Learning
Decision Trees

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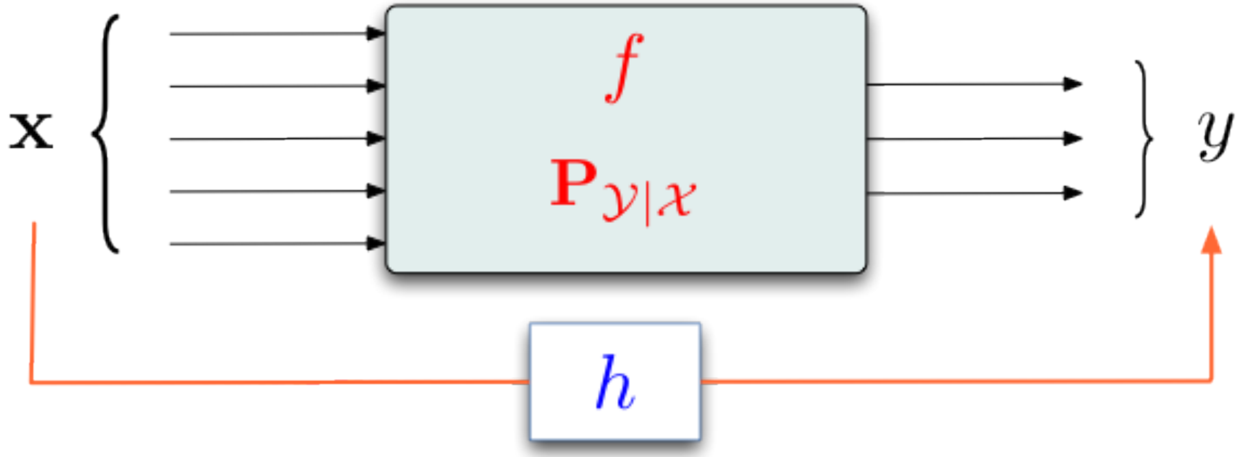
Apprentissage supervisé



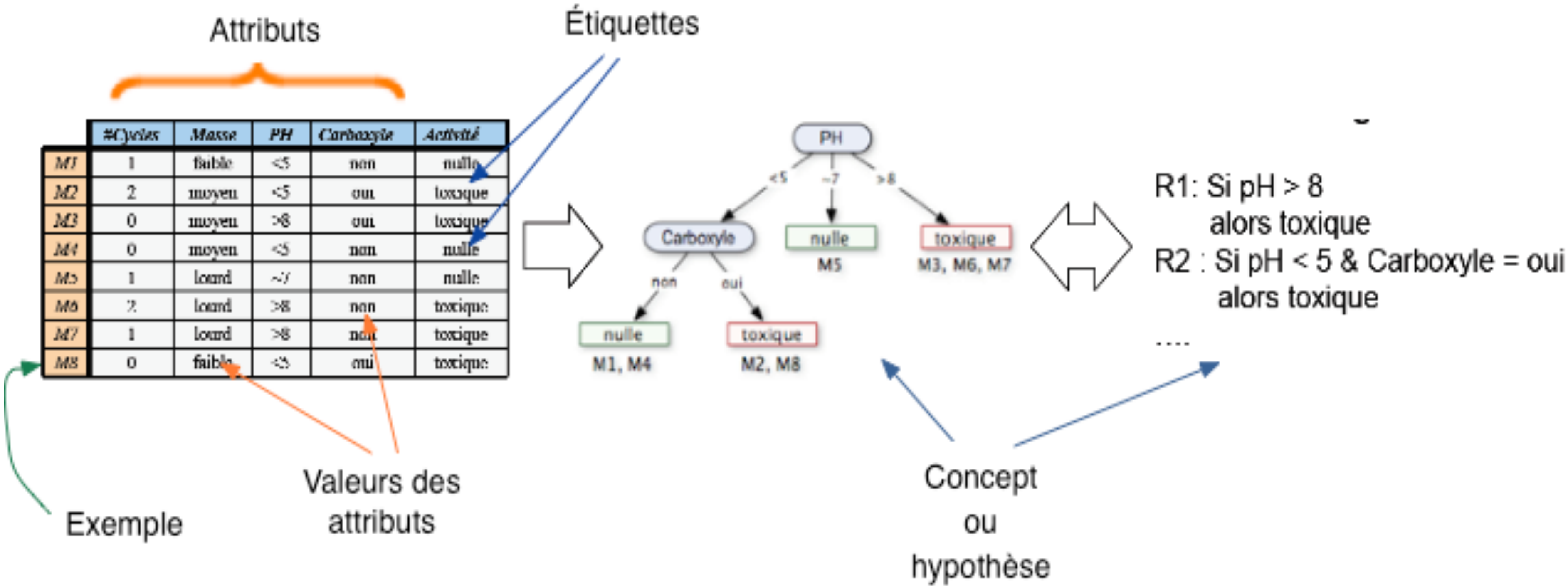
À partir :

- d'un échantillon d'apprentissage $S_m = \langle(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\rangle$
- de connaissances préalables sur le type de dépendances sur $\mathcal{X} \times \mathcal{Y}$

Trouver :

- une fonction h
- permettant la prédiction de y pour une nouvelle entrée x $h(\mathbf{x}) \approx y \ (= f(\mathbf{x}))$

Induction supervisée



	#Cycles	Masse	PH	Carboxyle	Activité
M1	1	faible	<5	non	nulle
M2	2	moyen	<5	oui	toxique
M3	0	moyen	>8	oui	toxique
M4	0	moyen	<5	non	nulle
M5	1	lourd	~7	non	nulle
M6	2	lourd	>8	non	toxique
M7	1	lourd	>8	non	toxique
M8	0	faible	<5	oui	toxique

Les données : organisation et types

Identifieur	Genre	Age	Niveau études	Marié ?	Nb enfants	Revenu	Profession	A prospecter ?
I_21	M	43	Bac+5	Oui	3	55 000	Architecte	OUI
I_34	M	25	Bac+2	Non	0	21 000	Infirmier	NON
I_38	F	34	Bac+8	Oui	2	35 000	Chercheuse	OUI
I_39	F	67	Bac	Oui	5	20 000	Retraitée	NON
I_58	F	56	CAP	Oui	4	27 000	Ouvrière	NON
I_73	M	40	Bac+3	Non	2	31 000	Commercial	OUI
I_81	F	51	Bac+5	Oui	3	75 000	Chef d'entreprise	OUI

Exemple
(*example, instance*)

Descripteur
Attribut
(*feature*)

Étiquette
(*label*)

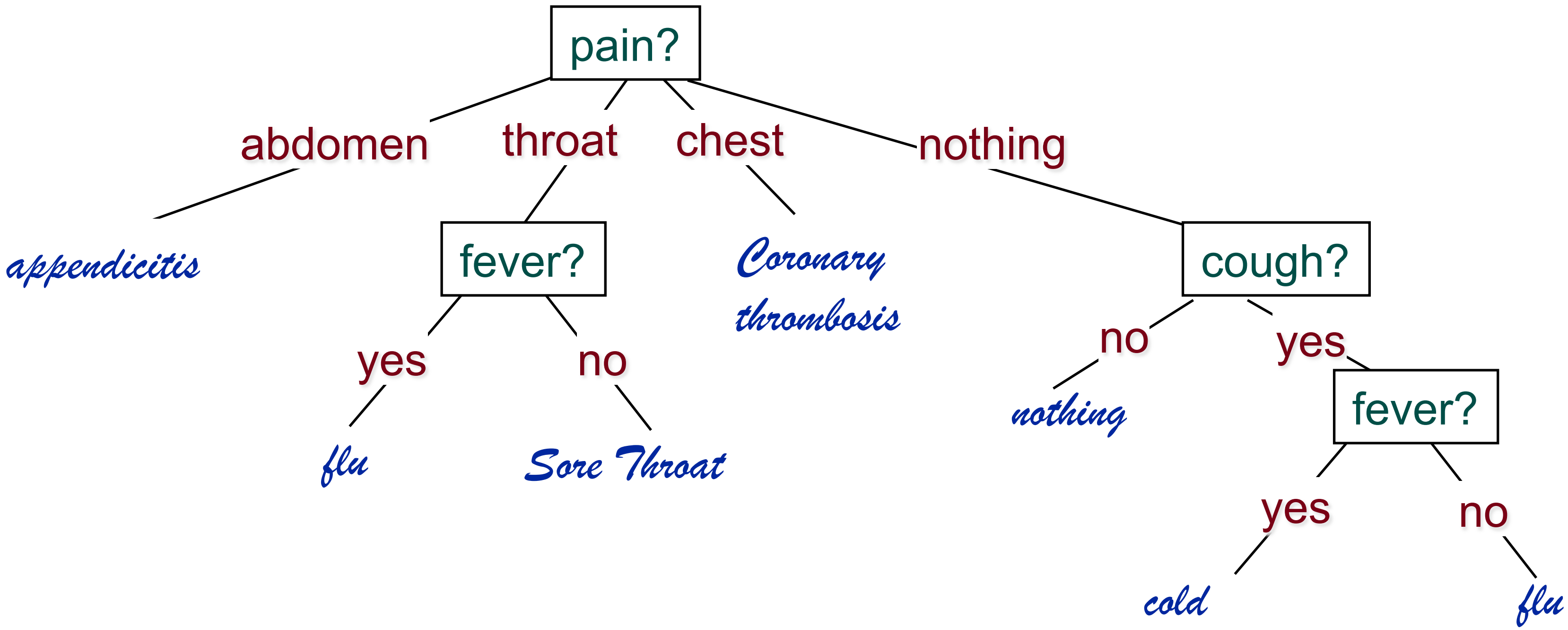
Outline

1. Decision trees
2. Learning decision trees
3. Pruning decision trees
4. Bias in decision trees and oblique trees
5. Regression trees

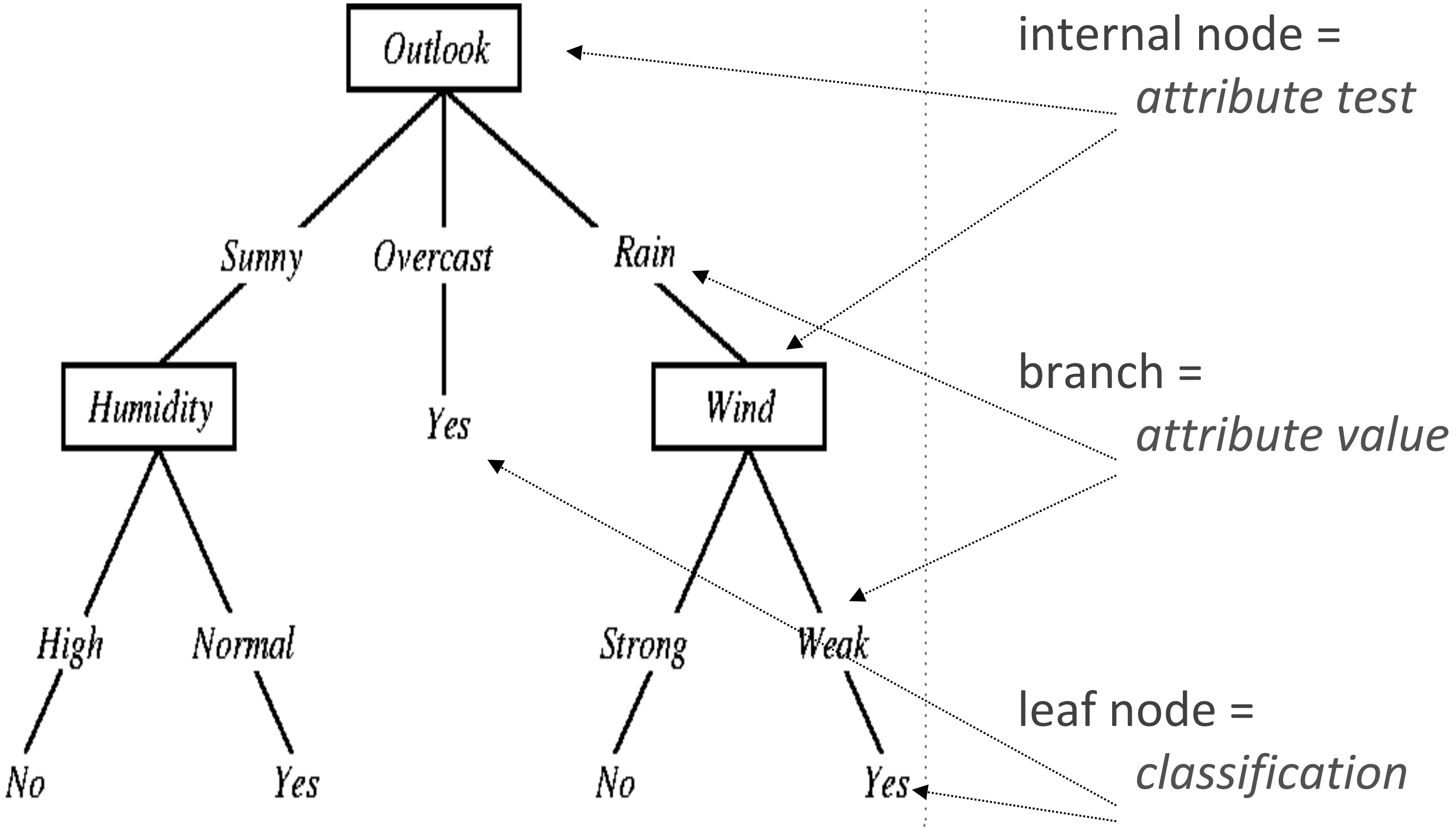
Decision trees

The structure of decision trees

- The internal nodes test attribute values
- A branch for each possible value of the tested attribute
- Leaves correspond to classes (labels)



Les arbres de décision : représentation



A Real Decision Tree

Decision Tree Trained on 1000 Patients:

```
+833+167 (tree) 0.8327 0.1673 0
fetal_presentation = 1: +822+116 (tree) 0.8759 0.1241 0
|   previous_csection = 0: +767+81 (tree) 0.904 0.096 0
|   |   primiparous = 0: +399+13 (tree) 0.9673 0.03269 0
|   |   primiparous = 1: +368+68 (tree) 0.8432 0.1568 0
|   |   |   fetal_distress = 0: +334+47 (tree) 0.8757 0.1243 0
|   |   |   |   birth_weight < 3349: +201+10.555 (tree) 0.9482 0.05176 0
|   |   |   |   birth_weight >= 3349: +133+36.445 (tree) 0.783 0.217 0
|   |   |   fetal_distress = 1: +34+21 (tree) 0.6161 0.3839 0
|   previous_csection = 1: +55+35 (tree) 0.6099 0.3901 0
fetal_presentation = 2: +3+29 (tree) 0.1061 0.8939 1
fetal_presentation = 3: +8+22 (tree) 0.2742 0.7258 1
```

