Machine Learning
机器学习

Lecture 4：决策树

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监督学习
Supervised Learning

- Given the training dataset of (data,label) pairs,

$$D = \{(x^{(i)}, y^{(i)})\}_{i=1.2,\ldots,N}$$

let the machine learn a function from data to label

$$y^{(i)} \approx f_\theta(x^{(i)})$$

- Function set $\{f_\theta(x^{(i)})\}$ is called hypothesis space
- Learning is referred to as updating the parameter θ to make the prediction closed to the corresponding label

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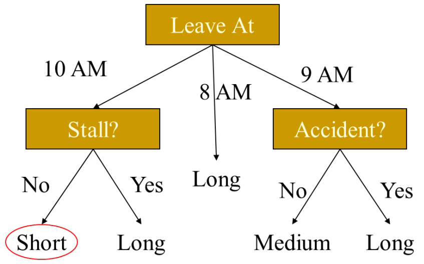
a decision tree



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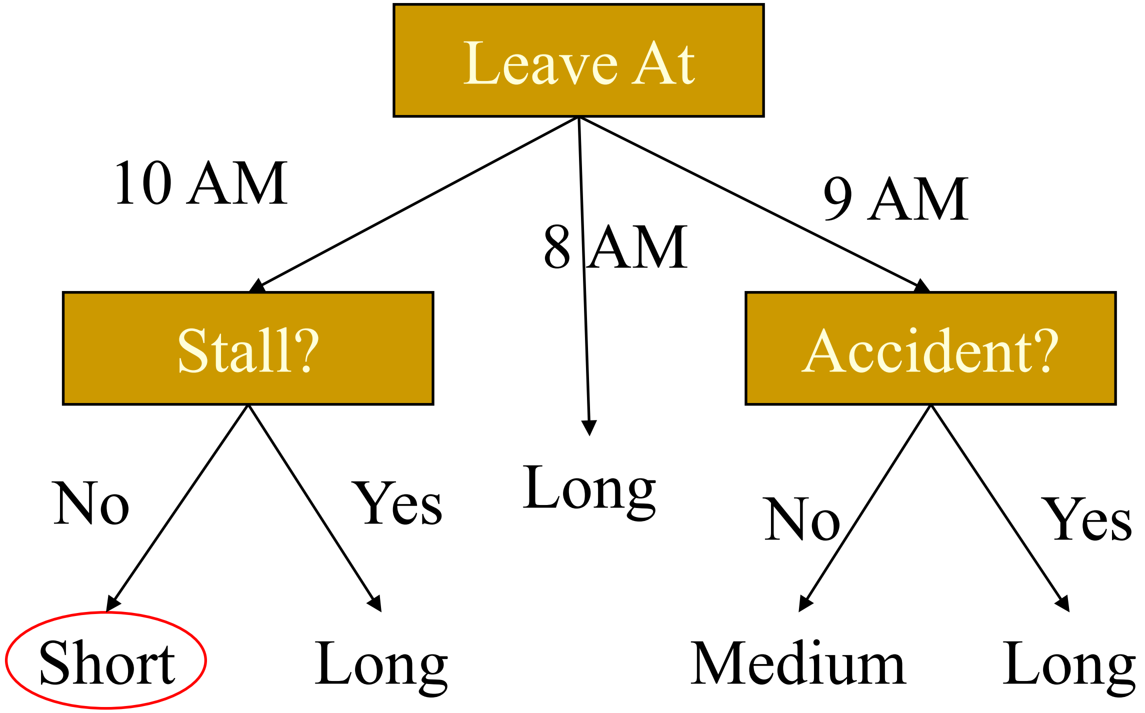
什么是决策树
What is a Decision Tree?

- Let’s look at a sample decision tree…

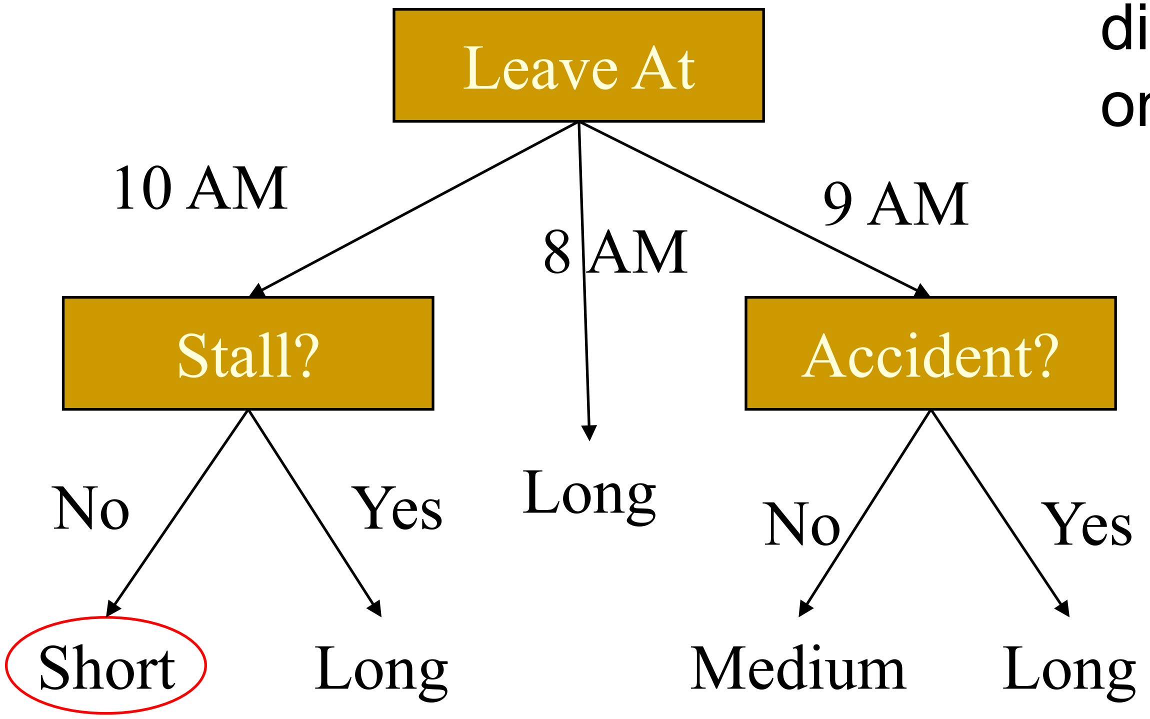
决策树举例
Predicting Commute Time



- *Decision tree representation:*
  – Each internal node tests an attribute
  – Each branch corresponds to attribute value
  – Each leaf node assigns a classification

If we leave at 10 AM and there are no cars stalled on the road, what will our commute time be?

决策树与规则集合
Representation as a Rule Set



Re-representation as if-then rules:
disjunction of conjunctions of constraints on the attribute value instances

```
if hour == 8am
    commute time = long
else if hour == 9am
    if accident == yes
        commute time = long
    else
        commute time = medium
else if hour == 10am
    if stall == yes
        commute time = long
    else
        commute time = short
```

If we leave at 10 AM and there are no cars stalled on the road, what will our commute time be?

决策树学习举例

- Problem: decide whether to wait for a table at a restaurant. What attributes would you use?

  Goal predicate: Will wait?

- Attributes
  1. Alternate: is there an alternative restaurant nearby?
  2. Bar: is there a comfortable bar area to wait in?
  3. Fri/Sat: is today Friday or Saturday?
  4. Hungry: are we hungry?
  5. Patrons: number of people in the restaurant (None, Some, Full)
  6. Price: price range ($, $$, $$$)
  7. Raining: is it raining outside?
  8. Reservation: have we made a reservation?
  9. Type: kind of restaurant (French, Italian, Thai, Burger)
  10. WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, >60)

决策树学习举例

- Examples (also called instances, observations, or samples) are described by features (also called attributes, or variables) and labels (also called targets or outcomes).
- E.g., situations where I will/won't wait for a table:

