

Bootstrap: example

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- Bootstrap samples:

3	4	6	10	3	9	10	7	7	1	m_1
2	8	6	2	10	10	2	9	5	6	m_2
2	9	4	4	7	7	2	3	6	7	m_3
6	1	3	3	9	3	8	10	10	1	m_4
3	7	10	3	2	8	6	9	10	2	m_5
	$\vdots$								$\vdots$	
7	10	3	4	9	10	10	8	6	1	m_B

Bootstrap: example

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1	2	3	4	5	6	7	8	9	10

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3	7	10	3	2	8	6	9	10	2	m_5
	$\vdots$								$\vdots$	
7	10	3	4	9	10	10	8	6	1	m_B

- We finally aggregate:

$$\widehat{m}_B(x) = \frac{1}{B}\sum_{k=1}^{B} m_k(x).$$

Bagging algorithm

- Estimates m_k are not fitted on the original dataset $\mathcal{D}_n = (X_1, Y_1), \ldots, (X_n, Y_n)$ but on bootstrap samples.

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- B a positive integer.

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Bagging

Inputs:

- a "simple machine" (a tree, 1NN rule...)
- B a positive integer.

For $k = 1, \ldots, B$:

1. Draw a bootstrap sample from $\mathcal{D}_n$.
2. Fit the simple machine on this bootstrap sample: $m_k(x)$.

Output: the aggregate estimate $\widehat{m}_B(x) = \frac{1}{B} \sum_{k=1}^{B} m_k(x)$.

How to choose B?

- 2 parameters have to be chosen: the number of iterations B and the simple machine.

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- As B increases, $\widehat{m}_B$ stabilizes.

Important conclusion

- B is not an important parameter, we have to choose it as large as possible (often 500).
- Bagging is random but it is less random when B is large.

Some properties

Bias and variance

For regression, we have $\mathbf{E}[\widehat{m}_B(x)] = \mathbf{E}[m_k(x)],\ \forall k = 1, \ldots, B$ and

$$\mathbf{V}[\widehat{m}_B(x)] \approx |\rho(x)|\mathbf{V}[m_k(x)]$$

where $\rho(x) = corr(m_k(x), m_{k'}(x))$ for $k \neq k'$.

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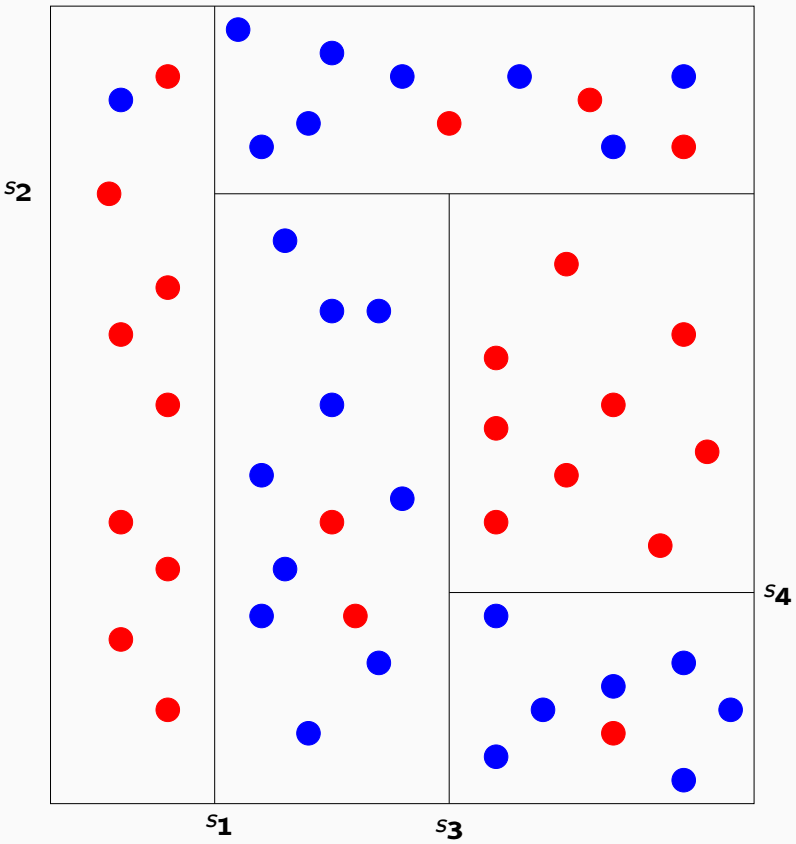
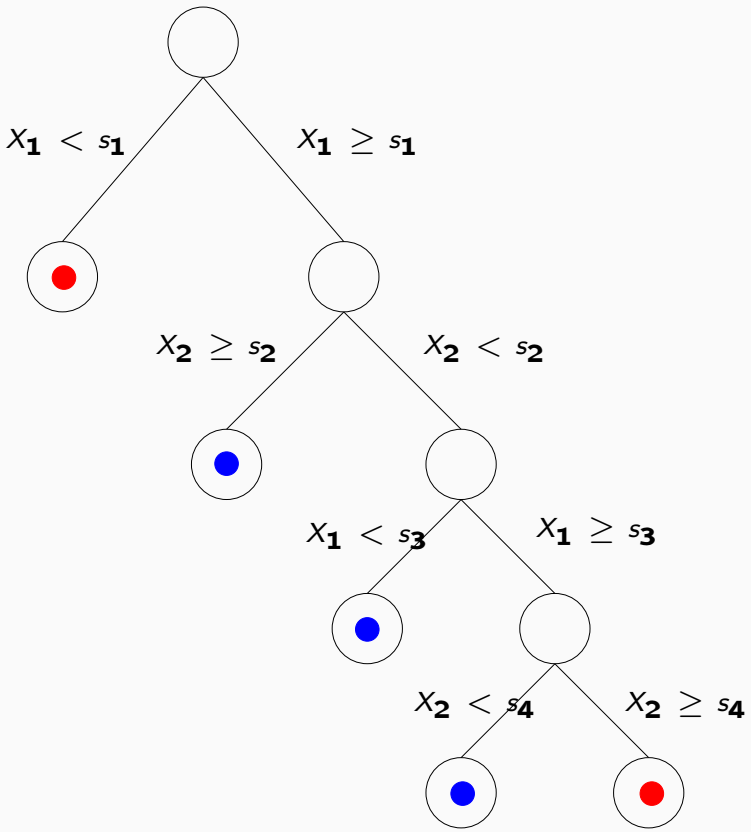
- Bias is not affected by the bagging process.
- Variance of the bagging estimate reduces when correlation between the simple machines decreases.
- Consequence: we need simple machines sensitive to small disturbances of the data.
- Trees are known to satisfy this property (drawback becomes an advantage...).