Expressiveness of decision trees

- **Any boolean function** can be represented by a decision tree
  - Reminder: with 6 boolean attributes, there are $2^6 = 64$ possible examples, and there exists approximately $2 \,.\, 10^{19}$ boolean functions!!
- Some functions can require very large decision trees
  - E.g. The "parity" function and the "majority" function may require exponentially large trees
  - Other functions can be represented with one node
- Limited to **propositional logic**. No relational representation
- A tree corresponds to a disjunction of rules

DT =
(**if** feather = no **then** label = **not bird**)
or (**if** feather = yes & color = brown **then** label = **not bird**)
or (**if** feather = yes & color = B&W **then** label = **bird**)
or (**if** feather = yes & color = yellow **then** label = **bird**)

Arbre de décision : exemple

Détection du spam

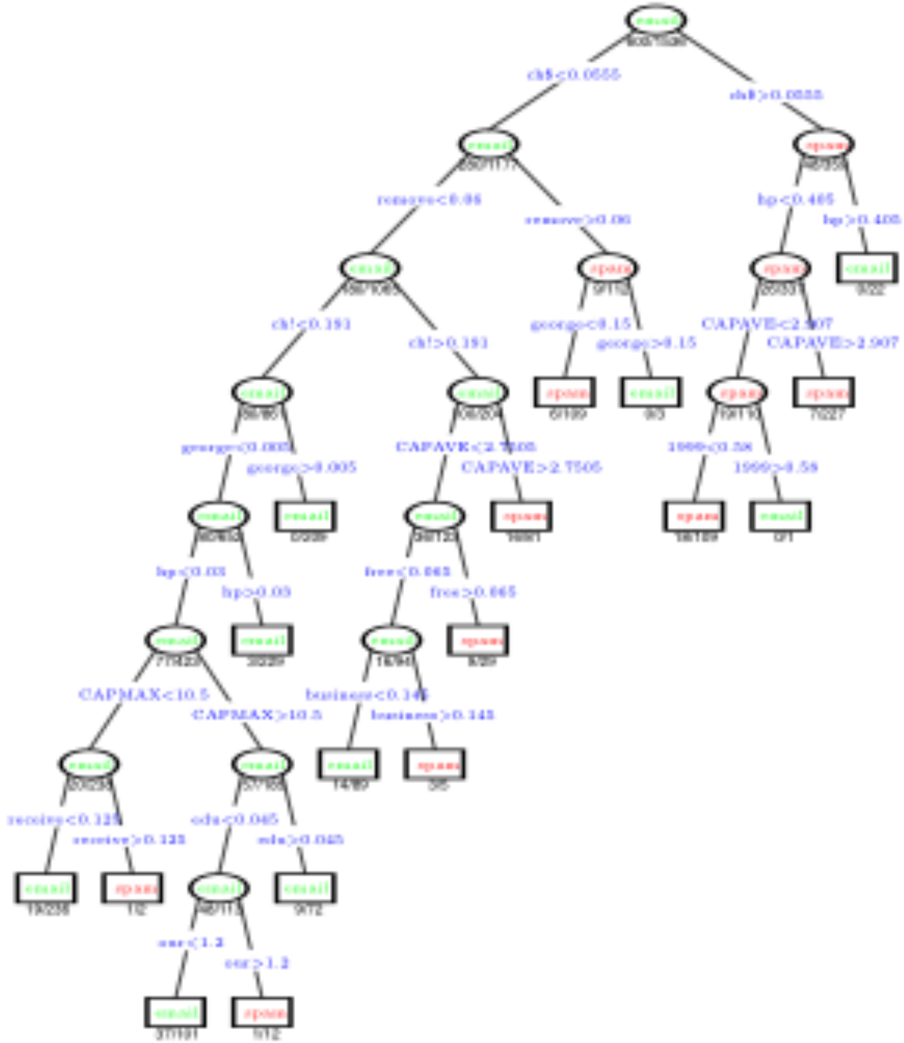
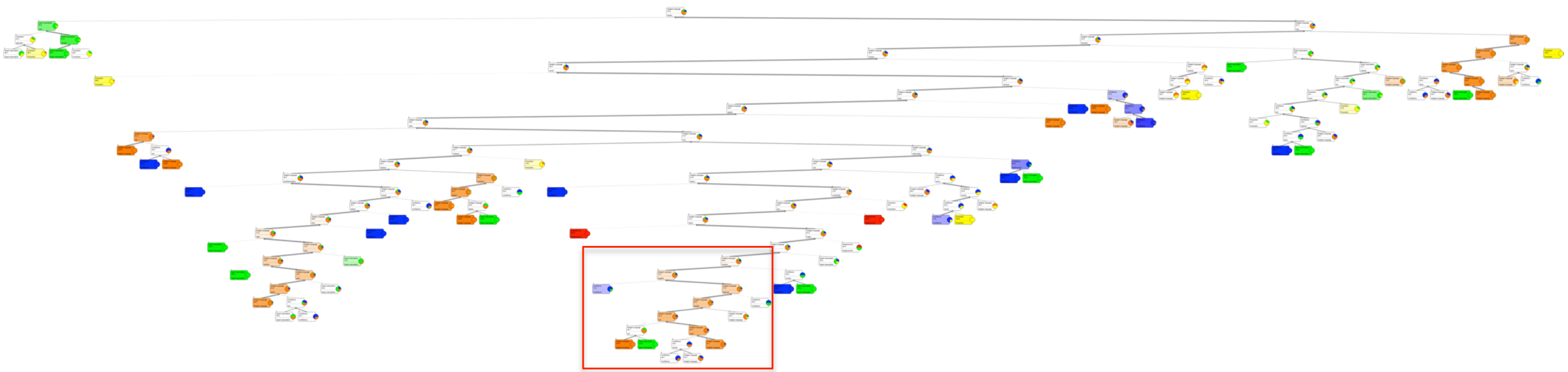
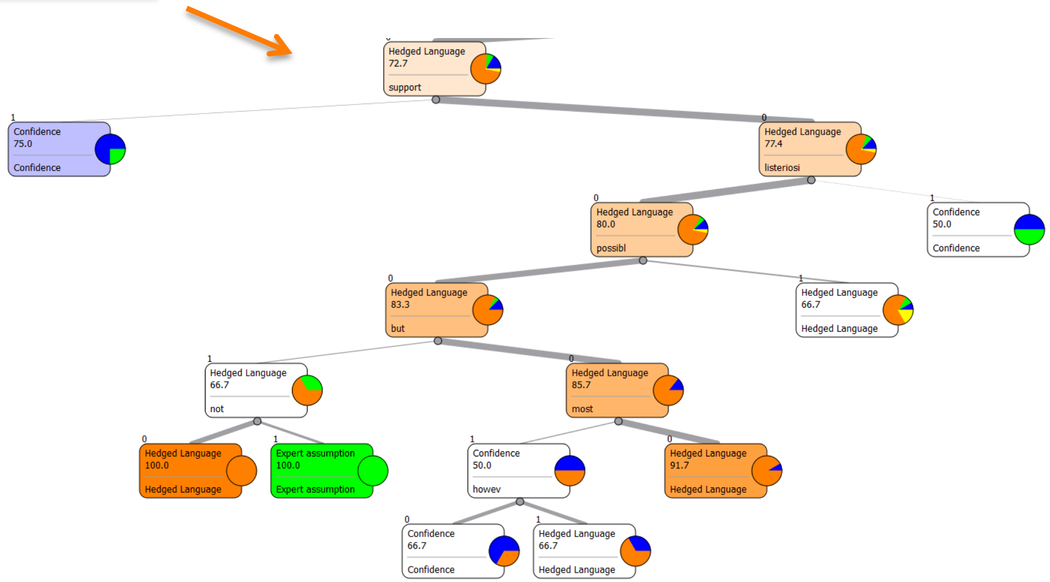


FIGURE 9.5. *The pruned tree for the* spam *example. The split variables are shown in blue on the branches, and the classification is shown in every node. The numbers under the terminal nodes indicate misclassification rates on the test data.*

Exemple : arbre de décision





Étude sur la différence d'appréciation des risques d'intoxication des deux côtés de l'Atlantique.

(ANR – Holyrisk (2010-2013))

On cherche à distinguer deux classes de textes

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Illustration

ID	color	root	sound	texture	umbilicus	surface	ripe
1	green	curly	muffled	clear	hollow	hard	true
2	dark	curly	dull	clear	hollow	hard	true
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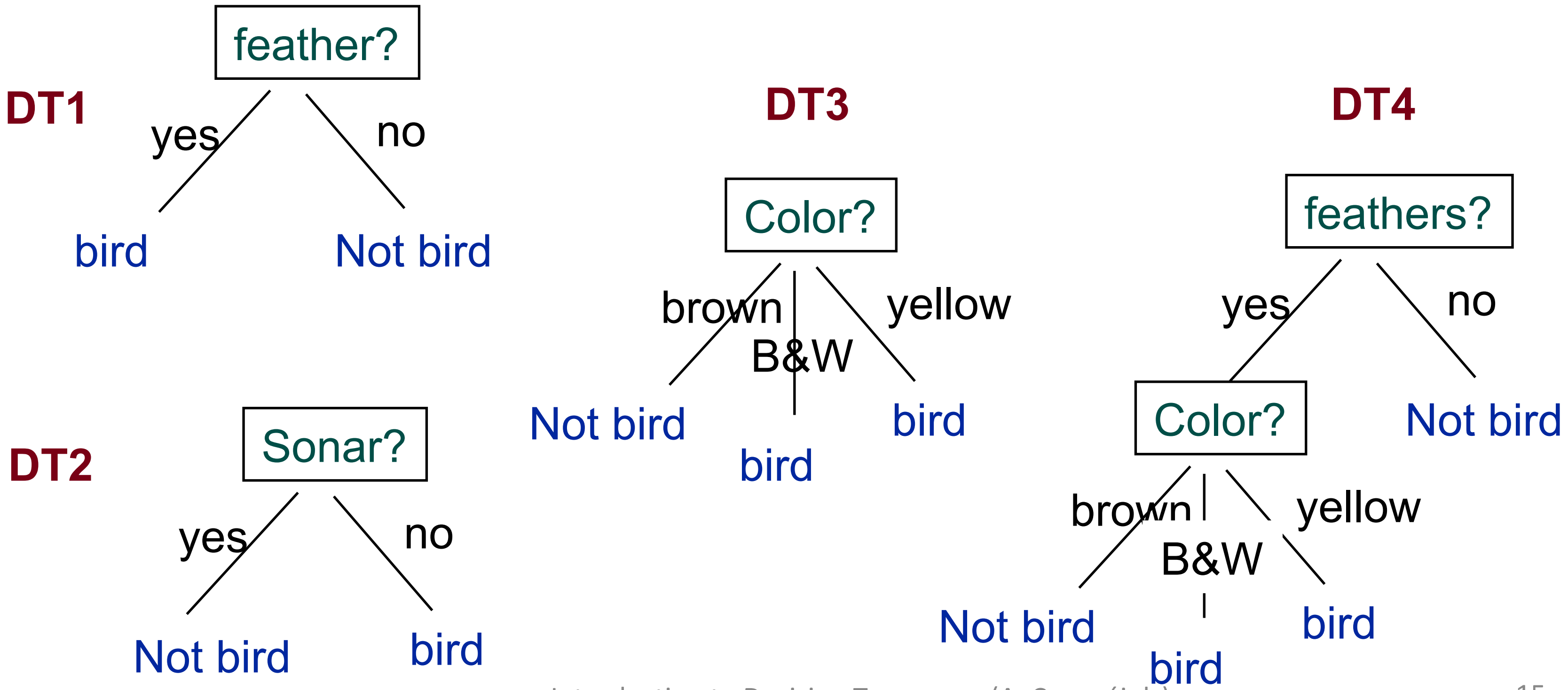
How to **learn** a decision tree?

...

Which tree to select from *H*?

	Color	Wings	Feathers	Sonar	**Concept**
x23	yellow	yes	yes	no	bird
x24	B&W	yes	yes	no	bird
x25	brown	yes	no	yes	Not bird

There exist **four trees** consistant with the data set



L’espace de recherche

- Toutes les séquences possibles de tous les tests (éventuellement répétés)

- Arbre de recherche GIGANTESQUE
  - Nombre de Catalan (n nœuds d’au plus deux descendants)

$$C_n = \frac{1}{n+1}\binom{2n}{n}$$

$n = 10$ => 16 796 arbres binaires

$n = 20$ => 6.56×10^9 arbres binaires

The search space

- Number of trees = Catalan's number

$$C_n = \frac{1}{n+1}\binom{2n}{n}$$

n attributes of
branching factor = 2

→ **Huge** search space!

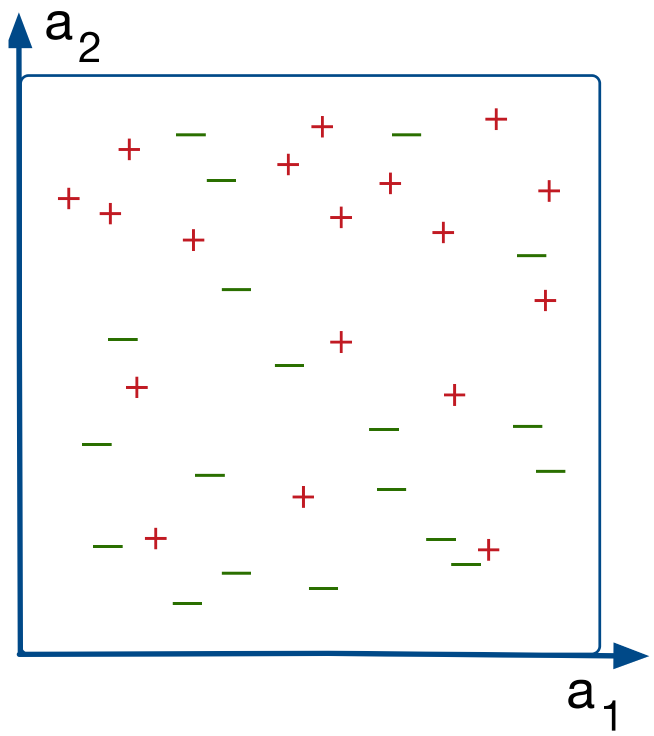
How to explore it?