12 examples

6 +
6 -

Example	Attributes										Target
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X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
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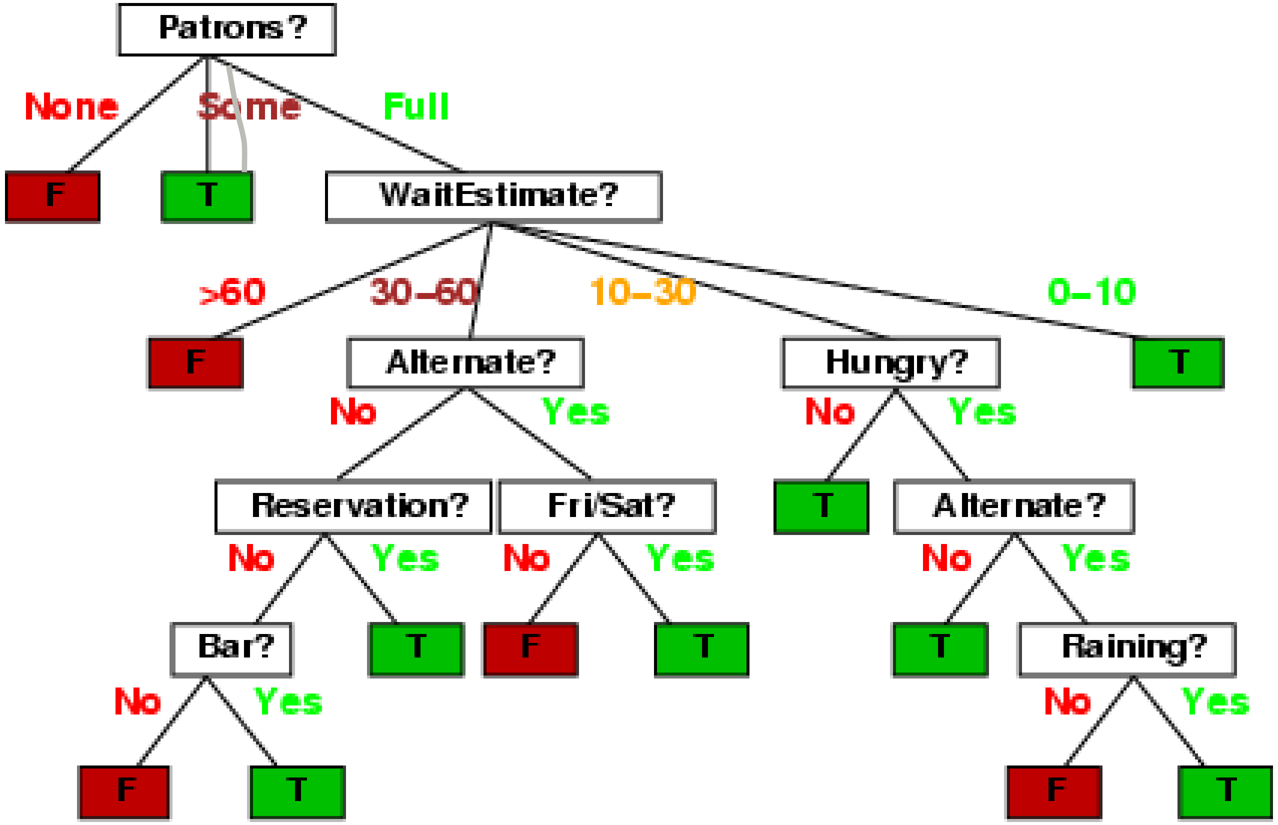
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

- Classification of examples is positive (T) or negative (F)

决策树学习举例

- One possible representation for hypotheses
- E.g., here is a tree for deciding whether to wait:



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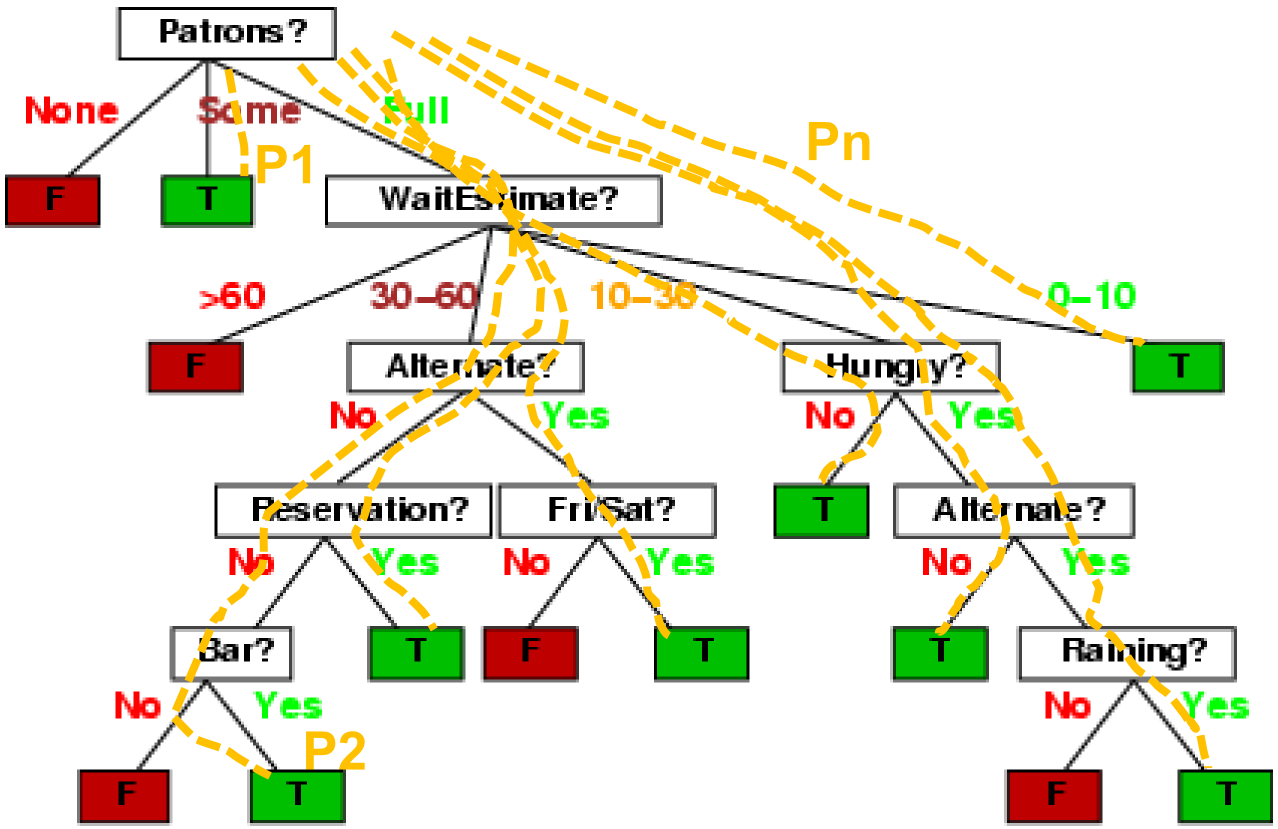

WillWait(s) ↔ (P1(s) ∨ P2(s) ∨ … ∨ Pn(s))

决策树的表达能力

Any particular decision tree hypothesis for WillWait goal predicate can be seen as

a disjunction of a conjunction of tests,

i.e., an assertion of the form:

$$\forall s \;\; WillWait(s) \leftrightarrow (P1(s) \vee P2(s) \vee \ldots \vee Pn(s))$$

Where each condition Pi(s) is a conjunction of tests corresponding to the path from the root of the tree to a leaf with a positive outcome.

决策树的表达能力

For 10 Boolean attributes, there are 2^{10} possible combinations of input values (features).

For each input combination, there are 2 possible outputs (0/1).

Input features	Output
0 0 0 0 0 0 0 0 0 0	0/1
0 0 0 0 0 0 0 0 0 1	0/1
0 0 0 0 0 0 0 0 1 0	0/1
0 0 0 0 0 0 0 1 0 0	0/1
…	
1 1 1 1 1 1 1 1 1 1	0/1

How many entries does this table have?

$$2^{10}$$

Decision trees can express any Boolean function

决策树的表达能力

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…	
1 1 1 1 1 1 1 1 1 1	0/1

How many entries does this table have?

2^{10}

Decision trees can express any Boolean function

Total number of distinct Boolean functions (and corresponding decision trees): Since there are 2^{10} possible input combinations, and each combination can yield one of two possible outputs (0 or 1), the total number of distinct Boolean functions is:

$$= 2^{2^{10}}$$

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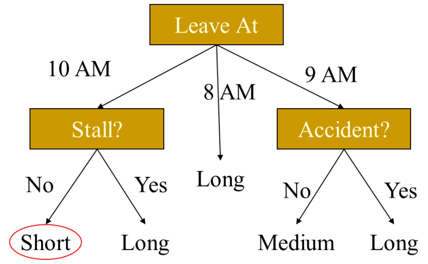
let the machine learn a function from data to label

$$y^{(i)} \approx \boxed{f_\theta(x^{(i)})} \Rightarrow$$

a decision tree



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决策树学习算法
Decision tree learning Algorithm

- Goal: Finding a decision tree that agrees with training set.

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Could we construct a decision tree that has one path to a leaf for each instance, where the path tests sets each attribute value to the value of the instance?

What is the problem with this from a learning point of view?

决策树学习算法
Decision tree learning Algorithm

- Goal: Finding a decision tree that agrees with training set.

Could we construct a decision tree that has one path to a leaf for each instance, where the path tests sets each attribute value to the value of the instance?

What is the problem with this from a learning point of view?

Problem: This approach would just memorize training instances. How to deal with new instances?

It doesn’t generalize!