Outline

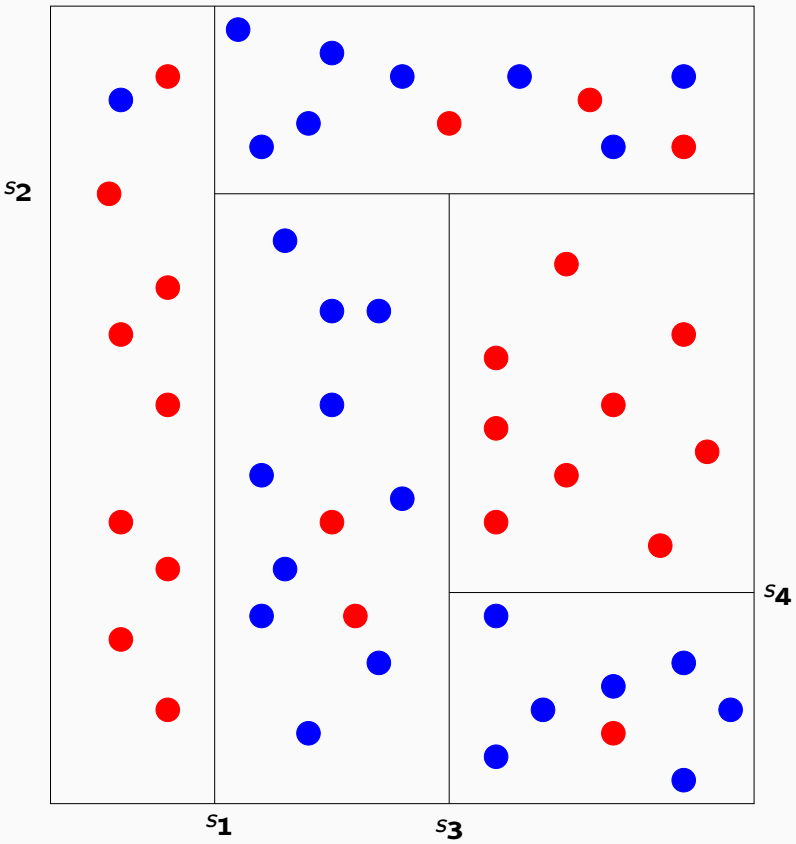
Outline

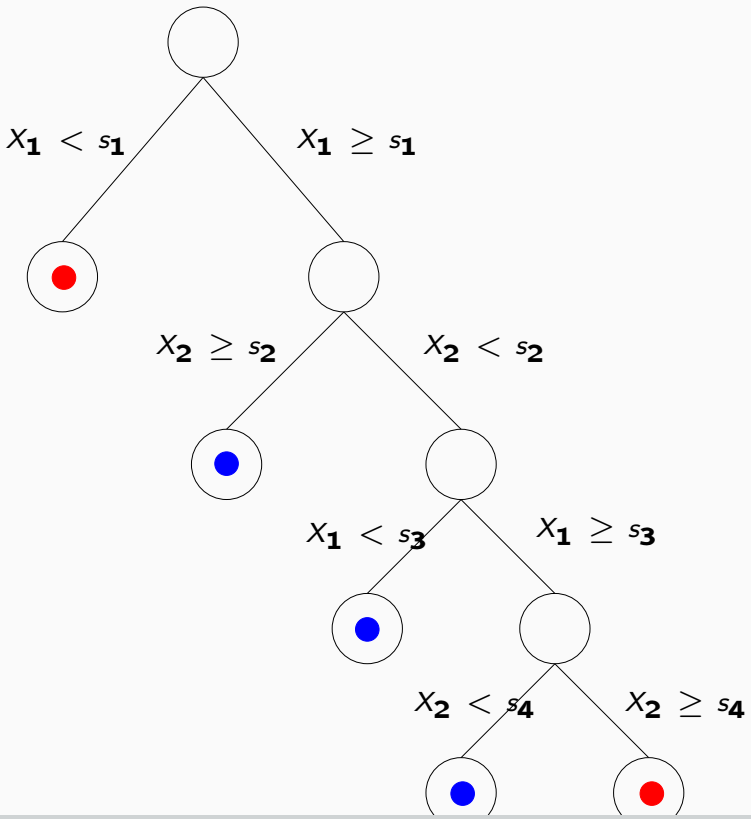
Tree (reminder)