A greedy iterative top-down strategy

- Principle

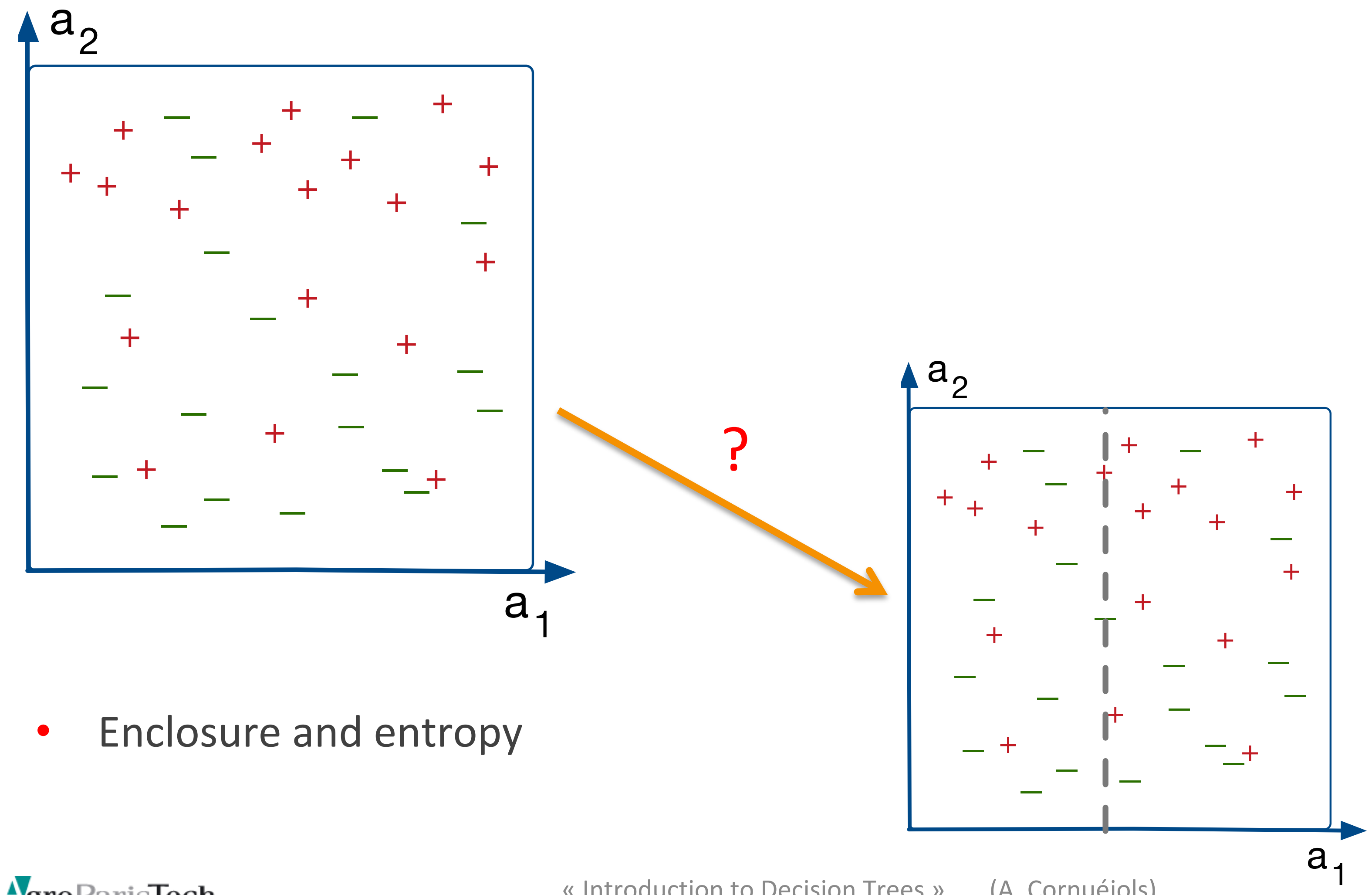
1. Select the **best attribute**
2. **Grow the tree** according to the choice
3. Now there are subsets of the data set at the leaves
4. Return to 1 **until stopping criterion**

How to chose the best separator?



- Enclosure and entropy

How to chose the best separator?



- Enclosure and entropy

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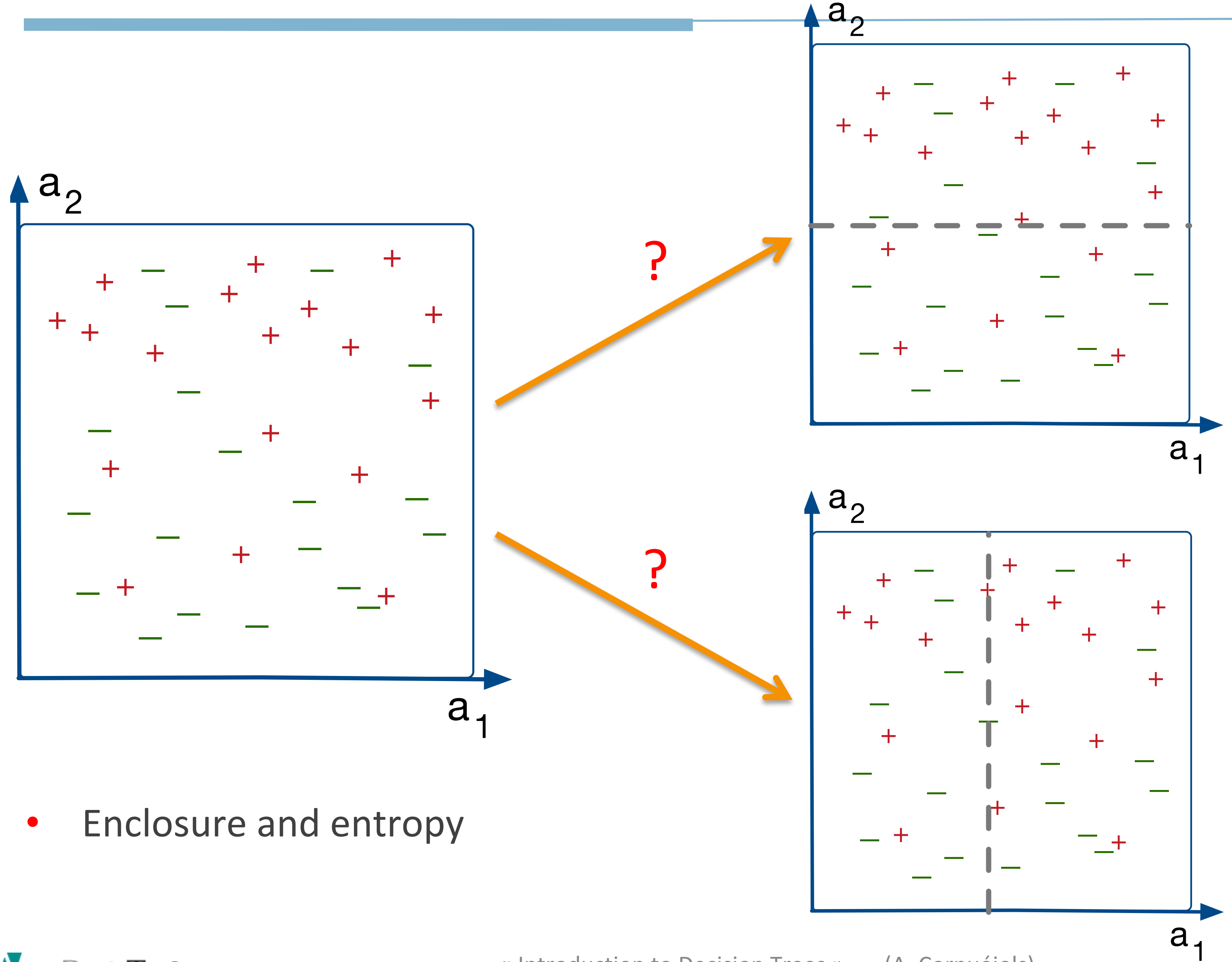


- Enclosure and entropy

Impurity measure: the entropy criterion

- Boltzmann entropy
- … used by Shannon
  - In 1949 Shannon proposed an entropy measure valid for discrete probability.
  - It expresses the quantity of information, that is the <u>number of bits</u> required to specify the distribution
  - The information entropy is:

$$\boxed{I = -\sum_{i=1..k} p_i \times \log_2(p_i)}$$

where p_i is the probability of class C_i.

Impurity measure: the entropy criterion

Information entropy of S (with C classes) :

$$I(S) = -\sum_{i=1}^{C} p(c_i) \cdot \log p(c_i)$$

$p(c_i)$: probability of the class c_i

- Zero if only one class
- Increasing as the classes are more equi-likely
- Equals $\log_2(k)$ when the k classes are equiprobables
- Unit: bit of information

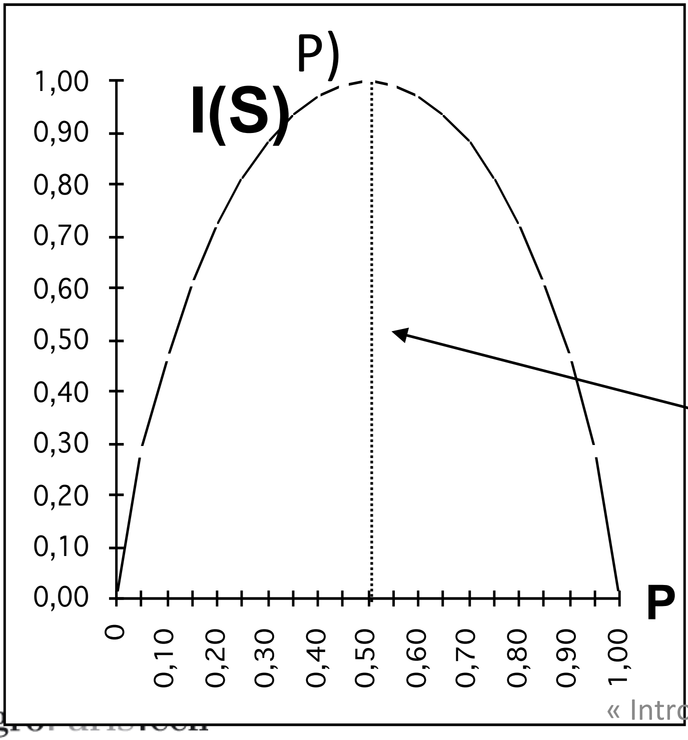
The entropy criterion for 2 classes

- For $C=2$: $I(S) = -p_+ \times \log_2(p_+) - p_- \times \log_2(p_-)$

  $p_+ = p/(p+n)$ and $p_- = n/(p+n)$

d'où $I(S) = -\frac{p}{(p+n)} \log\left(\frac{p}{(p+n)}\right) - \frac{n}{(p+n)} \log\left(\frac{n}{(p+n)}\right)$

and $I(S) = - P \log P - (1-P) \log(1-P)$



P=p/(p+n)=n/(n+p)=0.5
equiprobable

Entropy gain for one attribute

$$Gain(S, A) = I(S) - \sum_{v \in valeurs(A)} \frac{|S_v|}{|S|} \cdot I(S_v)$$

$|S_v|$: size of the sub-population in the branch *v* of *A*

Measures to what extent the knowledge of the value of attribute A
Brings information about the class of an example

Illustration

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$$\text{Ent}(D) = -\sum_{k=1}^{2} p_k \log_2 p_k = -\left(\frac{8}{17}\log_2\frac{8}{17} + \frac{9}{17}\log_2\frac{9}{17}\right) = 0.998$$

...

Illustration

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For the "color" attribute :

3 subsets D^1 `(color = green)`

D^2 `(color = dark)`

D^3 `(color = light)`

$$\mathrm{Ent}(D) = -\sum_{k=1}^{2} p_k \log_2 p_k = -\left(\frac{8}{17}\log_2\frac{8}{17} + \frac{9}{17}\log_2\frac{9}{17}\right) = 0.998$$

$$\mathrm{Ent}(D^1) = -\left(\frac{3}{6}\log_2\frac{3}{6} + \frac{3}{6}\log_2\frac{3}{6}\right) = 1.000$$

$$\mathrm{Ent}(D^2) = -\left(\frac{4}{6}\log_2\frac{4}{6} + \frac{2}{6}\log_2\frac{2}{6}\right) = 0.918$$

$$\mathrm{Ent}(D^3) = -\left(\frac{1}{5}\log_2\frac{1}{5} + \frac{4}{5}\log_2\frac{4}{5}\right) = 0.722$$

$$\begin{aligned}\mathrm{Gain}(D, \text{color}) &= \mathrm{Ent}(D) - \sum_{v=1}^{3}\frac{|D^v|}{|D|}\mathrm{Ent}(D^v)\\ &= 0.998 - \left(\frac{6}{17}\times 1.000 + \frac{6}{17}\times 0.918 + \frac{5}{17}\times 0.722\right)\\ &= 0.109.\end{aligned}$$

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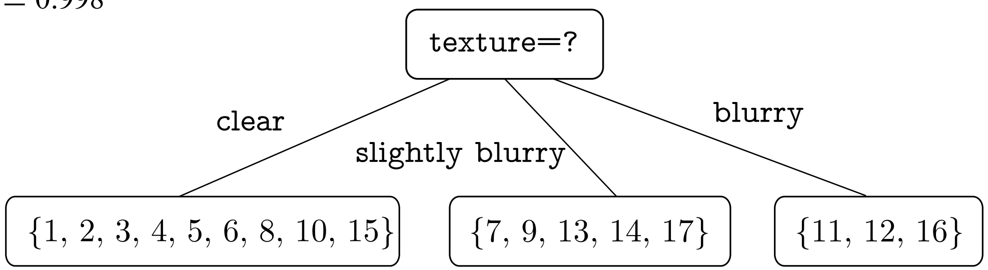
Information gain for the **other attributes**:

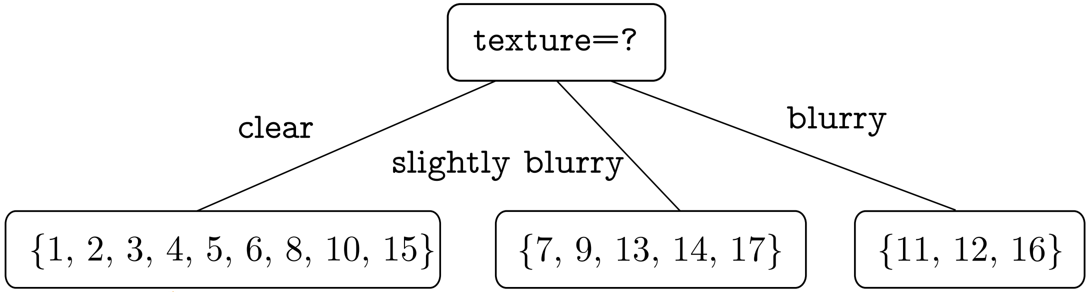
$\mathrm{Gain}(D, \mathrm{root}) = 0.143$; $\mathrm{Gain}(D, \mathrm{sound}) = 0.141$;
$\mathrm{Gain}(D, \mathrm{texture}) = 0.381$; $\mathrm{Gain}(D, \mathrm{umbilicus}) = 0.289$;
$\mathrm{Gain}(D, \mathrm{surface}) = 0.006$.