决策树学习算法
Decision tree learning Algorithm

- The basic idea behind any decision tree algorithm is as follows:
  - Choose the best attribute(s) to split the remaining instances and make that attribute a decision node
  - Repeat this process for recursively for each child
  - Stop when:
    - All the instances have the same target value
    - There are no more attributes
    - There are no more instances
    - Minimum sample size for a node (early stopping)
    - Maximum tree depth…

ID3 启发式算法
ID3 Heuristic algorithm

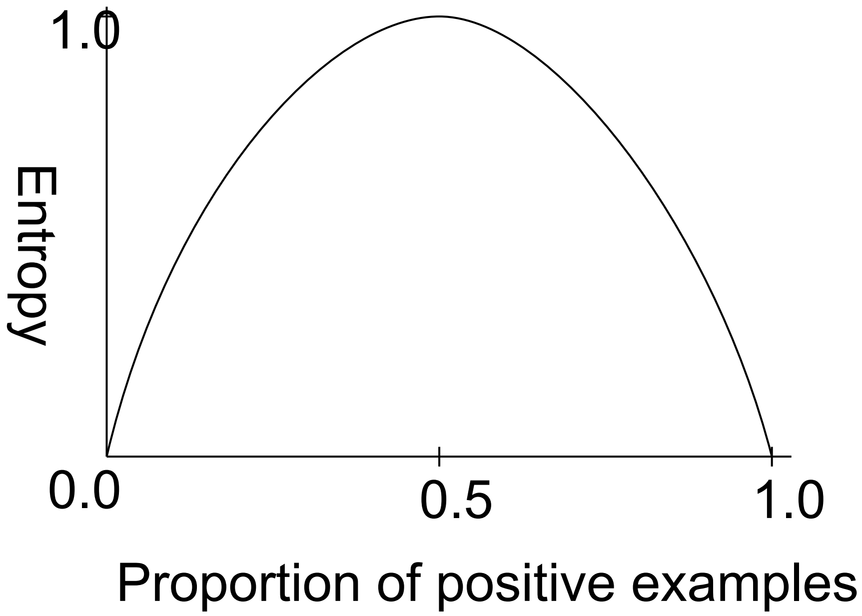
- How to determine the best attribute?

– ID3 splits attributes based on their entropy.
Entropy is the measure of randomness.

p(head)=0.5
p(tail)=0.5
H=1

p(head)=0.51
p(tail)=0.49
H=0.9997

熵函数
Entropy Function



For a collection D having positive and negative examples, entropy is given as:

$$Entropy(D) = -\frac{p}{p+n}\log_2\frac{p}{p+n} - \frac{\mathrm{n}}{p+n}\log_2\frac{n}{p+n}$$

p - # positive examples
n - # negative examples

Example taken from
Tom Mitchell's
Machine Learning

决策树学习举例

- Examples (also called instances, observations, or samples) are described by features (also called attributes, or variables) and labels (also called targets or outcomes).
- E.g., sit What's the entropy of this collection of examples?

12 examples

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	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
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$$Entropy(D) = -\frac{p}{p+n}\log_2\frac{p}{p+n} - \frac{n}{p+n}\log_2\frac{n}{p+n}$$

$$= -0.5\,log2(0.5) - 0.5\,log2(0.5) = 1$$

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$p = n = 6;$

$$\frac{P}{P+n} = \frac{n}{P+n}$$

$$= 0.5$$

X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
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熵的通用计算公式
General Formula for Entropy

- Calculation of entropy

$$Entropy(D) = -\sum_{k=1}^{|y|} p_k \log_2 p_k$$

  - D = the set of examples
  - p_k = the portion of examples in D that belong to class k.
  - $|y|$ = the number of distinct classes (i.e. the size of the range of the target value) .

It is applicable to both binary and multiclass classification problems.

ID3基于信息增益来选择属性
Choosing an attribute: Information Gain

- Intuition: the best attribute is the attribute that reduces the entropy (the uncertainty) the most.

- the information gain of a given attribute a relative to a collection of examples D is defined as:

$$Gain(D,a) = Entropy(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Entropy(D^v)$$

D^v is the subset of D where the attribute a takes on value V,
And V is the number of distinct values that the attribute a can take.

ID3
J. Ross Quinlan,1975

ID3算法构建决策树
Decision Tree Building: ID3 Algorithm

Start from the root node containing all data

- For each node, calculate the information gain of all available features
- Choose the feature with the highest information gain
- Split the data of at the node based on the selected feature (the feature is not reused in subsequent splits)
- Repeat the above steps recursively for each resulting node, until one of the following stopping conditions is met:
  - All instances at the node have the same target value.
  - No remaining features to split.
  - Maximum tree depth or minimum sample size for a node is reached.

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X_{12}	T	T	T	T	Full	\$	F	F	Burger	30–60	T

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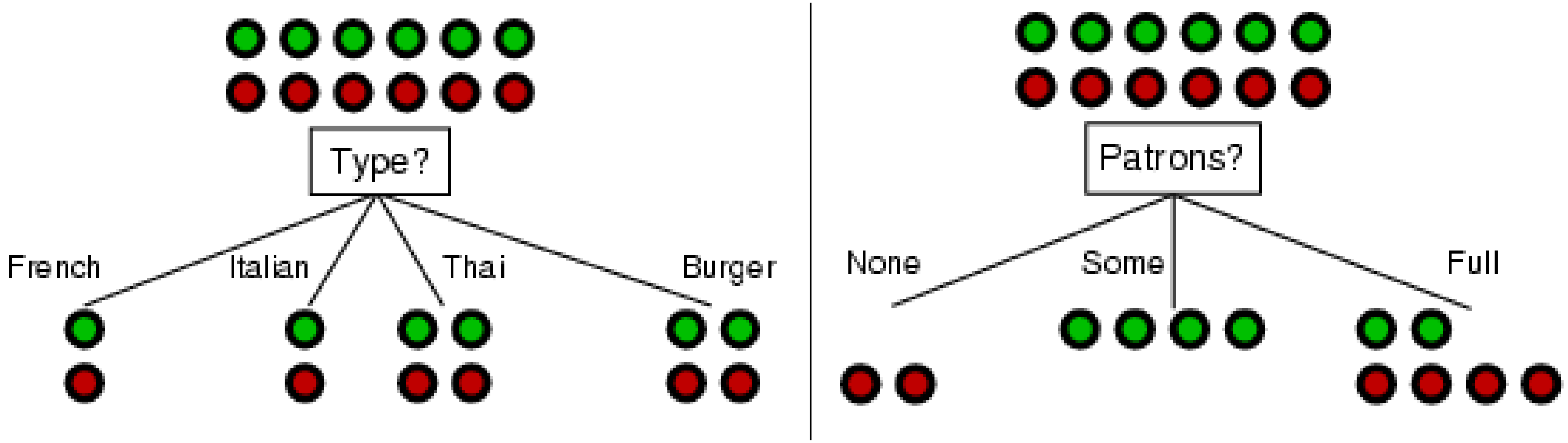
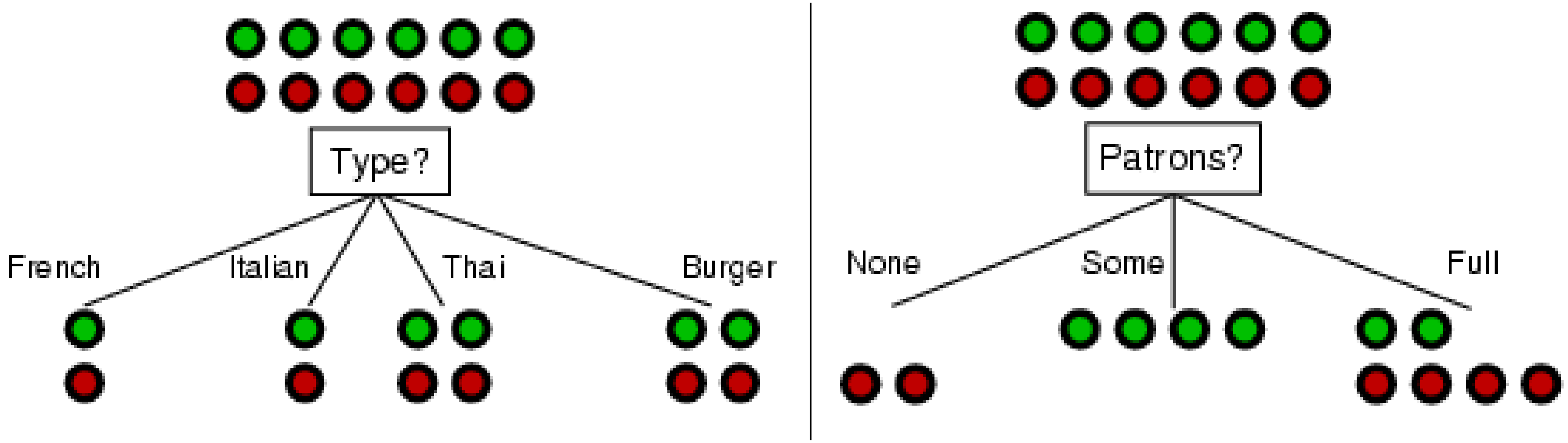
决策树学习举例

Which one should we pick?