Tree (reminder)





Important parameter: depth

- small: bias $\nearrow$, variance $\searrow$
- large: bias $\searrow$, variance $\nearrow$

- A random forest = a collection of trees.

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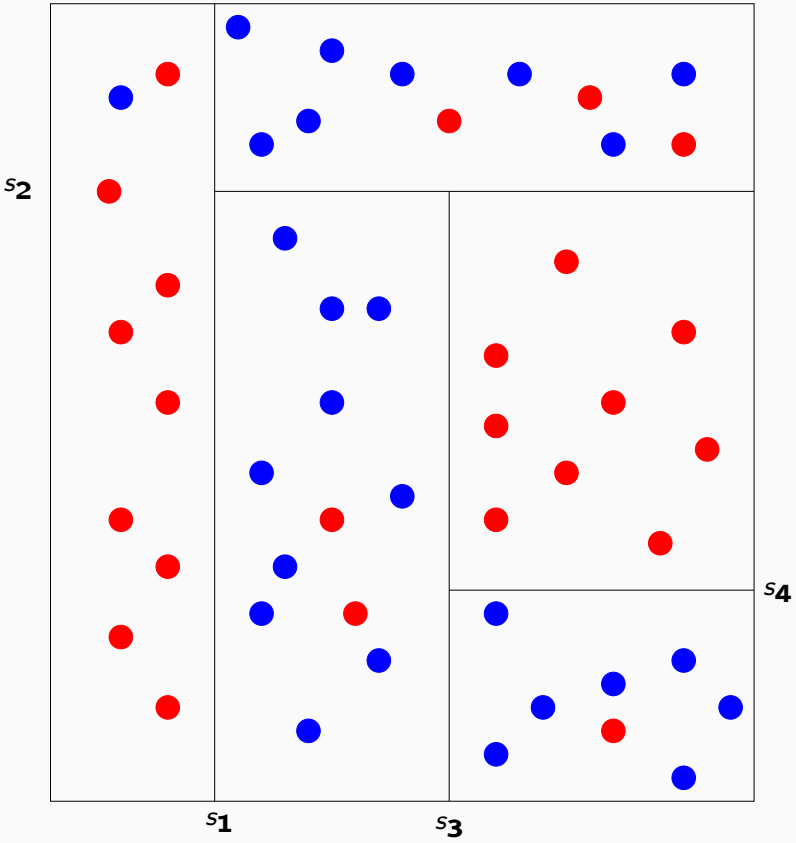
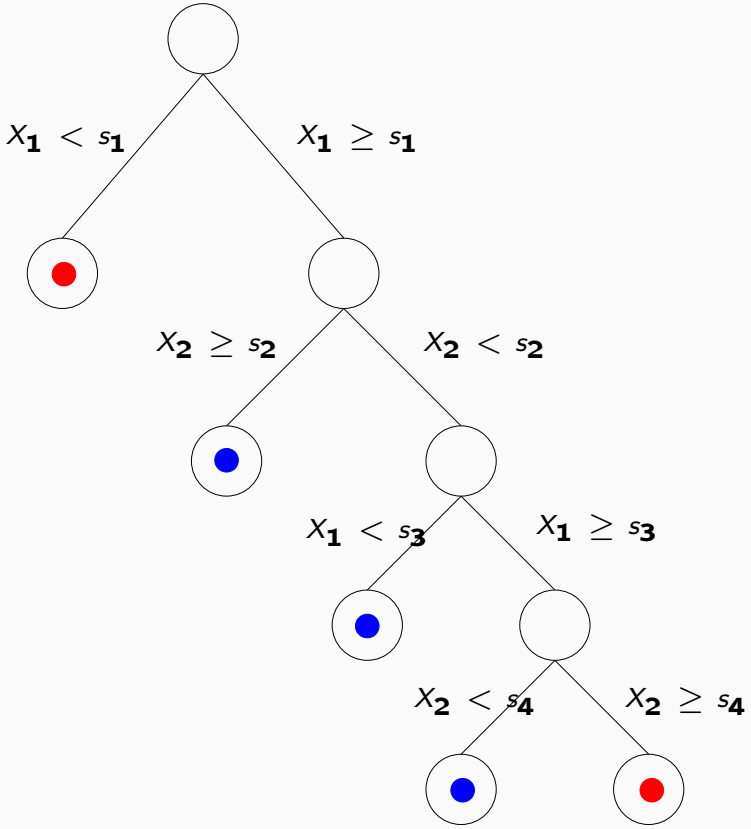
- References

  http://www.stat.berkeley.edu/~breiman/RandomForests/

  Robin Genuer's phd thesis [Genuer, 2010].