Texture is the best attribute

$$\mathrm{Ent}(D) = -\sum_{k=1}^{2} p_k \log_2 p_k = -\left(\frac{8}{17}\log_2\frac{8}{17} + \frac{9}{17}\log_2\frac{9}{17}\right) = 0.998$$



Illustration



$$D^1 = D^{\texttt{texture=clear}} = \{(1,+),(2,+),(3,+),(4,+),(5,+),(6,+),(8,-),(10,-),(15,-)\}$$

$\text{Gain}(D^1, \texttt{color}) = 0.043;$ $\quad$ $\text{Gain}(D^1, \texttt{root}) = 0.458;$

$\text{Gain}(D^1, \texttt{sound}) = 0.331;$ $\quad$ $\text{Gain}(D^1, \texttt{umbilicus}) = 0.458;$

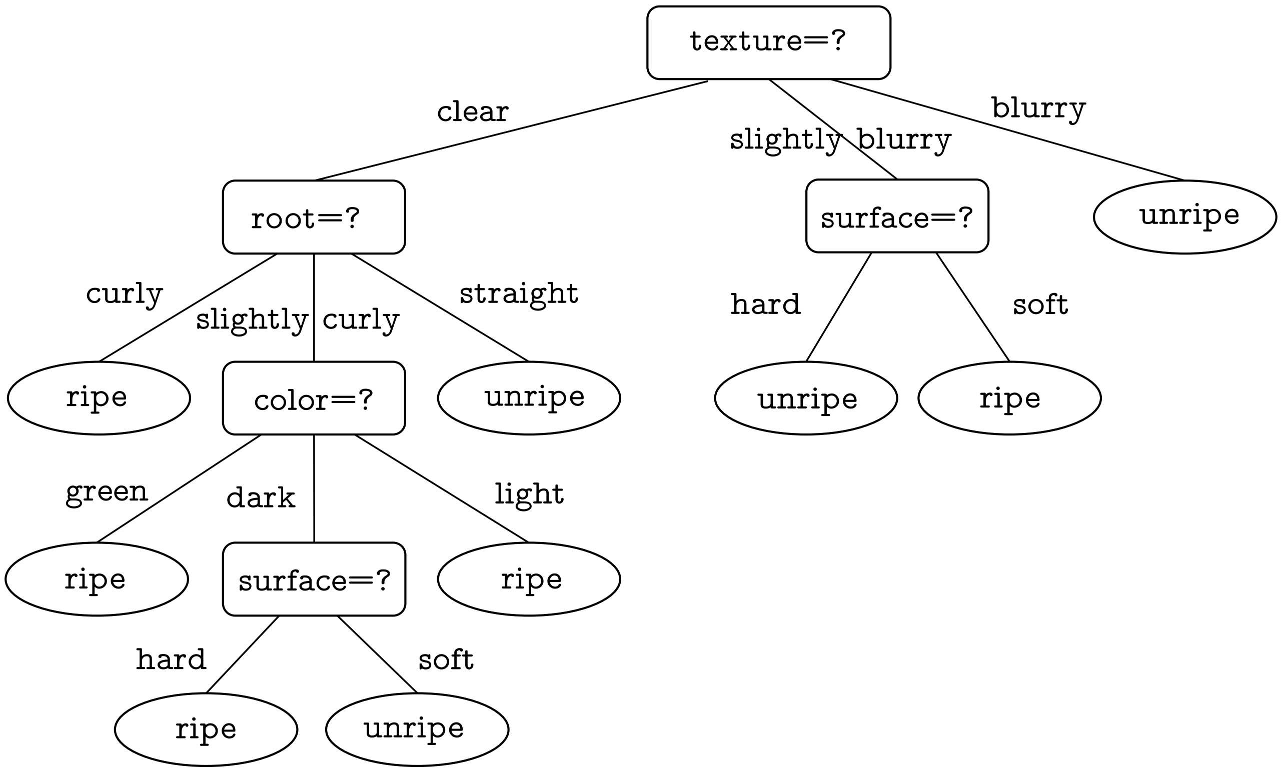
$\text{Gain}(D^1, \texttt{surface}) = 0.458.$

Root, surface and umbilicus are the best attributes

Any one of them can be chosen

…

Illustration



A possible final decision tree for the database

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Impurity measure: the Gini criterion

- Ideally:
  - The measure should be zero if the sub-populations are homogeneous (only one class)
  - The measure should be maximal if the classes are maximally mixed in the sub-populations

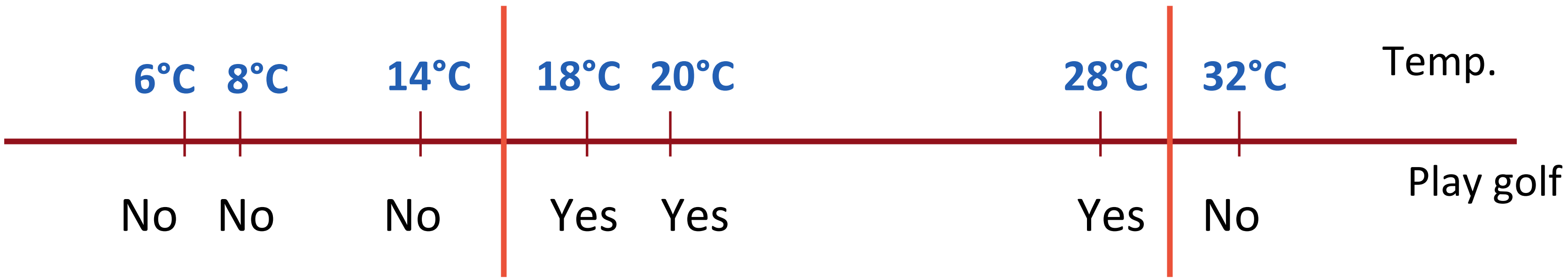
- Index Gini [Breiman et al.,84]

$$\boxed{Gini(D) = 1 - \sum_{j=1}^{k} (p_j)^2}$$

Some problems

And their solutions

Discretizing continuous attributes



Here, two candidate thresholds: 16°C and 30°C

The attribute $Temp_{>16°C}$ is the most informative, hence it is chosen

Different branching factors

- Problem:

  Entropy gain unduly favors the attributes with high branching factors

- Two solutions:
  - *Binarize all attributes*
    - *But the resulting tree lose interpretability*
  - *Introduce a normalizing factor to correct the bias*

$$Gain\_norm(S,A) = \frac{Gain(S,A)}{\sum_{i=1}^{nb\ valeurs\ de\ A} \frac{|S_i|}{|S|} \cdot \log \frac{|S_i|}{|S|}}$$

Missing values

- Given example $\langle\, x\,,\, c(x)\,\rangle$ with missing values for attribute A
- How can we compute $gain(S, A)$?

1. Take the **most frequent value** for A **in S**
2. Take the **most frequent value** for A in **the node**
3. Distribute the example into **fictive example**s with the possible values of A weighted by their respective frequencies

   - E.g. if 6 examples in this node take the value $A=a_1$ and 4 examples the value $A=a_2$
     $A(x) = a_1$ with prob=0.6 and $A(x) = a_2$ with prob=0.4
   - **When predicting**, give the label corresponding to the most likely leave

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1. Decision trees

2. Learning decision trees

3. **Pruning decision trees**

4. Bias in decision trees and oblique trees

5. Regression trees

Le problème de la généralisation

A-t-on appris un bon arbre de décision ?

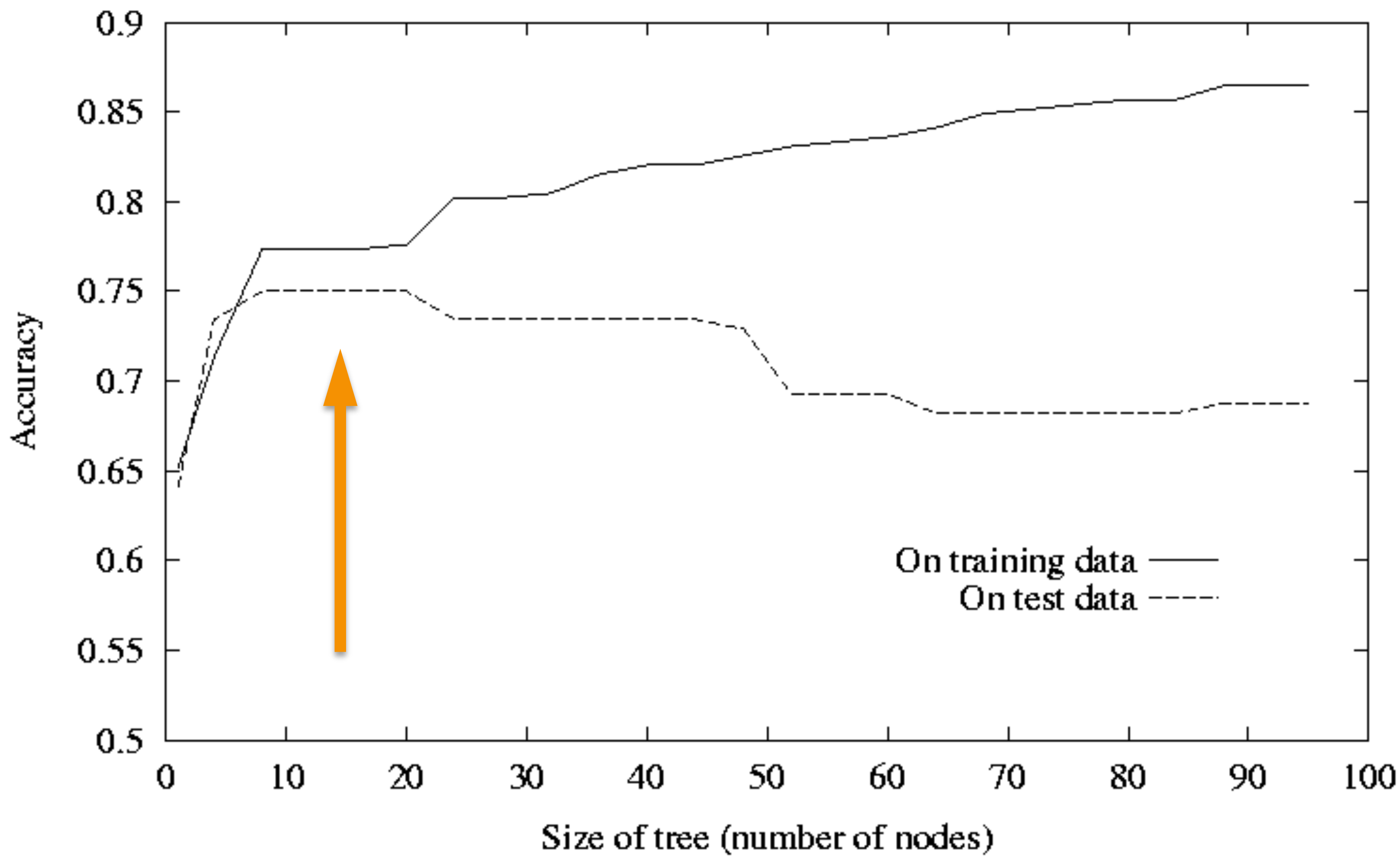
- Ensemble d'apprentissage. Ensemble test.
- Courbe d'apprentissage
- Méthodes d'évaluation de la généralisation
  - Sur un ensemble test
  - Validation croisée
  - "Leave-one-out"

Sur-apprentissage

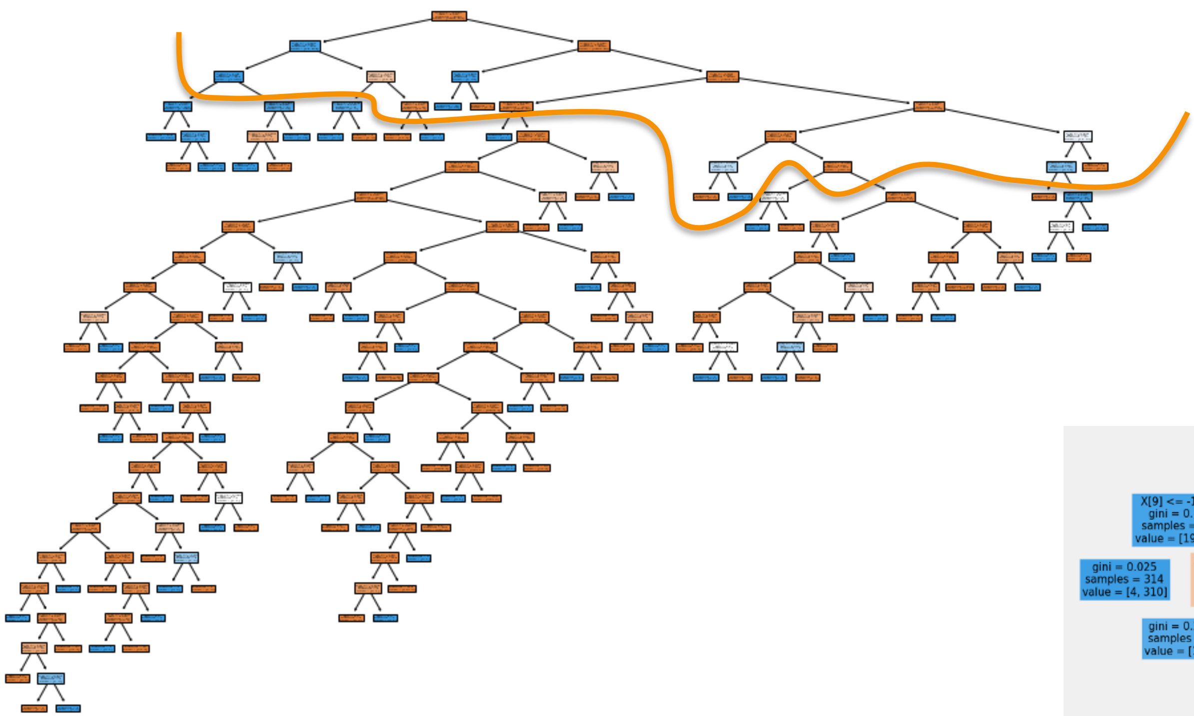
- Types de bruits
  - Erreurs de description
  - Erreurs de classification
  - “clashes”
  - valeurs manquantes

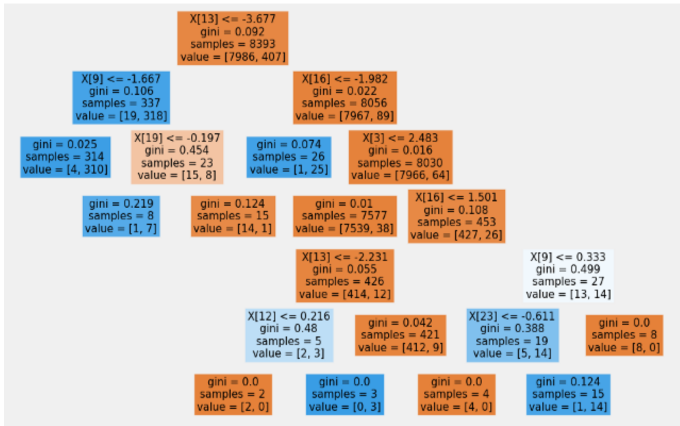
- Effet
  - **Arbre trop développé** : « touffus », trop profond