决策树学习举例

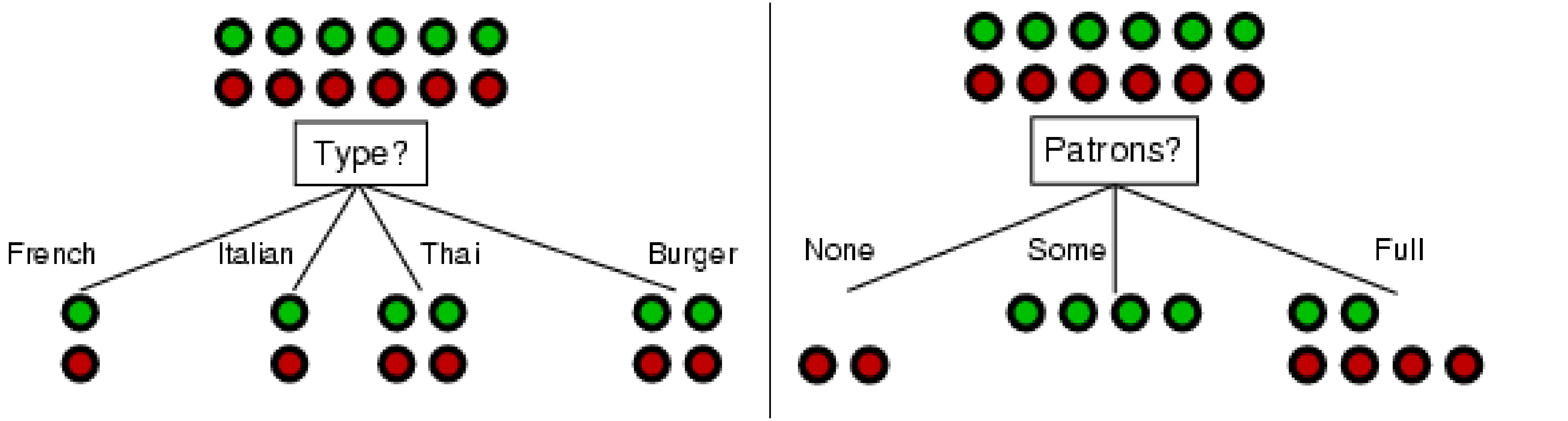
Goal: Choose the feature with the highest information gain



A perfect attribute would ideally divide the examples into sub-sets that are all positive or all negative… i.e. maximum information gain.

决策树学习举例

$$Gain(D,a) = Entropy(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Entropy(D)$$

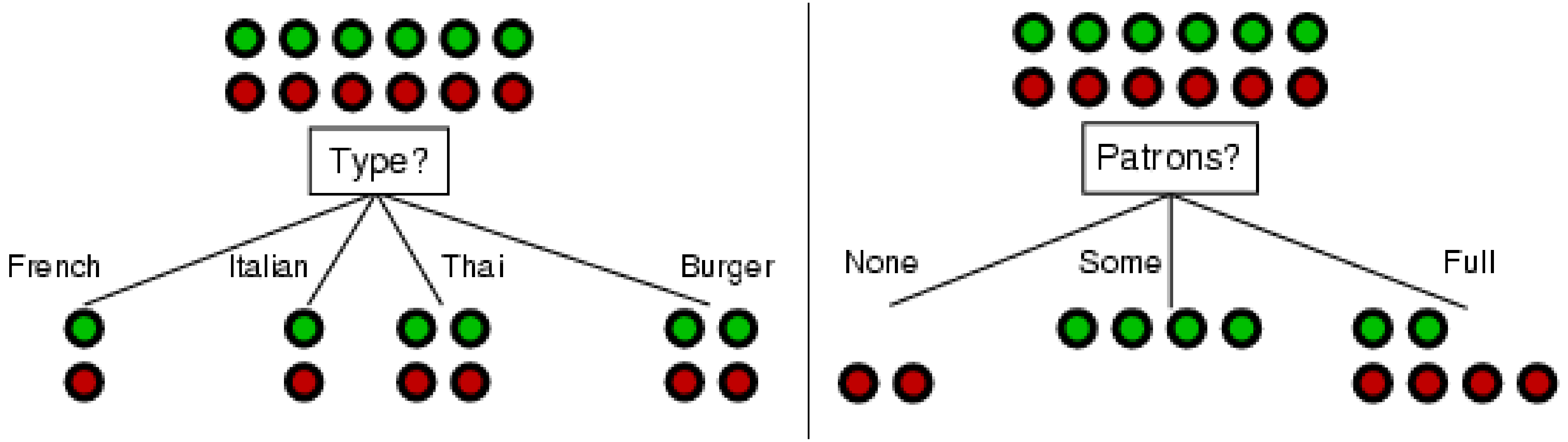


$$Gain(D,Type) = 1 - \left[\frac{2}{12} Entropy\left(\frac{1}{2},\frac{1}{2}\right) + \frac{2}{12} Entropy\left(\frac{1}{2},\frac{1}{2}\right) + \frac{4}{12} Entropy\left(\frac{1}{2},\frac{1}{2}\right) + \frac{4}{12} Entropy\left(\frac{1}{2},\frac{1}{2}\right)\right] = 0$$

$$Gain(D,Patrons) = 1 - \left[\frac{2}{12} Entropy(0,1) + \frac{4}{12} Entropy(1,0) + \frac{6}{12} Entropy\left(\frac{2}{6},\frac{4}{6}\right)\right] = 0.541$$

决策树学习举例

Patrons has the highest ‘information gain’ of all attributes and so is chosen as the root.



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奥卡姆剃刀原则
Principle of Occam's razor

Among competing hypotheses, the one with the fewest assumptions should be selected.

Recall the function set $\{f_\theta(x^{(i)})\}$ is called hypothesis space

$$\boxed{\min_\theta \frac{1}{N}\sum_{i=1}^{N} L(y^{(i)}, f_\theta(x^{(i)}))} + \boxed{\lambda\Omega(\theta)}$$

Inductive Bias

prefer/search bias

Original loss

Penalty on assumptions

Structural Risk Minimization, SRM

ID3的归纳偏置
Inductive Bias in ID3

ID3 algorithm prefers shorter trees by selecting attributes with higher information gain near the root. This helps in reducing the overall complexity of the tree.

- Occam’s razor: prefer the shortest hypothesis that fits the data
- The bias in ID3 is a preference for some hypotheses(prefer/search bias), rather than a restriction of hypothesis space H. The algorithm prioritizes certain types of models (e.g., shorter trees), but other hypotheses are still possible.

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Number
1
2
3
4
5
6
7
8
9
10
11
12

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If add an attribute—'number'

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X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30

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10

es

- Classi

Number has the highest 'information gain' of all attributes and so is chosen as the root.

If add an attribute—'number'

决策树学习举例

- Examples (also called instances, observations, or samples) are described by features (also called attributes, or variables) and lab… called targets or outcomes).

- E.g., situations where I will/won't wait for a table:

12 exa… …es

6
6

$$Gain(D, \text{number})$$
$$= Entropy(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Entropy(D)$$
$$= 1 - \left[\frac{6}{12} Entropy(1,0) + \frac{6}{12} Entropy(0,1)\right]$$
$$=1 - 0 \quad = \ 1$$

Number
1
2
3
4
5
6
7
8
9
10

Number has the highest 'information gain' of all attributes and so is chosen as the root.

- Classi…

If add an attribute—'number'

ID3基于信息增益来选择属性
Choosing an attribute: Information Gain

- Intuition: the best attribute is the attribute that reduces the entropy (the uncertainty) the most.

- the information gain of a given attribute a relative to a collection of examples D is defined as:

$$Gain(D,a) = Entropy(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Entropy(D^v)$$

D^v is the subset of D where the attribute a takes on value V,
And V is the number of distinct values that the attribute a can take.

ID3
J. Ross Quinlan,1975

信息增益率和C4.5算法
Information Gain Ratio and C4.5

$$Gain\_\mathrm{ratio}(D,a) = \frac{Gain(D,a)}{IV(a)}$$

$$a_* = \underset{a \in A}{\mathrm{argmax}}\, Gain\_\mathrm{ratio}\,(D,a)$$

$IV(a)$ = intrinstic value, the greater the possible number of attributes is, the greater the value is.

$$IV(a) = -\sum_{v=1}^{V} \frac{|D^v|}{|D|} \log_2 \frac{|D^v|}{|D|}$$

C4.5 is an extension of ID3
J. Ross Quinlan, The Morgan Kaufmann Series in Machine Learning, Pat Langley.
Gain Ratio for Attribute Selection

D^v is the subset of D where the attribute a takes on value V, and V is the number of distinct values that the attribute a can take.

决策树学习举例

- Examples (also called instances, observations, or samples) are described by features (also called attributes, or variables) and lab[...] called targets or outcomes).

- E.g., situations where I will/won't wait for a table:

12 exa

6

6

$$Gain(D, \text{number})$$
$$= Entropy(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Entropy(D)$$
$$= 1 - \left[\frac{6}{12} Entropy(1,0) + \frac{6}{12} Entropy(0,1)\right]$$
$$= 1 - 0 \quad = 1$$

Number
1
2
3
4
5
6
7
8
9
10

es

- Classi

Number has the highest 'information gain' of all attributes and so is chosen as the root.