- Trees are fitted as for the CART process (no pruning) with only one small variation.


s_2
s_4
s_1
s_3


$X_1 < s_1$
$X_1 \geq s_1$
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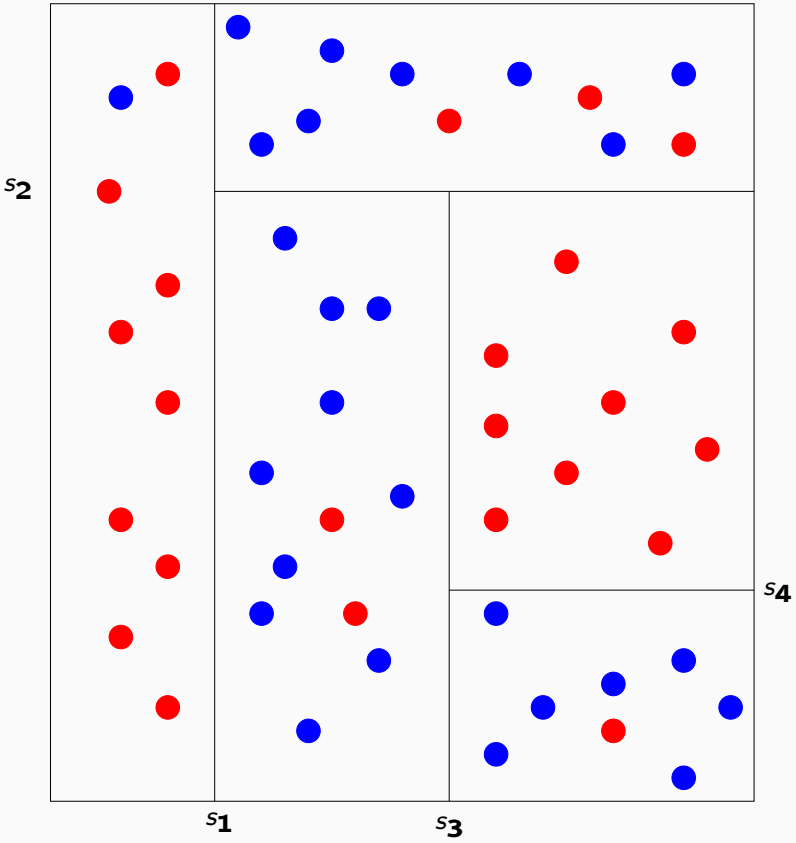
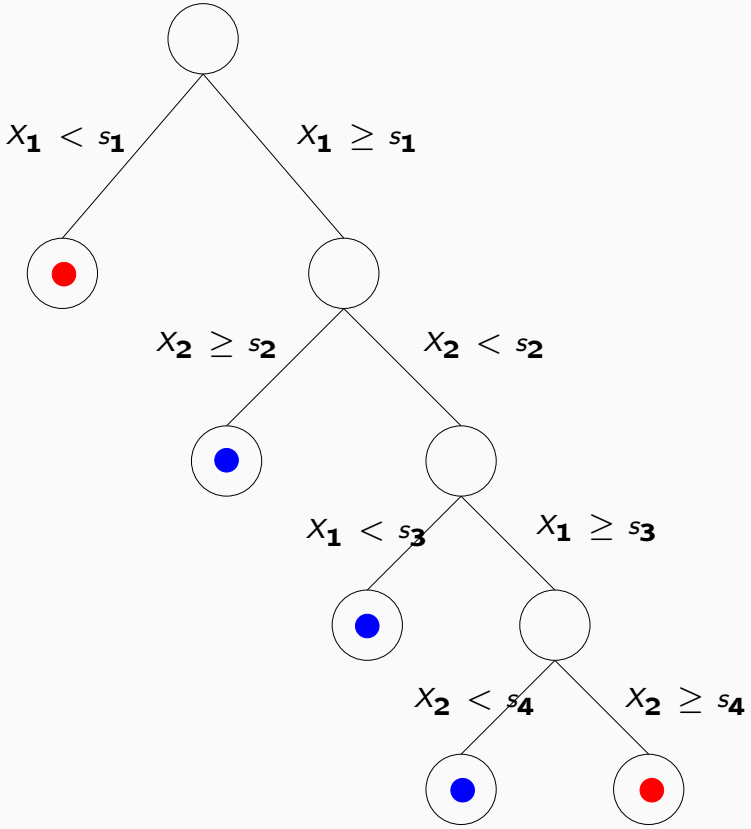
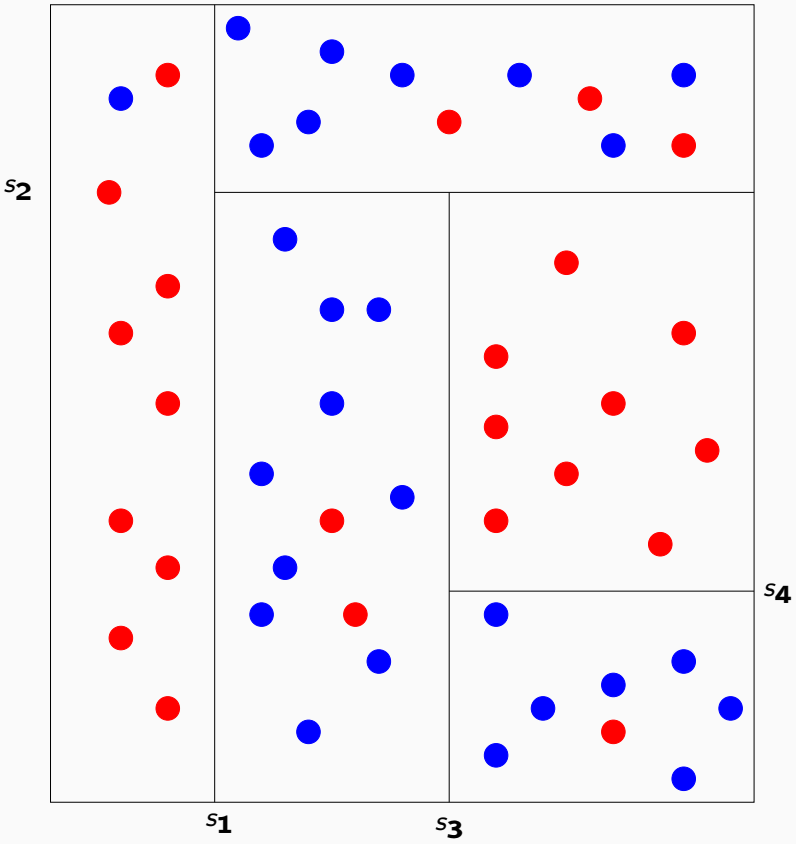
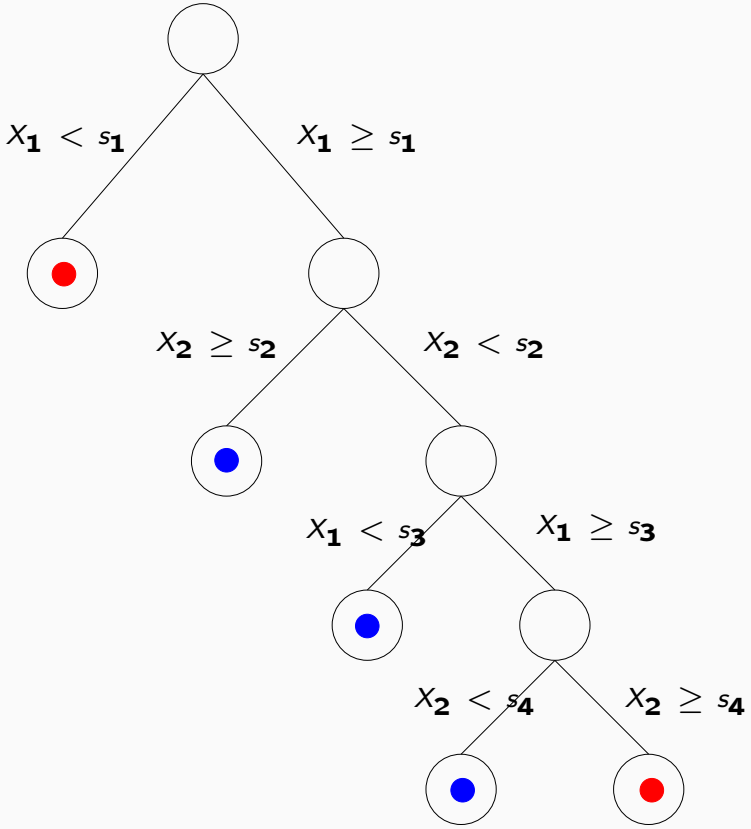