Overfitting



Overfitting in decision trees





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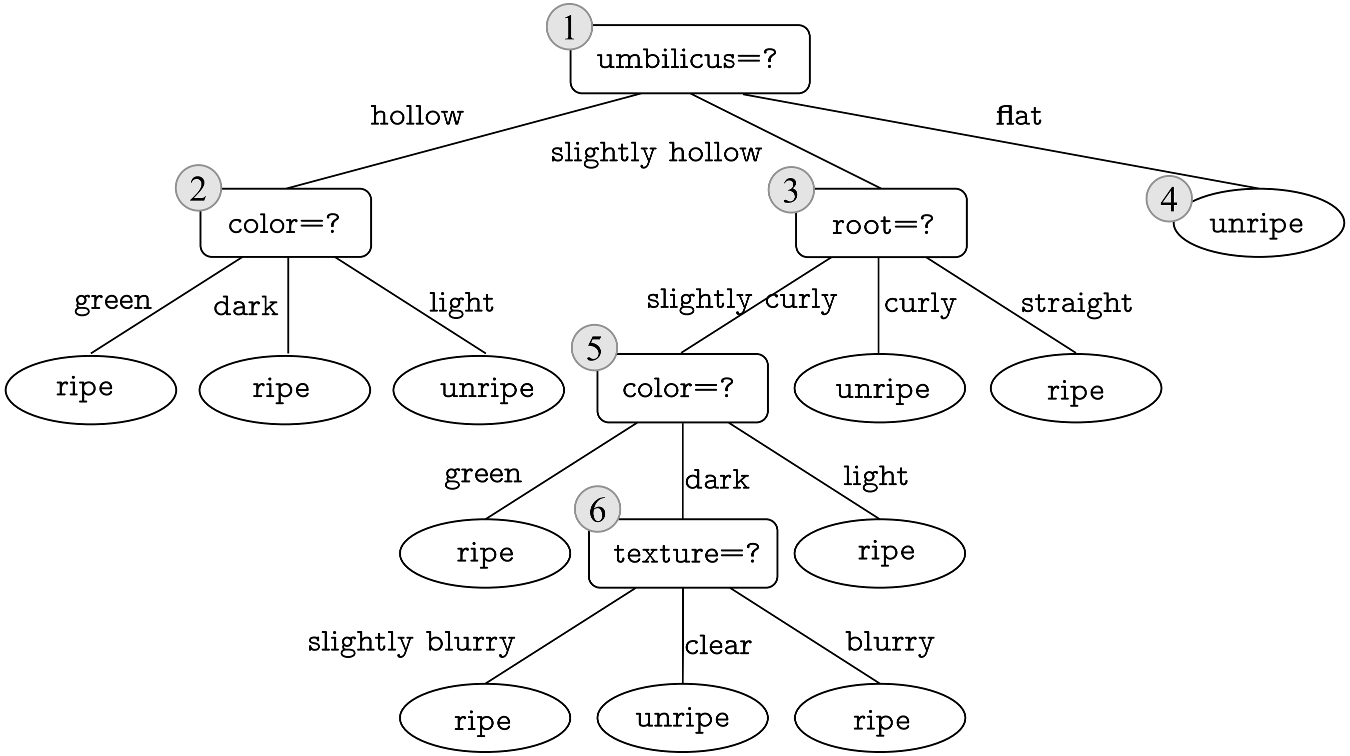
Pre and post pruning

- The unpruned decision tree



Pruning

- Splitting the watermelon data set into a training set and a validation set

Training set

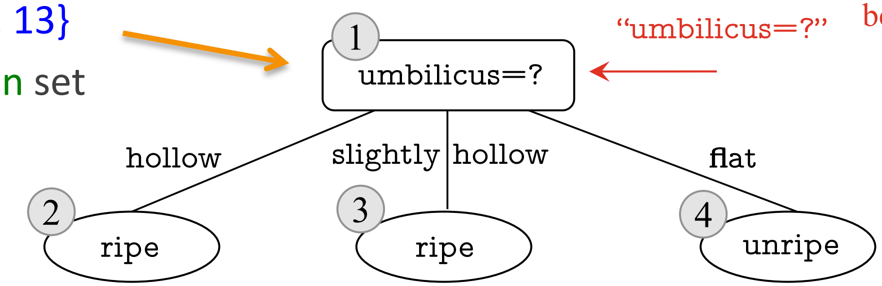
ID	color	root	sound	texture	umbilicus	surface	ripe
1	green	curly	muffled	clear	hollow	hard	true
2	dark	curly	dull	clear	hollow	hard	true
3	dark	curly	muffled	clear	hollow	hard	true
6	green	slightly curly	muffled	clear	slightly hollow	soft	true
7	dark	slightly curly	muffled	slightly blurry	slightly hollow	soft	true
10	green	straight	crisp	clear	flat	soft	false
14	light	slightly curly	dull	slightly blurry	hollow	hard	false
15	dark	slightly curly	muffled	clear	slightly hollow	soft	false
16	light	curly	muffled	blurry	flat	hard	false
17	green	curly	dull	slightly blurry	slightly hollow	hard	false

Validation set

ID	color	root	sound	texture	umbilicus	surface	ripe
4	green	curly	dull	clear	hollow	hard	true
5	light	curly	muffled	clear	hollow	hard	true
8	dark	slightly curly	muffled	clear	slightly hollow	hard	true
9	dark	slightly curly	dull	slightly blurry	slightly hollow	hard	false
11	light	straight	crisp	blurry	flat	hard	false
12	light	curly	muffled	blurry	flat	soft	false
13	green	slightly curly	muffled	slightly blurry	hollow	hard	false

Pre-pruning

{4, 5, 8, 9, 11, 12, 13}
from the validation set



validation accuracy
before splitting: 42.9%

Here, “umbilicus” should be chosen to split the the training set into 3 branches

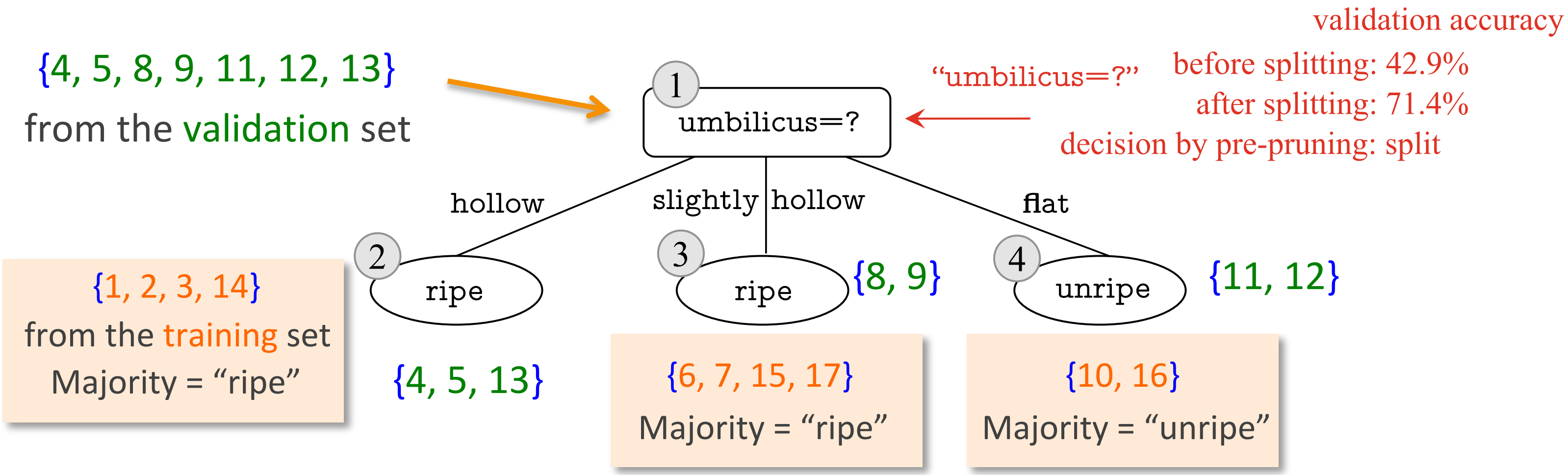
Should we do it?

Comparing the **validation** accuracy before splitting and after gives:

- **Before**: majority class “ripe” (decided on the training set) => {4, 5, 8} well-classified and {9, 11, 12, 13} missclassified on the validation set

$$\frac{3}{7} \times 100 \approx 42.9\%$$

Pre-pruning



The validation accuracy after splitting gives:

{(4, ripe), (5, ripe), (8, ripe), (9, unripe), (11, unripe), (12, unripe), (13, unripe)}

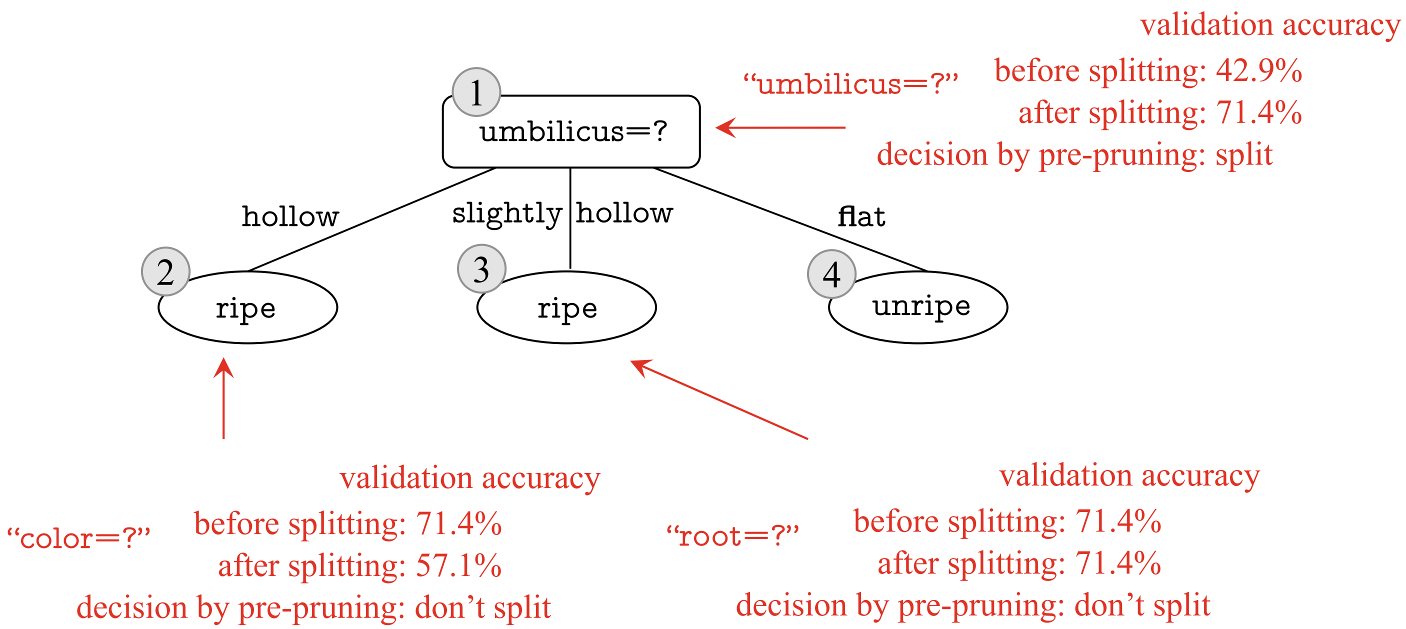
- **After**: => {4, 5, 8, 11, 12} well-classified and {9, 13} missclassified on the validation set

$$\frac{5}{7} \times 100 \approx 71.4\% \; > \; 42.9\%$$

Splitting improves the validation accuracy

Pre-pruning

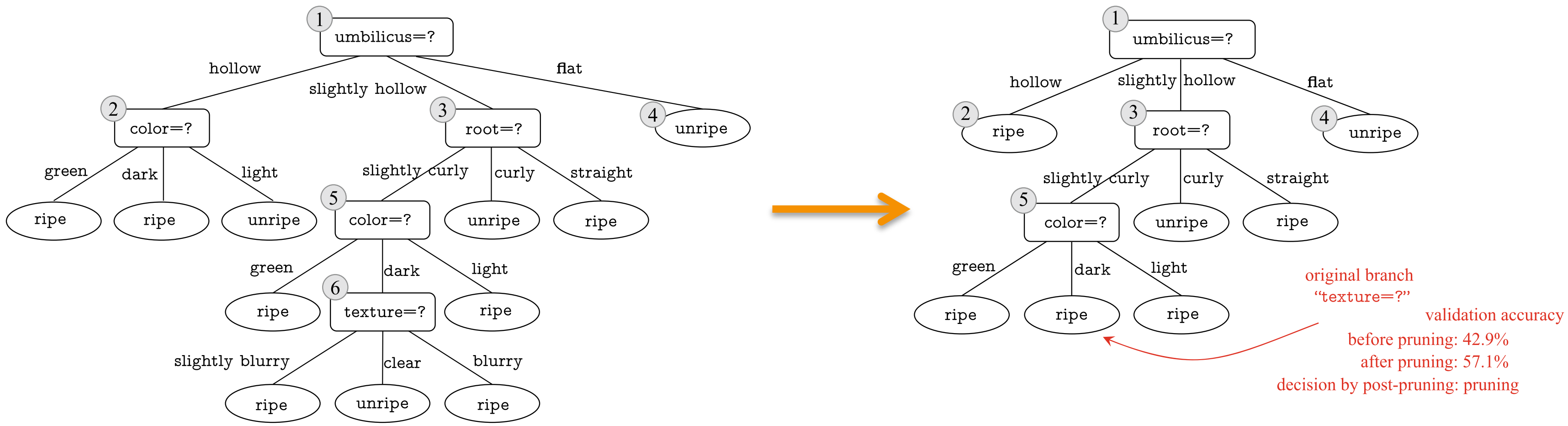
The **pre-pruned** decision tree



Here, gives a "decision stump": only one splitting node

Post-pruning

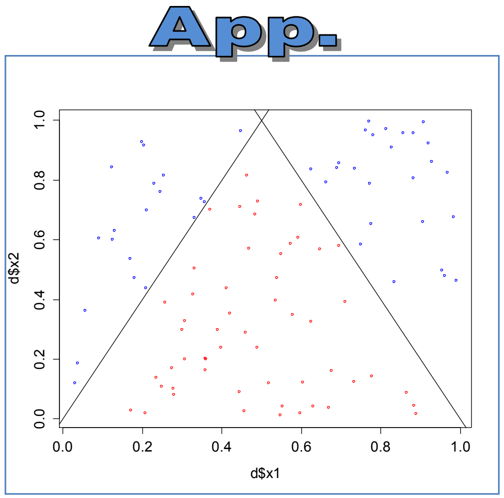
- Post-pruning allows a decision tree to **grow into a complete tree** (here, validation accuracy = 42.9%)
- And then examines the splitting nodes **starting from the deepest ones** (here node 6)
  - If the subtree led by node (6) is pruned, then it includes {7, 15} and the majority class is set to "ripe"
  - The validation accuracy increases to 57.1% and pruning is performed

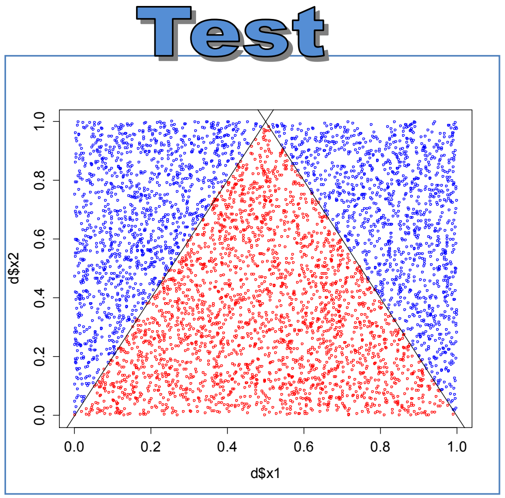


Outline

1. Decision trees
2. Learning decision trees
3. Pruning decision trees
4. Bias in decision trees and oblique trees
5. Regression trees