If add an attribute—'number'

决策树学习举例

- Examples (also called instances, observations, or samples) are described by features (also called attributes, or variables) and lab called targets or outcomes).
- E.g., s

12 exar es

6
6

- Classi

$$Gain\_ratio(D, number) = \frac{Gain(D,a)}{IV(a)}$$

$$= \frac{Gain(D,a)}{-\sum_{v=1}^{V}\frac{|D^v|}{|D|}\log_2\frac{|D^v|}{|D|}}$$

$$= \frac{1}{-12\frac{1}{12}\log_2\frac{1}{12}}$$

$$= \frac{1}{\log_2 12}$$

Est
0–10
30–60
>60
0–10
0–10
0–10
>60
10–30

Number
1
2
3
4
5
6
7
8
9
10

Number has the highest 'information gain' of all attributes and so is chosen as the root.

If add an attribute—'number'

基尼指数和CART算法
Gini index and CART

$$Gini\_\text{index}(D, a = v) = \frac{|D^l|}{|D|} Gini(D^l) + \frac{|D^r|}{|D|} Gini(D^r)$$

$$a_*, v_* = \underset{a \in A}{argmin}\, Gini_{index}(D, a = v)$$

D^l and D^r are the left and right subsets of D after splitting by a $= v$.

$Gini(D)$ reflects the probability that two samples randomly selected from D belong to different classes.

$$\text{Gini}(D) = \sum_{k=1}^{|y|} \sum_{\mathrm{k}' \neq k} p_k p_{\mathrm{k}'} = 1 - \sum_{k=1}^{|y|} p_k^2$$

CART
Breiman et al., 1984
Classification and Regression tree

Where p_k is the proportion of samples in class k in the dataset D

基尼指数和CART算法
Gini index and CART

Binary Tree

$$Gini\_index(D, a = v) = \frac{|D^l|}{|D|} Gini(D^l) + \frac{|D^r|}{|D|} Gini(D^r)$$

$$a_*, v_* = \underset{a \in A}{argmin}\, Gini_{index}\,(D, a = v)$$

D^l and D^r are the left and right subsets of D after splitting by a $= v$.

$Gini(D)$ reflects the probability that two samples randomly selected from D belong to different classes.

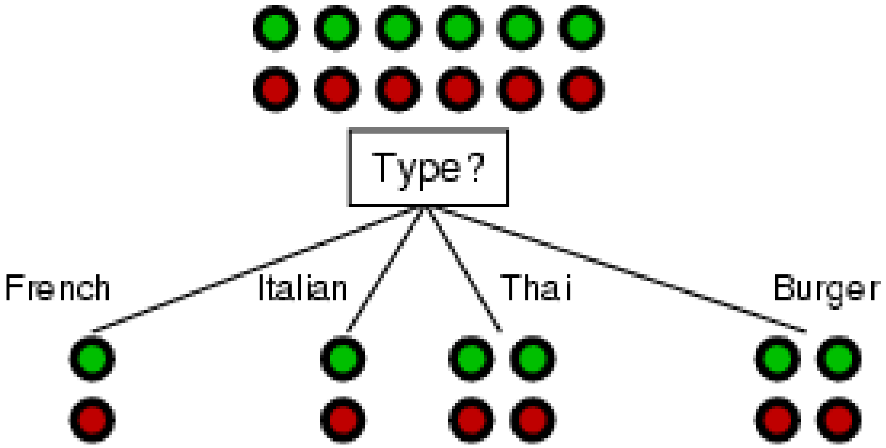
$$\mathrm{Gini}(D) = \sum_{k=1}^{|y|} \sum_{\mathrm{k}' \neq k} p_k p_{\mathrm{k}'} = 1 - \sum_{k=1}^{|y|} p_k^2$$

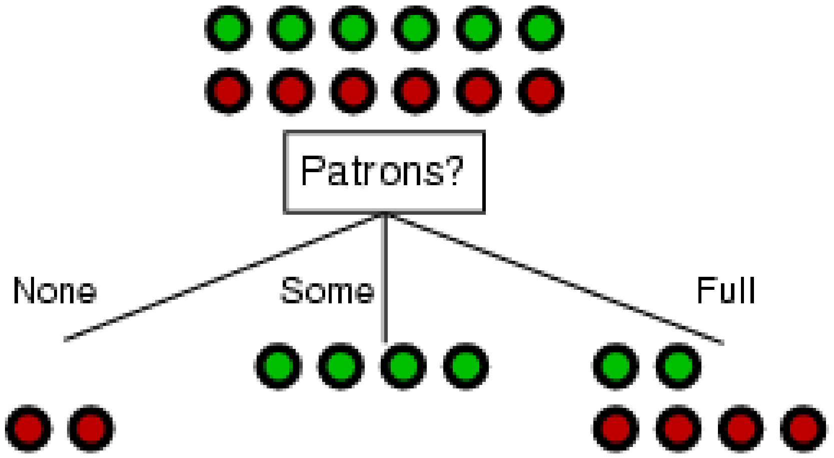
CART
Breiman et al., 1984
Classification and Regression tree

Where p_k is the proportion of samples in class k in the dataset D

决策树学习举例
Learning decision trees: An example

$$Gini\_\mathrm{index}(D, a = v) = \frac{|D^l|}{|D|} Gini(D^l) + \frac{|D^r|}{|D|} Gini(D^r)$$





$Gini\_index(D, Type = French) =$

$Gini\_index(D, Type = Italian) =$

$Gini\_index(D, Type = Thai) =$

$Gini\_index(D, Type = Burger) =$

$Gini\_index(D, Patrons = None) =$

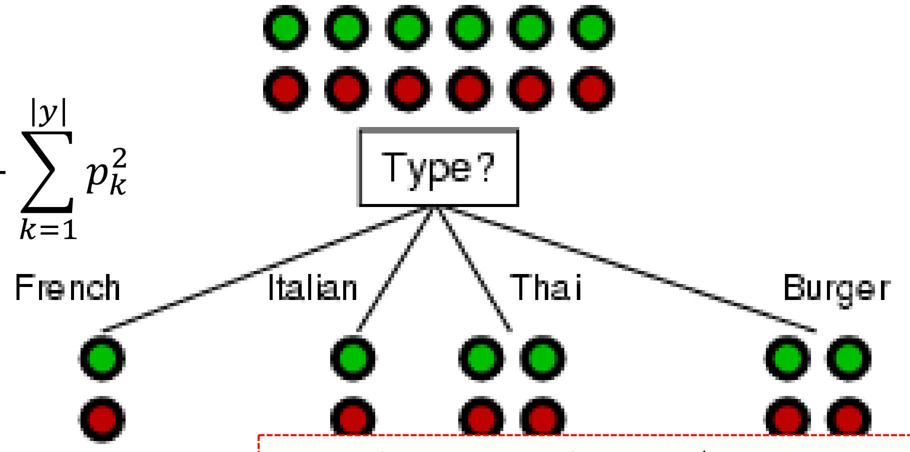
$Gini\_index(D, Patrons = some) =$

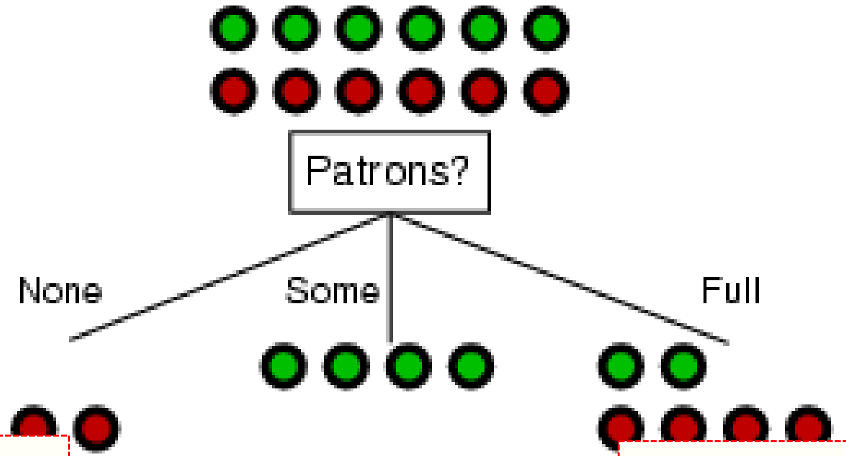
$Gini\_index(D, Patrons = Full) =$

决策树学习举例
Learning decision trees: An example

$$Gini\_\mathrm{index}(D, a = v) = \frac{|D^l|}{|D|} Gini(D^l) + \frac{|D^r|}{|D|} Gini(D^r)$$

$$\mathrm{Gini}(D) = 1 - \sum_{k=1}^{|y|} p_k^2$$





$Gini\_index(D, Type = French) =$

$$\frac{2}{12}\left(1 - \frac{1^2}{2} - \frac{1^2}{2}\right) + \frac{10}{12}\left(1 - \frac{5}{10}^2 - \frac{5}{10}^2\right) = 0.5$$

$Gini\_index(D, Type = Italian) =$

$Gini\_index(D, Type = Thai) =$

$$\frac{4}{12}\left(1 - \frac{2^2}{4} - \frac{2^2}{4}\right) + \frac{8}{12}\left(1 - \frac{4^2}{8} - \frac{4^2}{8}\right) = 0.5$$