Trees for the forest

- At each step, the best split is selected among $mtry \leq d$ inputs randomly chosen among the d inputs.





Trees for the forest

- At each step, the best split is selected among $mtry \leq d$ inputs randomly chosen among the d inputs.
- Goal: try to reduce correlations between the trees, to make the trees more different from each other.

Random forest algorithm

Inputs:

- B size of the forest;
- $mtry \in \{1, \ldots, d\}$ number of candidate inputs for each split.

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For $k = 1, \dots, B$:

1. Draw a bootstrap sample from $\mathcal{D}_n$;
2. Fit a tree according to the CART process, each split is chosen among $mtry$ variables randomly chosen among the d input variables. Denote by $T_k(x)$ the tree.

Output: the random forest $\widehat{T}_B(x) = \frac{1}{B} \sum_{k=1}^{B} T_k(x)$.

Comments

- The algorithm is for both regression and binary classfication:
  1. for regression, the RF estimates $m^\star(x) = \mathbf{E}[Y|X = x]$;
  2. for binary classification, the RF estimates $S^\star(x) = \mathbf{P}(Y = 1|X = x)$.

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- Simple algorithm. On R, you can use randomForest function from the randomForest package or the ranger function from the ranger package.
- Estimate known to be efficient for complex data and robust (wrt to the choice of its parameter).

Choice of the parameter

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Bagging decreases the variance:

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Consequence

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- Trees for forest are deep trees with a small number of observations in each terminal node.
- By default randomForest fit trees with (only) 5 observations in terminal nodes for regression and 1 for supervised classification.

Choice of *mtry*

- This parameter (slightly) governs the bias/variance trade-off of the forest.

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Conclusion

- We can look at the performances of the forest for many values of mtry.
- By default $mtry = d/3$ for regression and $\sqrt{d}$ for supervised classification.

Application on the spam dataset

```
> library(randomForest)
> forest1 <- randomForest(type~.,data=spam)
> forest1

Call:
 randomForest(formula = type ~ ., data = spam)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 7

        OOB estimate of  error rate: 5.26%
Confusion matrix:
     0   1 class.error
0 1352  42  0.03012912
1   79 827  0.08719647
```

Outline

Random forest performance

- As for other machine learning algorithms, we need criteria to measure performances of a random forest.

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- **Examples:**
  - Quadratic risk $\mathbf{E}[(Y - \widehat{T}_B(X))^2]$ for regression;
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- **Examples:**
  - Quadratic risk $\mathbf{E}[(Y - \widehat{T}_B(X))^2]$ for regression;
  - Misclassification error $\mathbf{P}(Y \neq \widehat{T}_B(X))$ for supervised classification.
- These criteria can be estimated by validation hold out or cross validation.
- Bootstrap step in bagging algorithms proposes another way to estimate these criteria: OOB (Out Of Bag).

Ouf Of Bag error

- For each (X_i, Y_i), construct its random forest predictor by averaging only those trees corresponding to bootstrap samples in which (X_i, Y_i) does not appear:

$$\hat{Y}_i = \frac{1}{|\mathcal{I}_B|} \sum_{k \in \mathcal{I}_B} T_k(X_i)$$

where $\mathcal{I}_B$ is the set of trees such that (X_i, Y_i) is Out Of Bag.

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Out Of Bag estimates

- OOB quadratic risk: $\frac{1}{n} \sum_{i=1}^{n} (\hat{Y}_i - Y_i)^2$.
- OOB misclassification error: $\frac{1}{n} \sum_{i=1}^{n} \mathbf{1}_{\hat{Y}_i \neq Y_i}$.

Example

3	4	6	10	3	9	10	7	7	1	m_1
2	8	6	2	10	10	2	9	5	6	m_2
2	9	4	4	7	7	2	3	6	7	m_3
6	1	3	3	9	3	8	10	10	1	m_4
3	7	10	3	2	8	6	9	10	2	m_5
7	10	3	4	9	10	10	8	6	1	m_6

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3	7	10	3	2	8	6	9	10	2	m_5
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- (X_1, Y_1) does not appear in bootstrap samples 2, 3 and 5, thus

$$\hat{Y}_1 = \frac{1}{3}(m_2(X_1) + m_3(X_1) + m_5(X_1)).$$

- We do the same for all the observations $\Longrightarrow \hat{Y}_2, \ldots, \hat{Y}_n$.

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- We do the same for all the observations $\Longrightarrow \hat{Y}_2, \ldots, \hat{Y}_n$.
- We obtain the OOB quadratic risk:

$$\frac{1}{n}\sum_{i=1}^{n}(\hat{Y}_i - Y_i)^2.$$

Example

- Spam dataset with $mtry = 1$:

```
> forest2 <- randomForest(Y~.,data=spam,mtry=1)
> forest2

Call:
 randomForest(formula = Y ~ ., data = dapp, mtry = 1)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 1

        OOB estimate of  error rate: 8.04%
Confusion matrix:
     0   1 class.error
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1  158 748  0.17439294
```

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Confusion matrix:
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```

Conclusion

OOB misclassification error: 8.04% for $mtry = 1$ and 5.26% for $mtry = 7$.

Outline

- Single trees are highly interpretable.
- Linear combinations of trees (random forests) loose this important features.

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- There exists a score which measures importance of each inputs.

- As for OOB error, this score is based on the fact for some observations does not appear in bootstrap samples.

- Let OOB_k denotes the OOB sample of the k-th tree.

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- Let E_{OOB_k} the quadratic error of the k-th tree measured on OOB_k:

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Definition

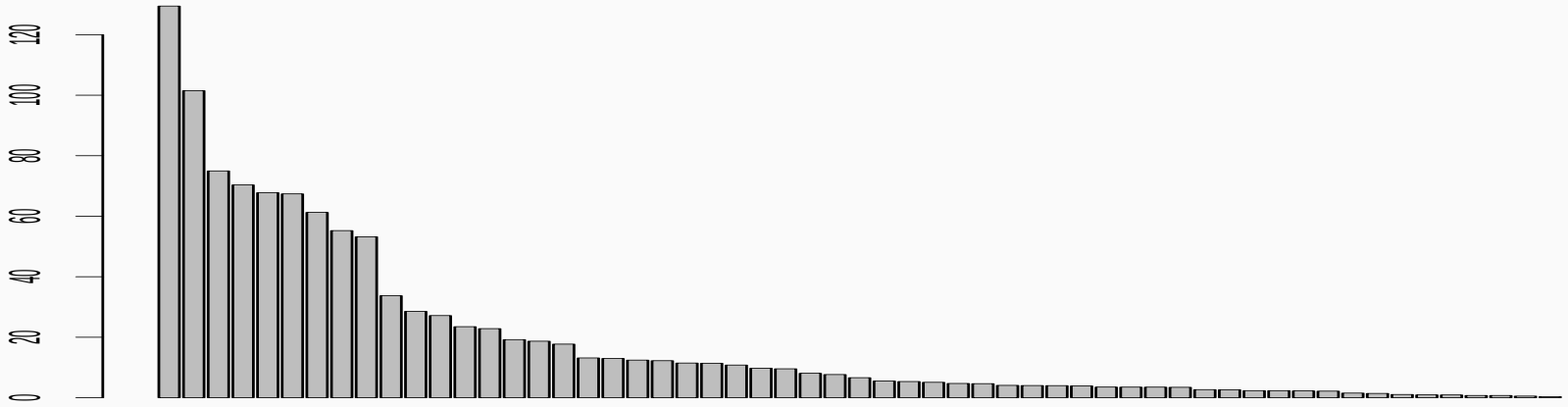
The variable importance score for the j variable is defined by

$$Imp(X_j) = \frac{1}{B} \sum_{k=1}^{B} (E_{OOB_k}^j - E_{OOB_k}).$$

Example

- It is easy to obtain variable importance score with randomForest

```
> imp <- importance(forest1)
> imp1 <- sort(imp,decreasing=TRUE)
> ord <- order(imp,decreasing=TRUE)
> ord
 [1] 52 53 55  7 56 16 21 25 57  5 24 19 26 23 46 27 11  8 50 12 37  3 18  6 45
[26] 17 10  2 28 42 49 35  1 36 39 13 54  9 30 33 22 51 29 14 43 44 31 20 48 15
[51] 40  4 41 34 32 38 47
> barplot(imp1,beside=TRUE)
```



Comparison - spam dataset

- We make a comparison between some statistical learning algorithms on the spam dataset.