Arbre de décision





Y = « bleu »

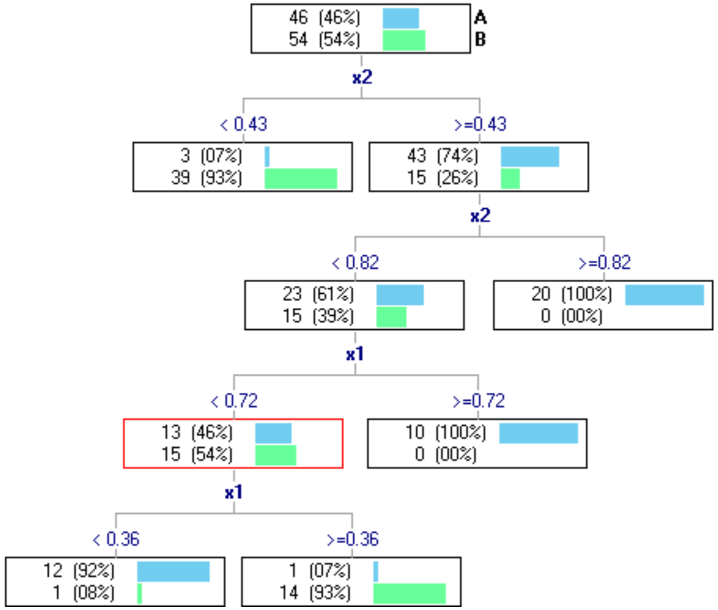
si (1) x2 > 2 * x1 pour x1 < 0.5

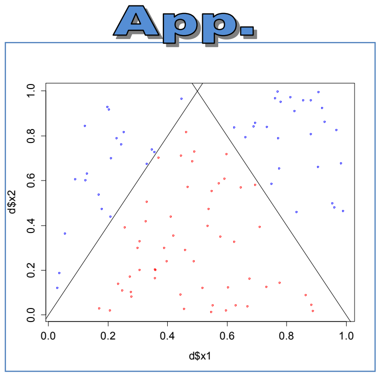
ou (2) x2 > (2 – 2 * x1) pour x1 ≥ 0.5

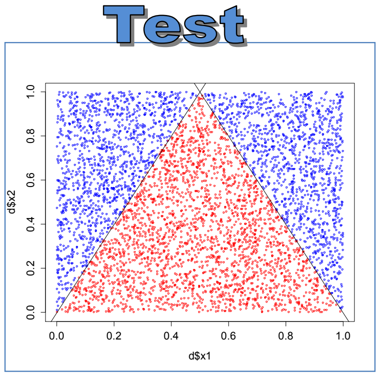
« rouge » autrement

...

Arbre de décision







Y = « bleu »

si (1) x2 > 2 * x1 pour x1 < 0.5

ou (2) x2 > (2 – 2 * x1) pour x1 ≥ 0.5

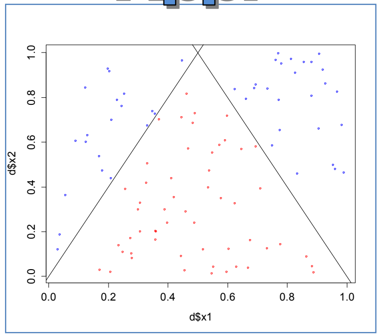
« rouge » autrement

Arbre profond : biais faible, variance forte

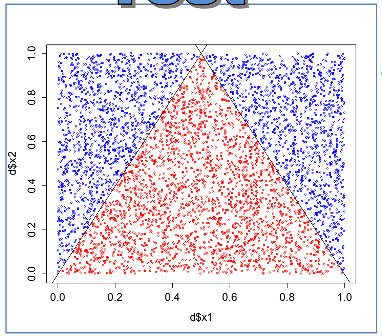
Arbre court : biais fort, variance faible

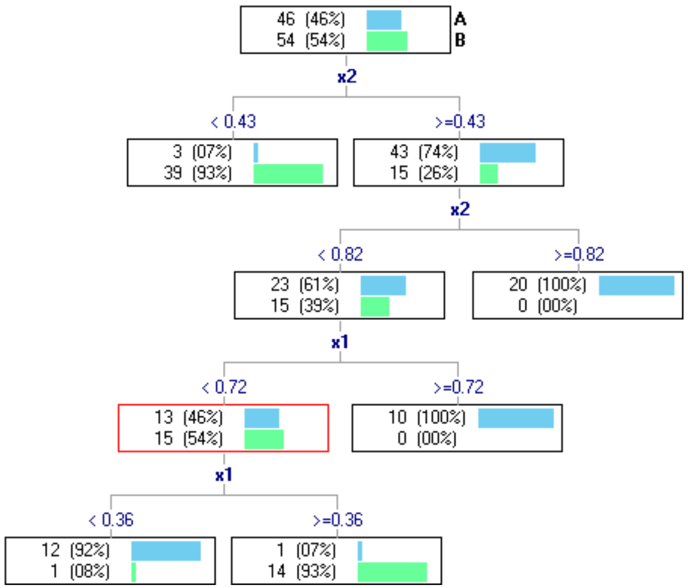
- toto

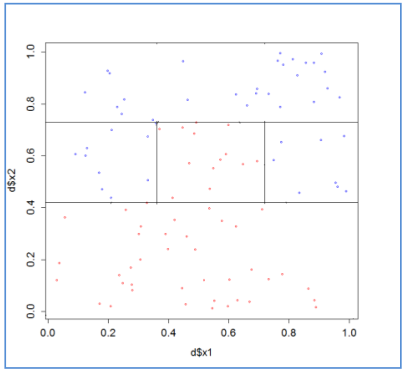
App.



Test

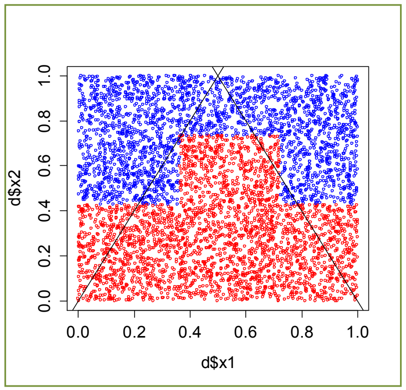






TRAIN

(5 feuilles dans l'arbre = 5 zones sont définies)



TEST

ε = 0.1632

Arbre profond : biais faible, variance forte

Arbre court : biais fort, variance faible

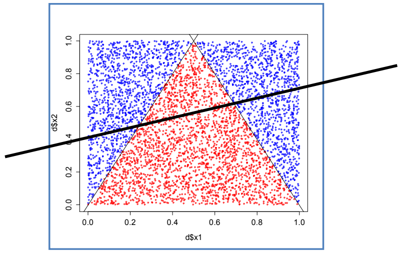
- toto

Composantes de l’erreur

L’erreur résulte de deux composantes

Biais

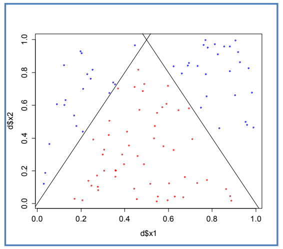
Traduit l’incapacité du modèle à traduire le concept (la « vraie » fonction) reliant Y aux X.



Un classifieur linéaire ne peut pas fonctionner ici. Impossible de trouver une droite permettant de séparer les points bleus des rouges.

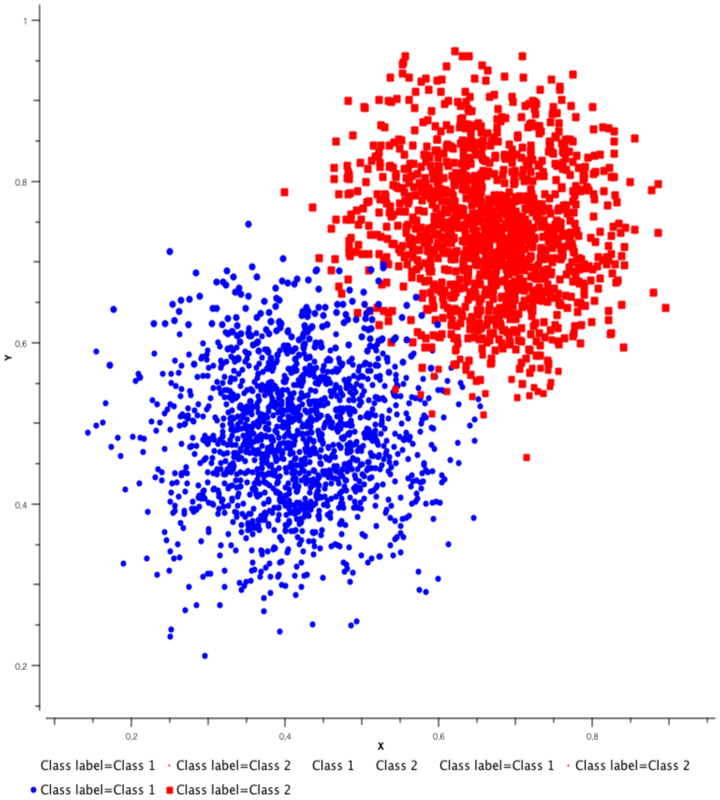
Variance

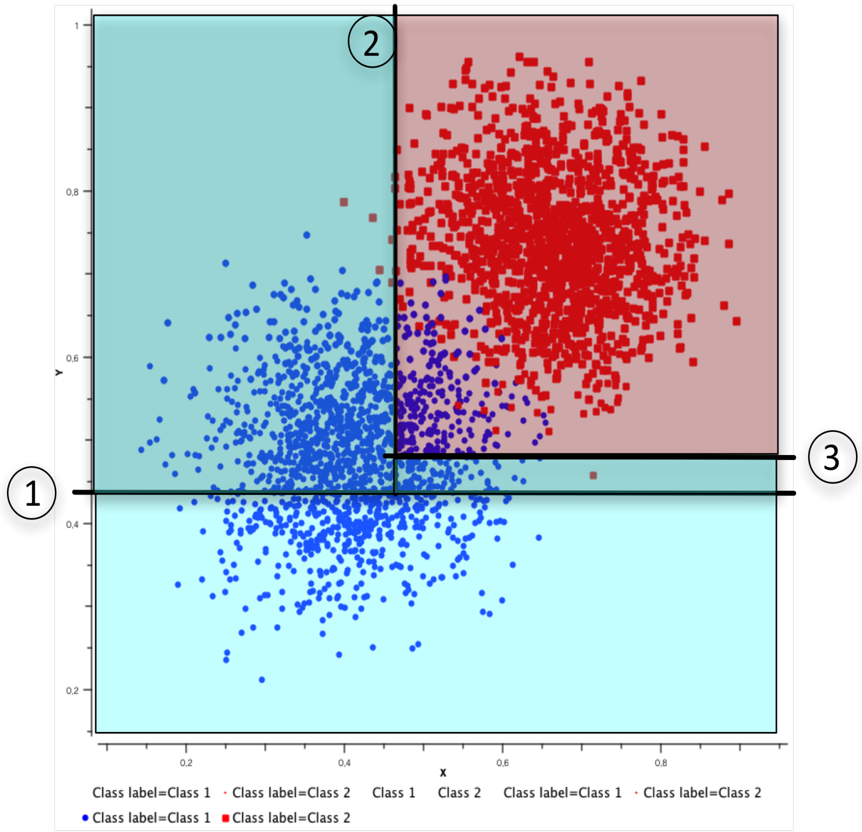
Sensibilité (variabilité par rapport) aux fluctuations d’échantillonnage.



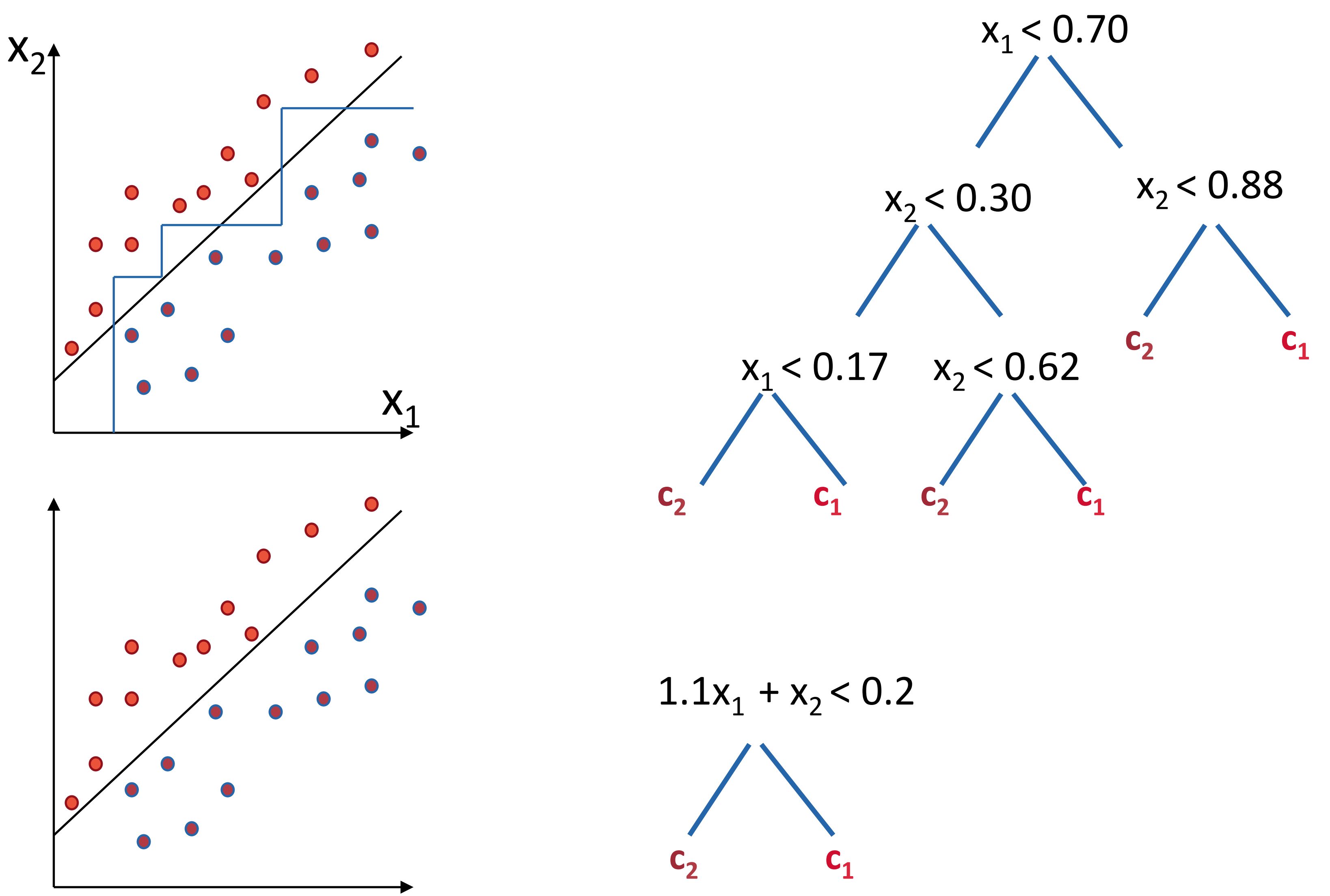
Le faible effectif de l’échantillon d’apprentissage ne permet pas de trouver avec exactitude les « bonnes » frontières.