$Gini\_index(D, Type = Burger) =$

$i\_index(D, Patrons = None) =$

$$\frac{2}{12}0 + \frac{10}{12}\left(1 - \frac{6}{10}^2 - \frac{4}{10}^2\right) = 0.40$$

$i\_index(D, Patrons = some) =$

$$\frac{4}{12}0 + \frac{8}{12}\left(1 - \frac{2^2}{8} - \frac{6^2}{8}\right) = 0.25$$

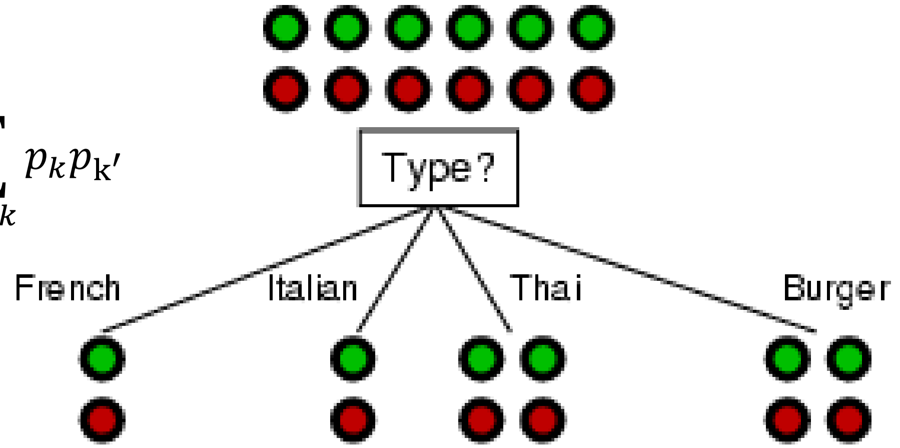
$i\_index(D, Patrons = Full) =$

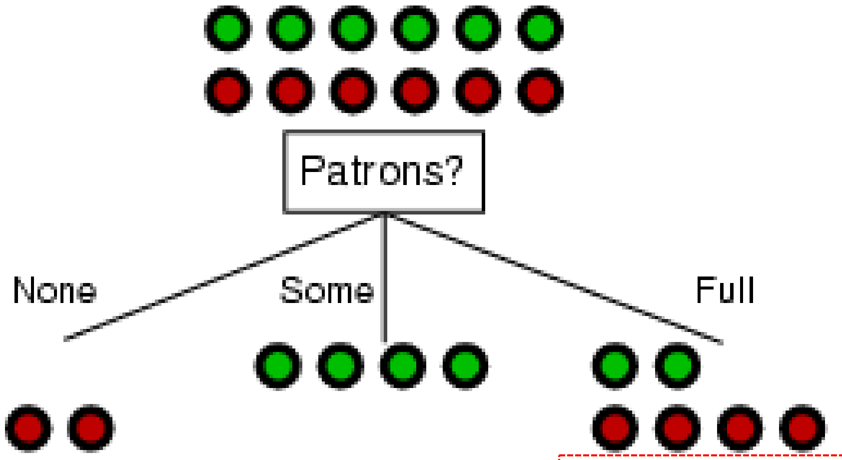
$$\frac{6}{12}\left(1 - \frac{2^2}{6} - \frac{4^2}{6}\right) + \frac{6}{12}\left(1 - \frac{2^2}{6} - \frac{4^2}{6}\right) = 0.44$$

决策树学习举例
Learning decision trees: An example

$$Gini\_index(D, a = v) = \frac{|D^l|}{|D|} Gini(D^l) + \frac{|D^r|}{|D|} Gini(D^r)$$

$$\text{Gini}(D) = \sum_{k=1}^{|y|} \sum_{k' \neq k} p_k p_{k'}$$





$Gini\_index(D, Type = Frenc$

$$\frac{2}{12}\left(2\frac{1}{2}\frac{1}{2}\right) + \frac{10}{12}\left(2\frac{5}{10}\frac{5}{10}\right) = 0.5$$

$Gini\_index(D, Type = Italia$

$Gini\_index(D, Type = Thai) =$

$$\frac{4}{12}(2\frac{2}{4}\frac{2}{4}) + \frac{8}{12}(2\frac{4}{8}\frac{4}{8}) = 0.5$$

$Gini\_index(D, Type = Burger) =$

$ini\_index(D, Patrons = None$

$$\frac{2}{12}0 + \frac{10}{12}(2\frac{6}{10}\frac{4}{10}) = 0.40$$

$ini\_index(D, Patrons = some) =$

$$\frac{4}{12}0 + \frac{8}{12}(2\frac{2}{8}\frac{6}{8}) = 0.25$$

$ini\_index(D, Patrons = Full) =$

$$\frac{6}{12}(2\frac{2}{6}\frac{4}{6}) + \frac{6}{12}(2\frac{2}{6}\frac{4}{6})) = 0.44$$

均方误差和CART算法
Mean Squared Error (MSE) and CART

$$a_*, v_* = \underset{a \in A}{argmin} \left[\min_{c^l} \sum_{x^i \in D^l} \left(y^i - c^l\right)^2 + \min_{c^r} \sum_{x^i \in D^r} \left(y^i - c^r\right)^2 \right]$$

a_*, v_* are the optimal attribute and split point that minimize the total Mean Squared Error (MSE).

D^l and D^r are the left and right subsets of D after splitting on attribute a with a thereshold v.
c^l and c^r are predicted values for the left and right subsets, respectively.
y^i represents the actual target value for the i-th sample.

The CART can be applied to regression task!

均方误差和CART算法
Mean Squared Error (MSE) and CART

$$a_*, v_* = \underset{a \in A}{argmin} \left[\min_{c^l} \sum_{x^i \in D^l} \left(y^i - c^l\right)^2 + \min_{c^r} \sum_{x^i \in D^r} \left(y^i - c^r\right)^2 \right]$$

c^l and c^r are predicted values for the left and right subsets, respectively.
y^i represents the actual target value for the i-th sample.

To minimize the Mean Squared Error (MSE), the predicted value is typically the mean of the target values in the subset.

$$\frac{\partial \sum_{x^i \in D^l} \left(y^i - c^l\right)^2}{\partial c^l} = -2 \sum_{x^i \in D^l} \left(y^i - c^l\right) = 0$$

$$\Downarrow$$

$$c_l = \frac{1}{N^l} \sum_{x^i \in D^l} y^i$$

$$\frac{\partial \sum_{x^i \in D^l} \left(y^i - c^r\right)^2}{\partial c^r} = -2 \sum_{x^i \in D^r} \left(y^i - c^r\right) = 0$$

$$\Downarrow$$

$$c_l = \frac{1}{N^r} \sum_{x^i \in D^r} y^i$$

均方误差和CART算法
MSE and CART

$$a_*, v_* = \underset{a \in A}{argmin} \left[\min_{c^l} \sum_{x^i \in D^l} \left(y^i - c^l\right)^2 + \min_{c^r} \sum_{x^i \in D^r} \left(y^i - c^r\right)^2 \right]$$

$$c_l = \frac{1}{N^l} \sum_{x^i \in D^l} y^i, \qquad c_l = \frac{1}{N^r} \sum_{x^i \in D^r} y^i$$

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
mse	15.72	12.07	8.36	5.78	3.91	1.93	8.01	11.73	15.74

$s = 1.5, R_1 = \{1\}, R_2 = \{2,3,4,5,6,7,8,9,10\},$

$c_1 = 5.56, \ c_2 = 7.5$

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l									

c^r									

MSE									

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56								
c^r	7.5								
MSE	15.72								

=(5.7+5.91+6.4+6.8+7.05+8.9+8.7+9+9.05)/9

$$\sum_{x^i \in D^l}\left(y^i - c^l\right)^2 + \sum_{x^i \in D^l}\left(y^i - c^l\right)^2$$

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56	5.63	5.72	5.89	6.07	6.24	6.62	6.88	7.11
c^r	7.5	7.73	7.99	8.25	8.54	8.91	8.92	9.03	9.05
MSE	15.72	12.07	8.36	5.78	3.91	1.93	8.01	11.73	15.74

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56	5.63	5.72	5.89	6.07	6.24	6.62	6.88	7.11
c^r	7.5	7.73	7.99	8.25	8.54	8.91	8.92	9.03	9.05
MSE	15.72	12.07	8.36	5.78	3.91	1.93	8.01	11.73	15.74

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56	5.63	5.72	5.89	6.07	6.24			

c^r	6.37	6.54	6.75	6.93	7.05	8.91			

MSE	1.31	0.75	0.28	0.44	1.01	1.93			

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56	5.63	5.72	5.89	6.07	6.24			
c^r	6.37	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
MSE	1.31	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]			

=(5.7+5.91+6.4+6.8+7.05)/5

均方误差和CART算法
MSE and CART

x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56	5.63	5.72	5.89	6.07	6.24			
c^r	6.37	6.54	6.75	6.93	7.05	8.91			
MSE	1.31	0.75	0.28	0.44	1.01	1.93			