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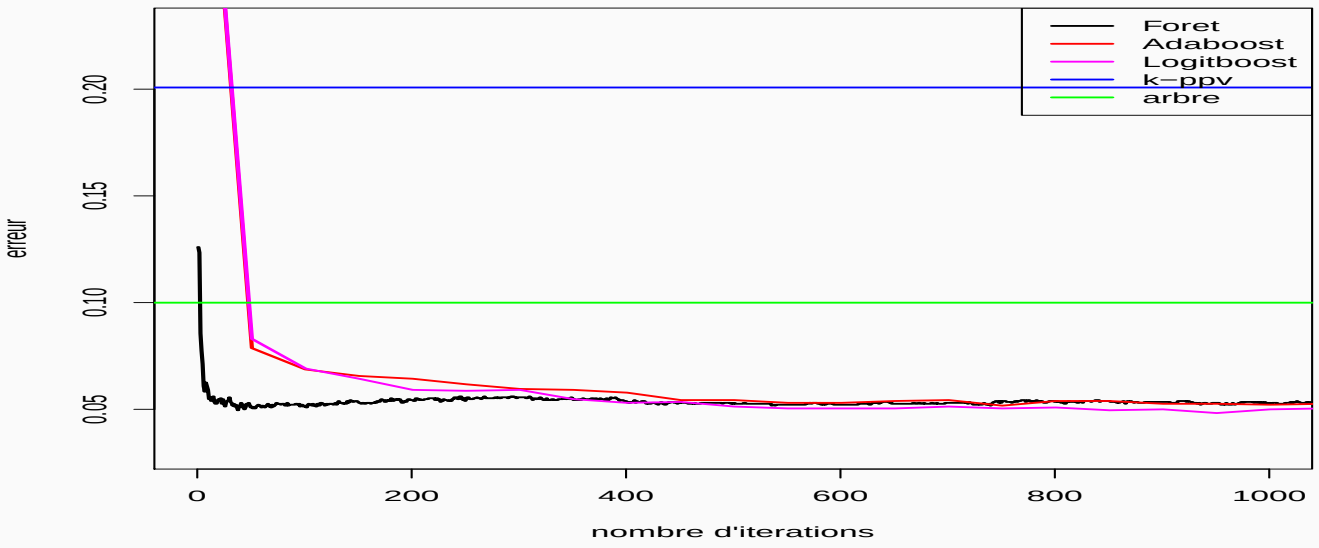
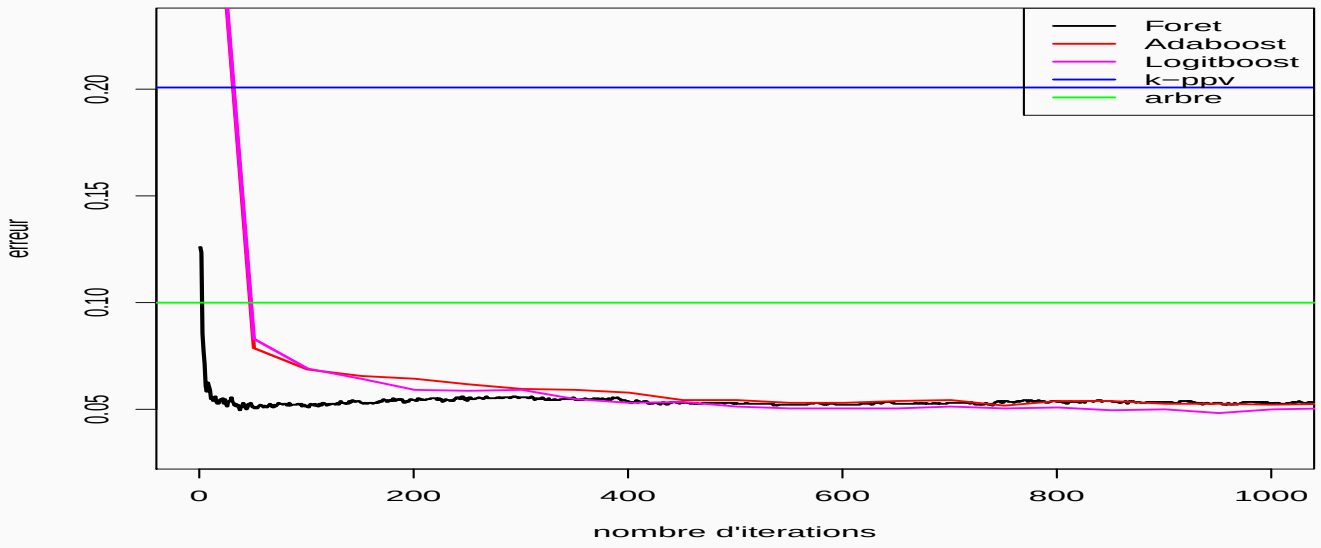
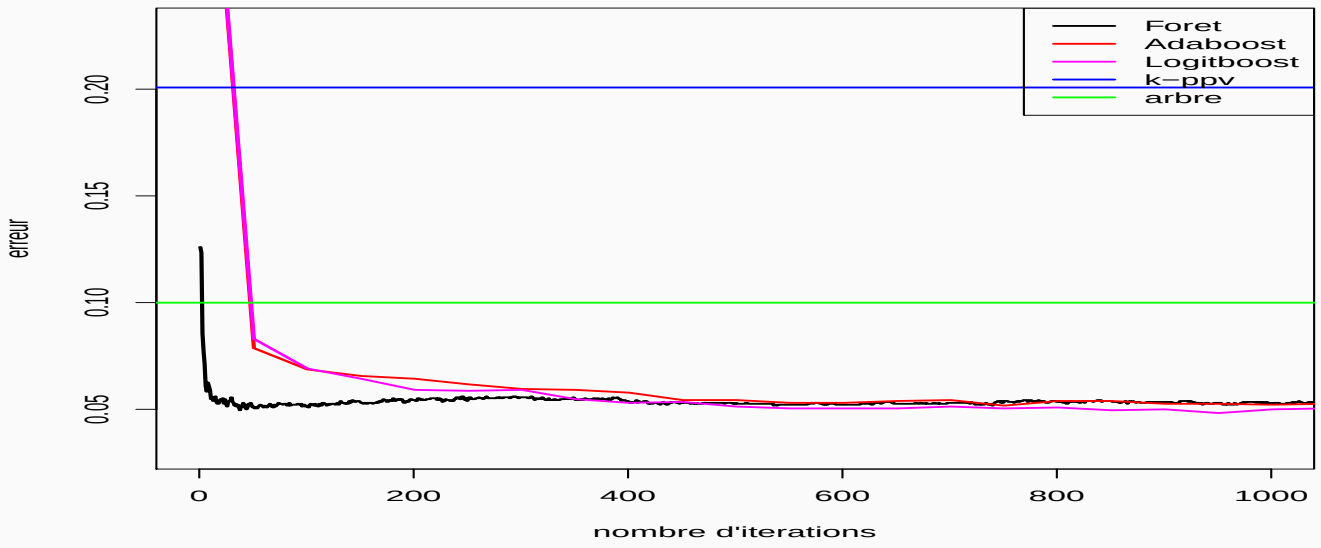
- We make a comparison between some statistical learning algorithms on the spam dataset.
- To do that, we split the data into a
  - a training set of size 2300 to fit and calibrate the models;
  - a test set of size 2301 to estimate misclassification error of each model

$$L_n(\hat{g}) = \frac{1}{n_{test}} \sum_{i \in \mathcal{D}_{test}} \mathbf{1}_{\hat{g}(X_i) \neq Y_i}.$$


Foret
Adaboost
Logitboost
k−ppv
arbre
erreur
0.05
0.10
0.15
0.20
0
200
400
600
800
1000
nombre d'iterations



Method	M. error
Random Forest	0.050
Adaboost	0.052
Logitboost	0.048
k-NN	0.200
Tree	0.100



Method	M. error
Random Forest	0.050
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k-NN	0.200
Tree	0.100

- Exercise 5-IML3

Outline

References i

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