Oblique trees



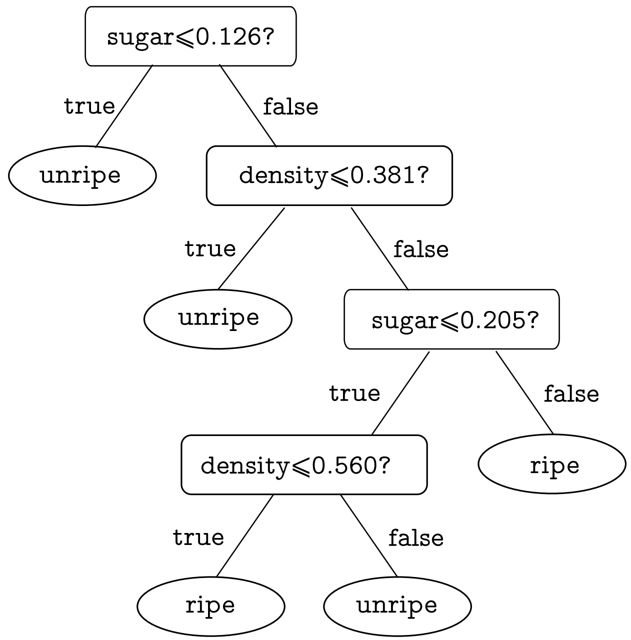


Oblique trees



Oblique decision trees

ID	density	sugar	ripe
1	0.697	0.460	true
2	0.774	0.376	true
3	0.634	0.264	true
4	0.608	0.318	true
5	0.556	0.215	true
6	0.403	0.237	true
7	0.481	0.149	true
8	0.437	0.211	true
9	0.666	0.091	false
10	0.243	0.267	false
11	0.245	0.057	false
12	0.343	0.099	false
13	0.639	0.161	false
14	0.657	0.198	false
15	0.360	0.370	false
16	0.593	0.042	false
17	0.719	0.103	false



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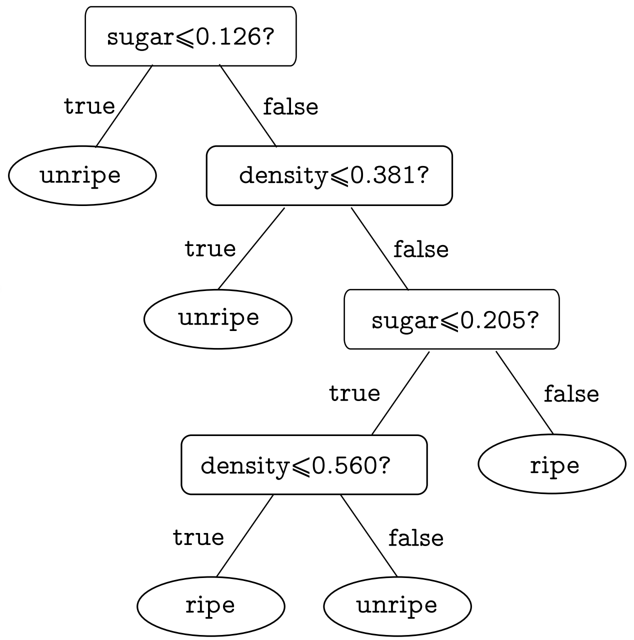

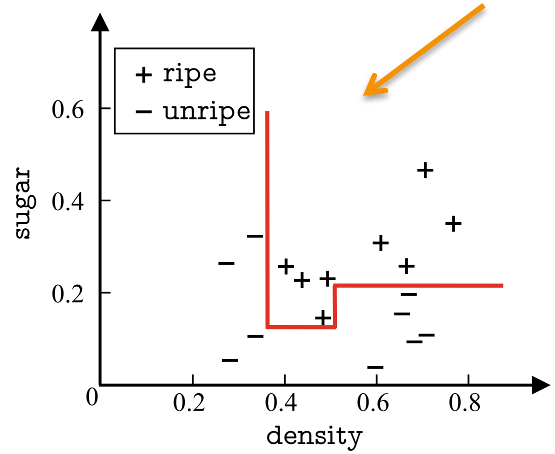

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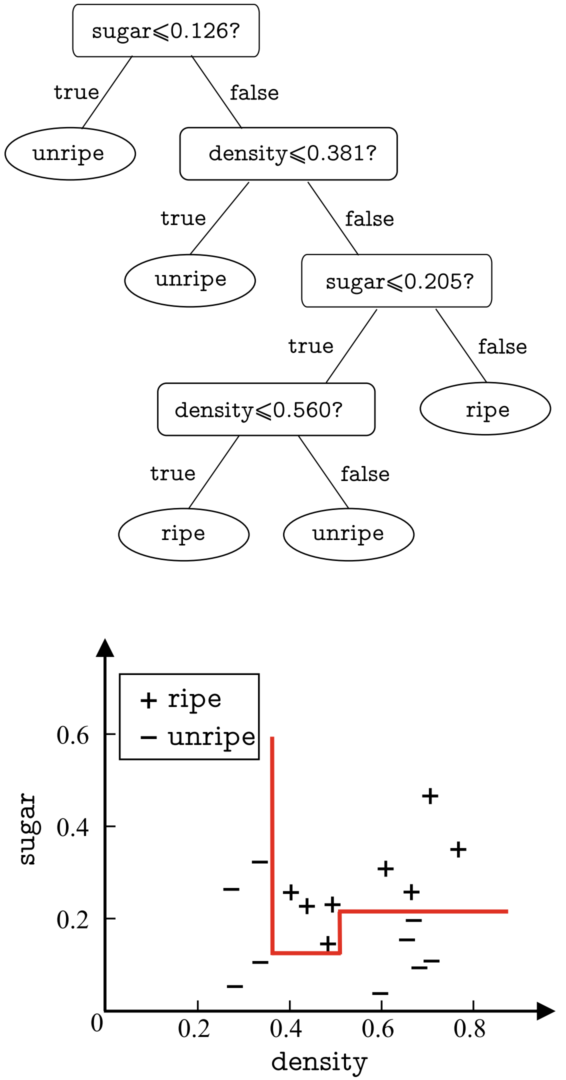
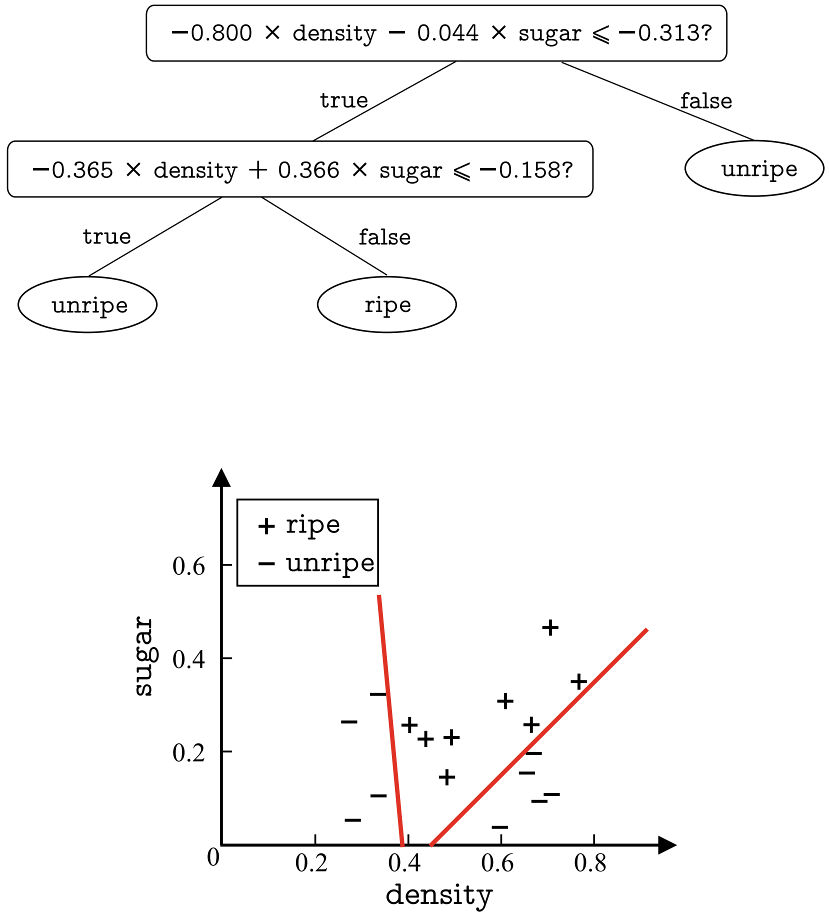
Oblique decision trees





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Bilan sur les arbres de décision

1. Avantages
   - **Interprétables**
     - Sélection automatique de variables « pertinentes »
     - Les branches des arbres peuvent se lire comme des règles
   - Non paramétrique
     - Traitement indifférencié des différents types de variables prédictives
     - Robuste face aux données aberrantes
     - Solutions pour traiter les données manquantes
   - Complexité calculatoire faible

2. Inconvénients
   - Problèmes de **stabilité** sur les petites bases de données
     (feuilles à très petits effectifs)
   - Méthode **gloutonne** et **myope**
     (pb pour identifier des interactions entre variables (e.g. le XOR)

Outline

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Limites des méthodes classiques de régression

- *Y* comme fonction linéaire d'une variable à valeur réelle

$$Y \;=\; \beta_0 \,+\, \beta_1\, X \,+ \varepsilon$$

- Régression multiple : Y fonction linéaire d'un ensemble de variables indépendantes $\mathbf{Y} \;=\; \beta_0 \,+\, \beta_1\, \mathbf{X} \,+ \varepsilon$

- Régression non linéaire $\mathbf{Y} \;=\; \beta_0 \,+\, \beta_1\, \mathbf{X} \,+\, \beta_2\, \mathbf{X}\mathbf{X}^\top \,+\, \varepsilon$

Immensité de l'espace de recherche si on cherche à prendre en compte toutes les combinaisons des attributs

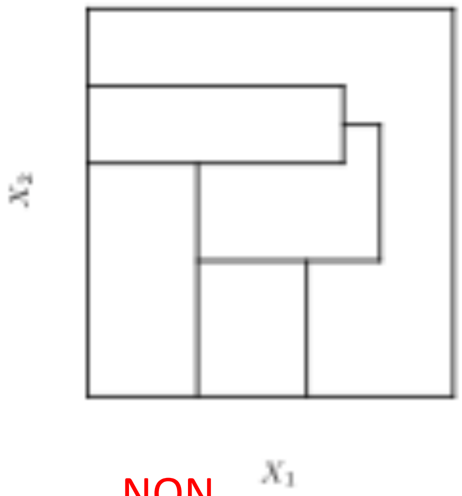
Régression linéaire vs. arbres de régression

- **Modèle global** défini sur l'ensemble de l'espace de description

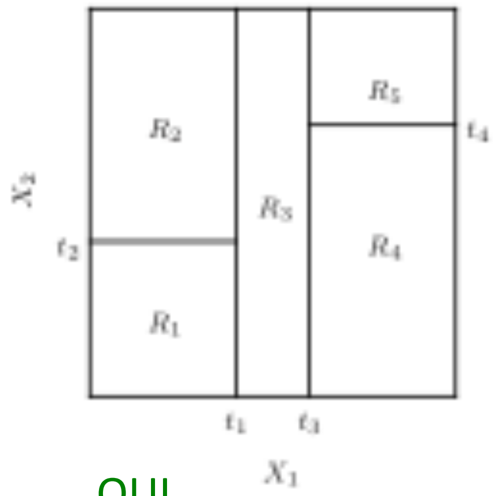
- Partition de l'espace avec des **modèles locaux**

Arbres de décision : quels concepts ?