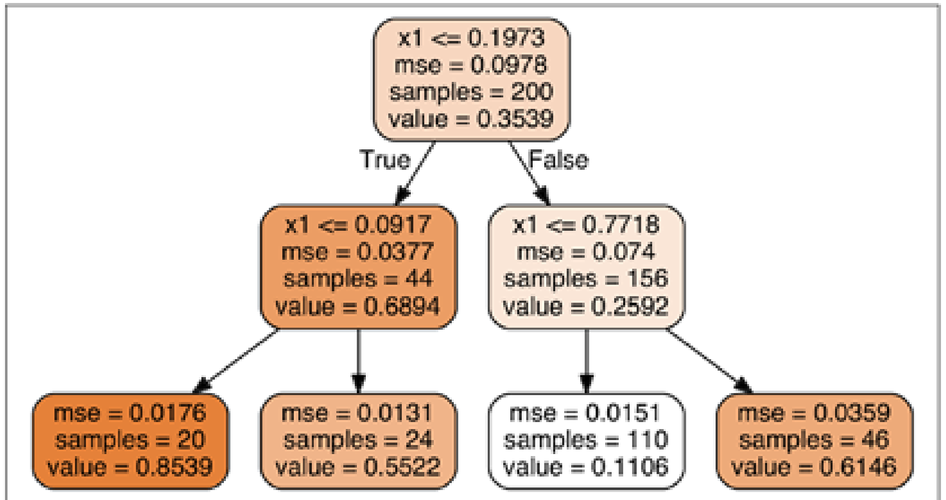
均方误差和CART算法
MSE and CART

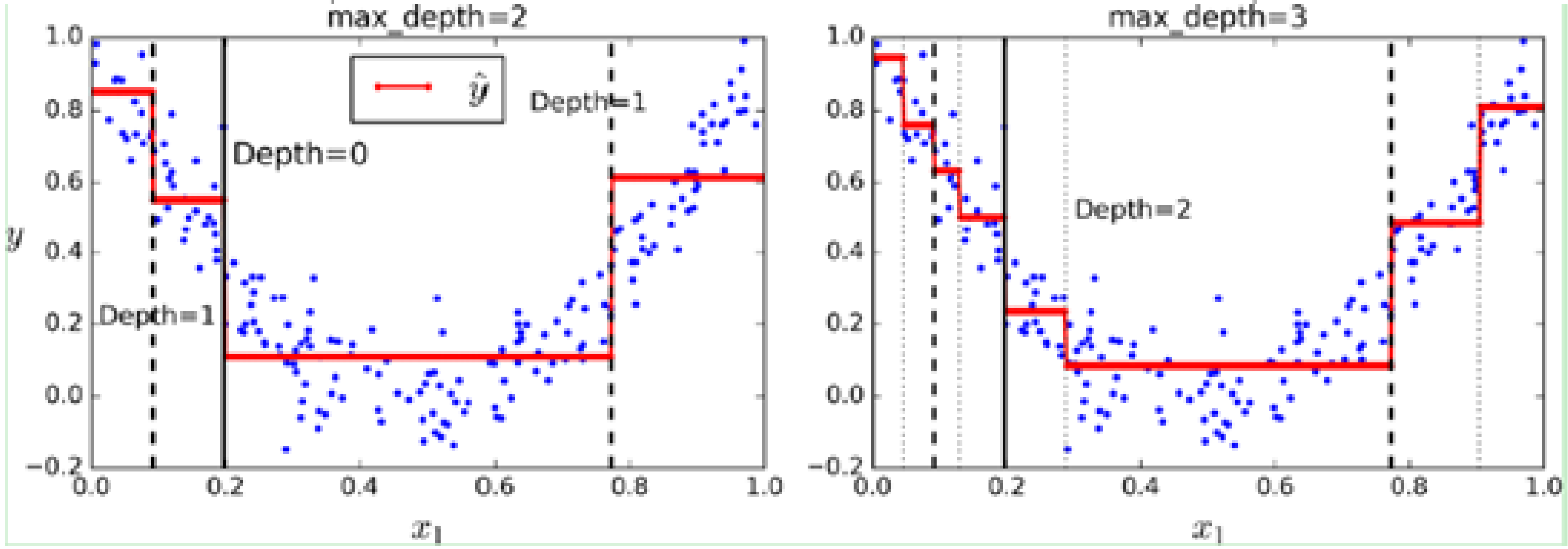
x	1	2	3	4	5	6	7	8	9	10
y	5.56	5.7	5.91	6.4	6.8	7.05	8.9	8.7	9	9.05

v	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
c^l	5.56	5.63	5.72	5.89	6.07	6.24			
c^r	6.37	6.54	6.75	6.93	7.05	8.91			
MSE	1.31	0.75	0.28	0.44	1.01	1.93			

$$
\mathrm{T} = \begin{cases} 5.72 & x \le 3.5 \\ 6.75 & 3.5 < x \le 6.5 \\ 8.91 & x > 6.5 \end{cases}
$$

CART算法
Classification and Regression Tree





The CART can be applied to regression task!

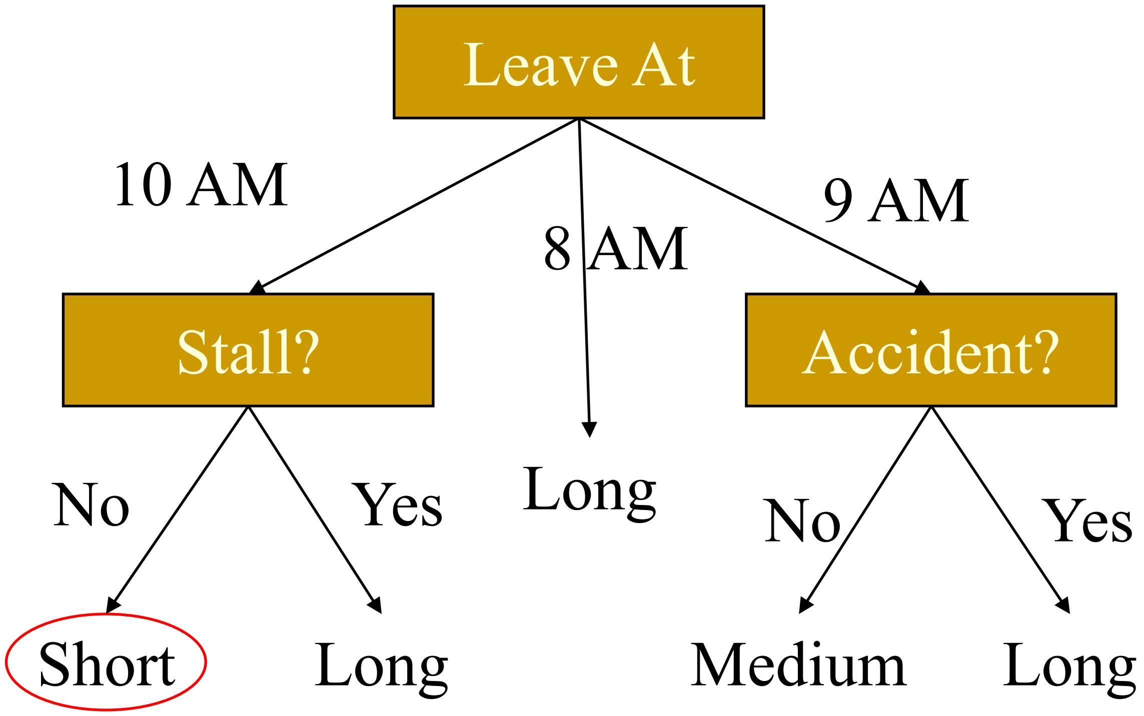
决策树经典算法小结
Summary of DT algorithms

	support task	criterion structure	tree structure	continous attribute value	missing attribute value	pruning	attribute multiple use
ID3	classification	Gain information	multiple Tree	No support	No support	No support	No support
C4.5	classification	Gain information rate	multiple Tree	support	support	support	No support
CART	Classification; regression	Gini index; mean square error	binary tree	support	support	support	support

连续值问题
Continuous attribute Problem

- Consider the attribute commute time, If we broke down leave time to the minute, we might get this:

8:00 (L), 8:02 (L), 8:07 (M), 9:00 (S), 9:20 (S), 9:25 (S), 10:00 (S), 10:02 (M)



连续值问题
Continuous attribute Problem

- Consider the attribute commute time, If we broke down leave time to the minute, we might get this:

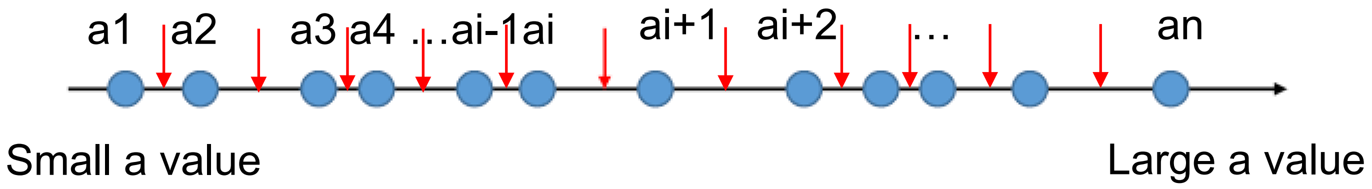
8:00 (L), 8:02 (L),| 8:07 (M),| 9:00 (S), 9:20 (S), 9:25 (S), 10:00 (S),| 10:02 (M)

cut points cut points cut points

discretization

Since entropy is very low for each branch, we have n branches with n leaves. This would not be helpful for predictive modeling.