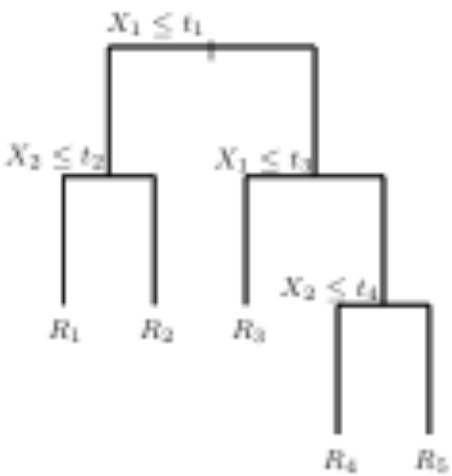
Domaine continu

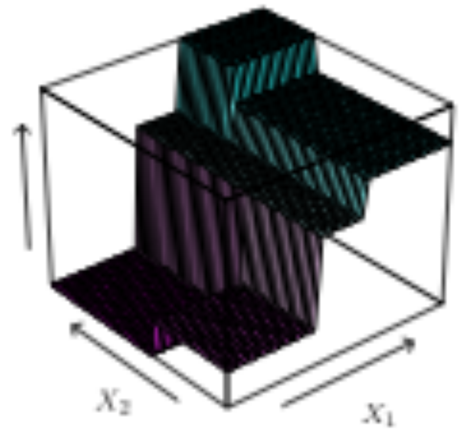


NON

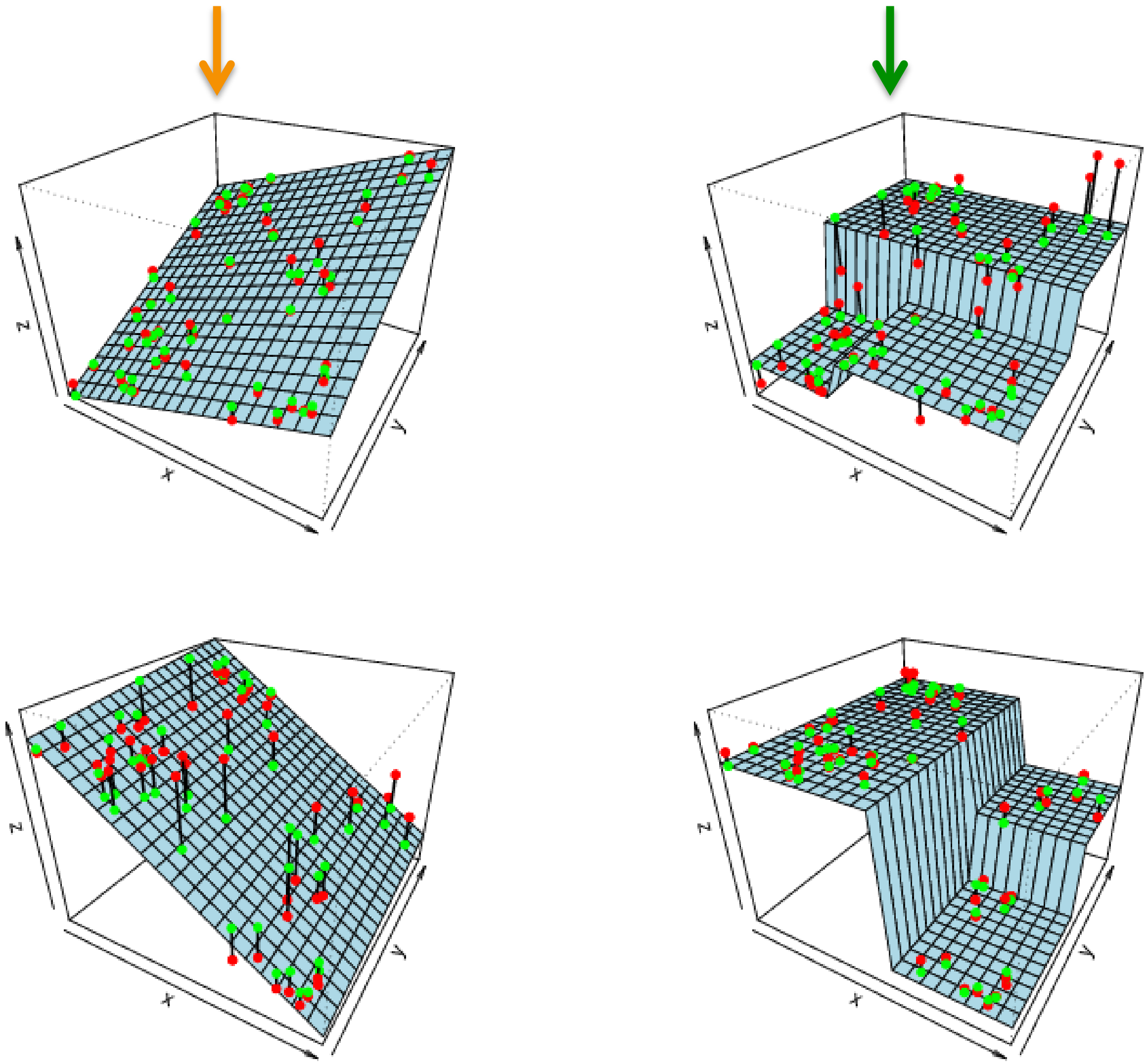


OUI





Régression linéaire vs. Arbre de régression



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Particularités des **arbres de régression**

- Les attributs et la classe sont à **valeur continue**
- On associe à chaque région R_i de X une valeur constante c_i.
- On cherche en général à minimiser l'*erreur quadratique* :

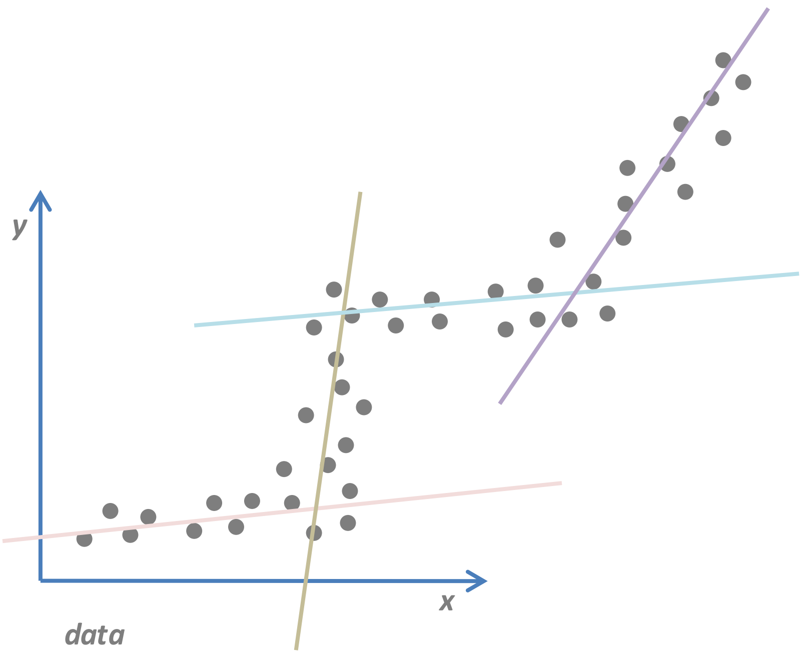
$$MSE = \sum_{i=1}^{m} \sum_{k=1}^{K} \mathcal{I}(R_k)(y_i - c_k)^2$$

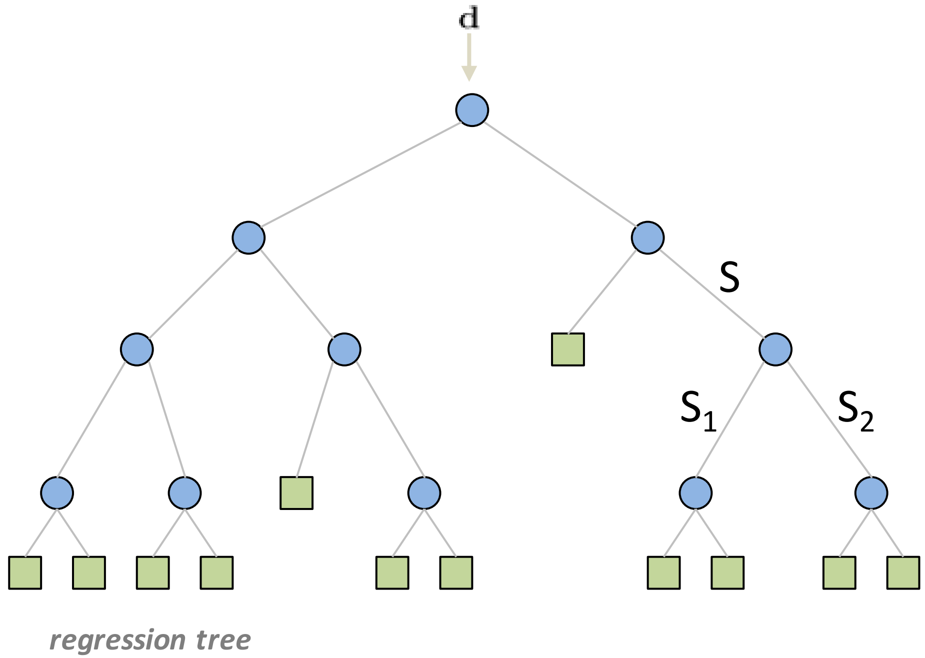
Induction des arbres de régression

- **Choix de l'attribut** et du **point de division** minimisant la somme des écarts quadratique à la moyenne dans chacune des régions de l'espace créées

- **Arrêt** lorsque
  - **Plus assez de points** par région
  - **Différence** des moyennes entre régions **sous un seuil fixé**

Regression trees (model trees)





- Real-valued output *y*
- Object function: maximize $Err(S) - \sum_{i=1}^{2} \frac{|S_i|}{|S|} Err(S_i)$

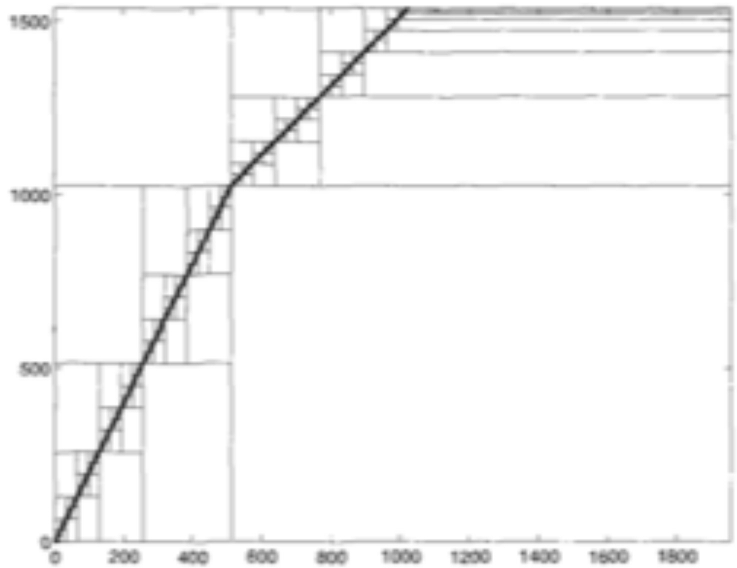
measure of fit of model

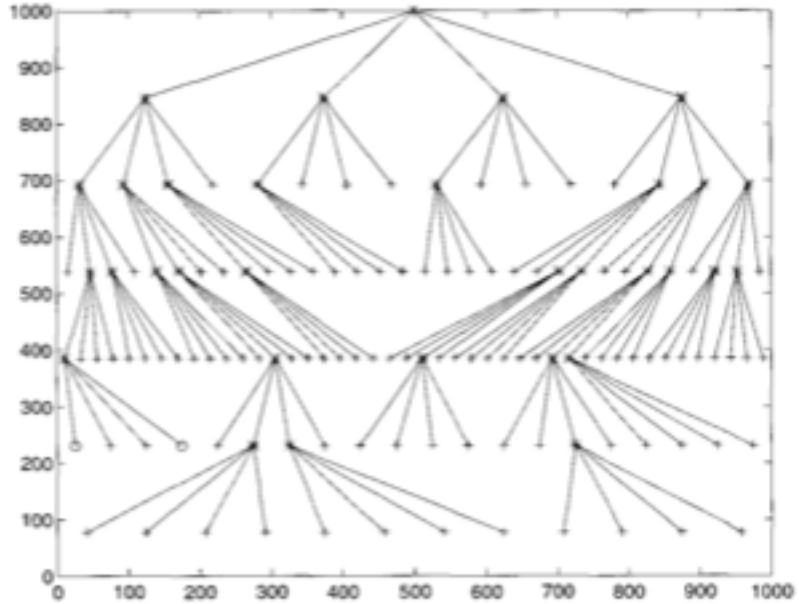
$$Err(S) = \sum_{j \in S} \left(y_j - y(x_j)\right)^2$$

e.g. linear model y = ax+b,
Or just constant model

AgroParisTech

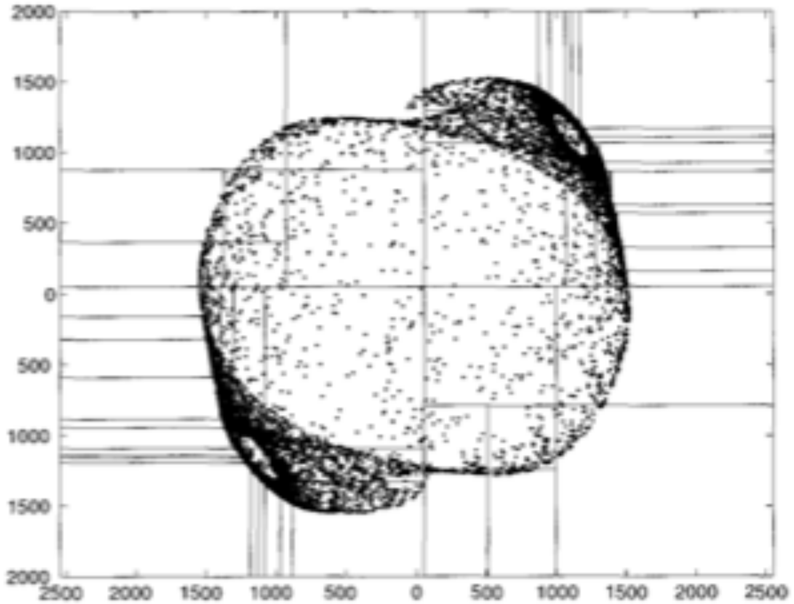
Arbres de régression : exemple

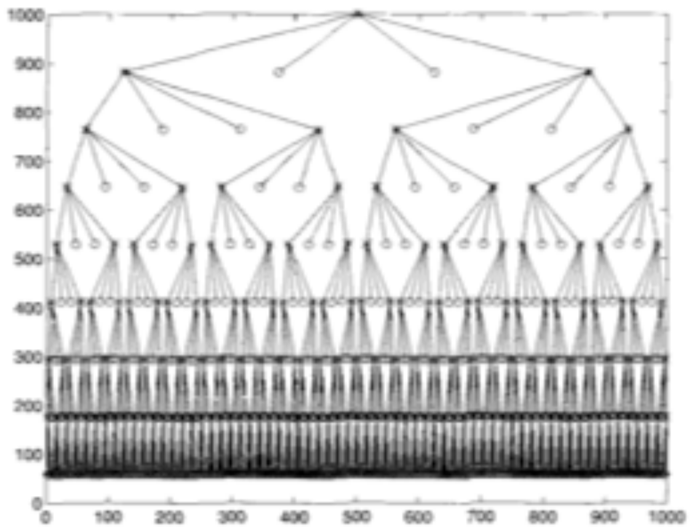




Tiré de [Anne-Emmanuelle BADEL*, Olivier MICHEL* et Alfred HERO, « Arbres de régression modélisation non paramétrique et analyse des séries temporelles », 1996]

Arbres de régression : exemple





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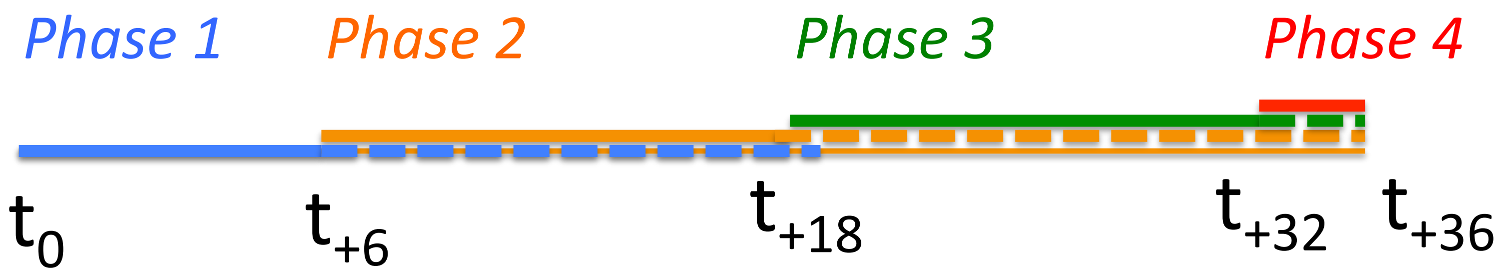
Quand utiliser des arbres de régression

- La régression classique ne marche pas
  - Dimension de l'espace d'entrée élevée
- L'interprétabilité du modèle est importante
- Le problème se prête bien à une division selon les axes

Conclusions

Conclusions

- Good if
  - Vectorial input space
  - The target concept corresponds to recursive boxes with borders parallel to the axes
- Very simple
- Computational complexity of learning in $O(A^2 . m)$
  - A attributes
  - m examples


Phase 1
Phase 2
Phase 3
Phase 4
t0
t+6
t+18
t+32
t+36

- ..