连续值离散化
Continuous attribute discretization



Calculate candidate cut points

$$T_a = \left\{ \frac{a^i + a^{i+1}}{2} \mid 1 \leq i \leq n-1 \right\}$$

the best partition point(s) are selected according to

$$T_a^* = \underset{T_a}{argmin}\, Gini\_\text{index} \quad \text{(CART)}$$

$$T_a^* = \underset{T_a}{\text{argmax}}\, Gain\_\text{ratio} \quad \text{(C4.5)}$$

缺失值处理
Strategies for missing attribute values

$\tilde{D}$ —— the subset of D in which samples that have no missing values in the attribute a
$\tilde{D}^v$ —— the subset of $\tilde{D}$ in which samples that have v values in the attribute a
$\tilde{D}_k$ —— the subset of $\tilde{D}$ in which samples belonging to a class k
w_x —— the weight to each sample x

Q1：如何在属性缺失的情况下进行划分属性选择？

$$\rho = \frac{\sum_{x \in \tilde{D}} w_x}{\sum_{x \in D} w_x}$$

$$\tilde{p}_k = \frac{\sum_{x \in \tilde{D}_k} w_x}{\sum_{x \in \tilde{D}} w_x} \quad (1 \leq k \leq |\mathcal{Y}|)$$

$$\tilde{r}_v = \frac{\sum_{x \in \tilde{D}^v} w_x}{\sum_{x \in \tilde{D}} w_x} \quad (1 \leq v \leq V)$$

$\sum_{k=1}^{|\mathcal{Y}|} \tilde{p}_k = 1, \sum_{v=1}^{V} \tilde{r}_v = 1.$

Calculate Gain according to

$$\begin{aligned} \mathrm{Gain}(D, a) &= \rho \times \mathrm{Gain}(\tilde{D}, a) \\ &= \rho \times \left(\mathrm{Ent}(\tilde{D}) - \sum_{v=1}^{V} \tilde{r}_v \mathrm{Ent}(\tilde{D}^v) \right) \end{aligned}$$

$$\mathrm{Ent}(\tilde{D}) = -\sum_{k=1}^{|\mathcal{Y}|} \tilde{p}_k \log_2 \tilde{p}_k$$

Q2：如何在属性缺失的情况下进行划分属性选择？

C4.5:
Probability weights

Assign x(with missing attribute a) to each of the possible value With a probability $\tilde{r}_v \cdot w_x$

缺失值处理
Strategies for missing attribute values

$\tilde{D}$ —— the subset of D in which samples that have no missing values in the attribute a

$\tilde{D}^v$ —— the subset of $\tilde{D}$ in which samples that have v values in the attribute a

$\tilde{D}_k$ —— the subset of $\tilde{D}$ in which samples belonging to a class k

w_x —— the weight to each sample x

A1：根据缺失率的大小对信息增益率进行打折

$$\rho = \frac{\sum_{x \in \tilde{D}} w_x}{\sum_{x \in D} w_x}$$

考虑样本权重后的具有完整属性值的样本比例

$$\tilde{p}_k = \frac{\sum_{x \in \tilde{D}_k} w_x}{\sum_{x \in \tilde{D}} w_x} \quad (1 \leq k \leq |\mathcal{Y}|)$$

具有完整属性值的类别 k 的加权样本比例

$$\tilde{r}_v = \frac{\sum_{x \in \tilde{D}^v} w_x}{\sum_{x \in \tilde{D}} w_x} \quad (1 \leq v \leq V)$$

具有特定属性值 v 的加权样本比例

$$\sum_{k=1}^{|\mathcal{Y}|} \tilde{p}_k = 1, \ \sum_{v=1}^{V} \tilde{r}_v = 1.$$

Calculate Gain according to

$$\begin{aligned}\mathrm{Gain}(D, a) &= \rho \times \mathrm{Gain}(\tilde{D}, a) \\ &= \rho \times \left(\mathrm{Ent}(\tilde{D}) - \sum_{v=1}^{V} \tilde{r}_v \mathrm{Ent}(\tilde{D}^v)\right)\end{aligned}$$

$$\mathrm{Ent}(\tilde{D}) = -\sum_{k=1}^{|\mathcal{Y}|} \tilde{p}_k \log_2 \tilde{p}_k$$

C4.5:
Probability weights

Assign x(with missing attribute a) to each of the possible value With a probability $\tilde{r}_v \cdot w_x$

A2：将缺失属性的样本按属性值的分布进行分配

缺失值处理
Strategies for missing attribute values

ID	A	B	C	
1	T	NaN	F	Y
2	T	F	NaN	N
3	F	F	F	Y
4	F	T	T	N

ID	A	C
1	T	F
3	F	F
4	F	T

If A=T : C=F
else : C=T
error:30%

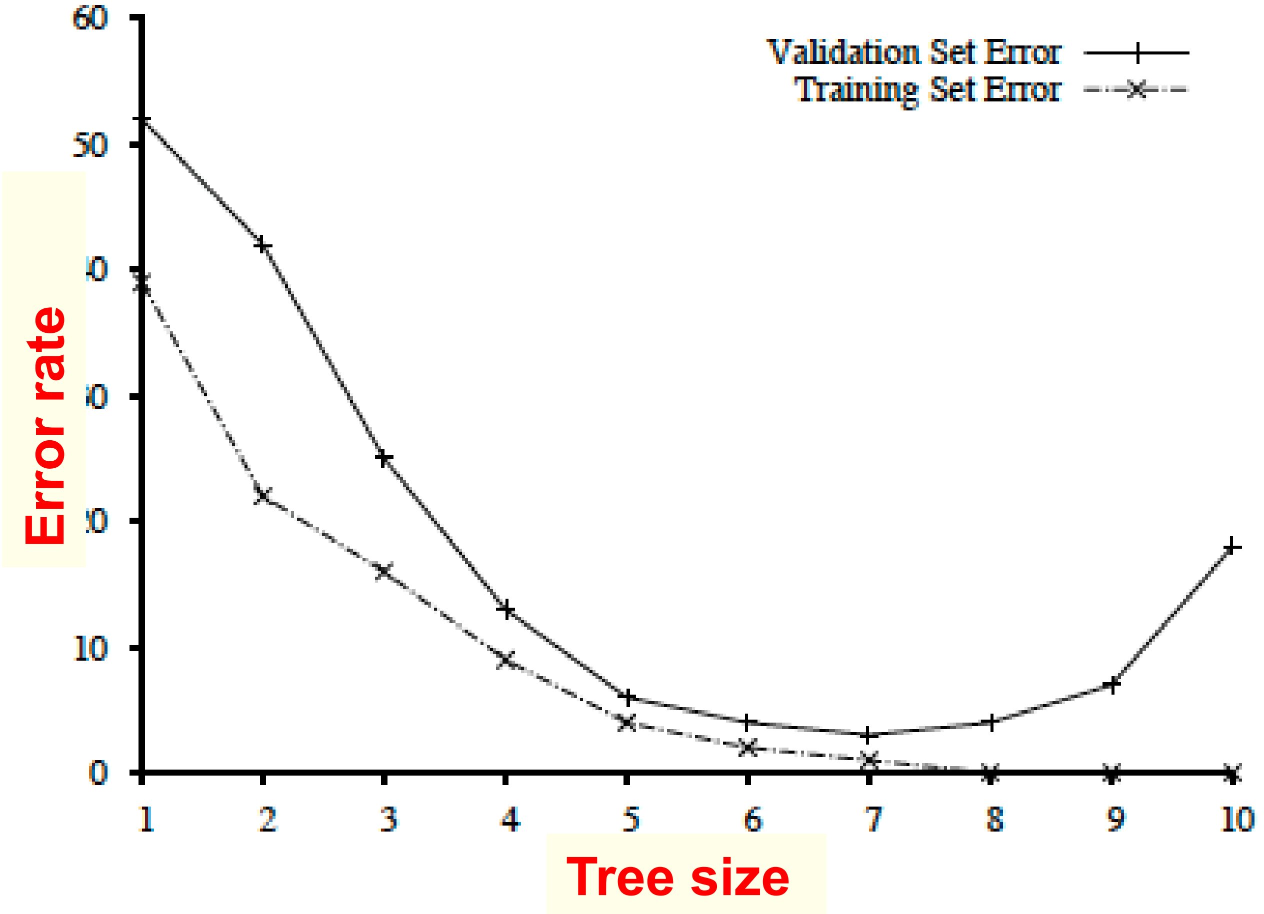
ID	B	C
3	F	F
4	T	T

If B=F : C=F
else : C=T
error:0%

Surrogate Variables order: B<A

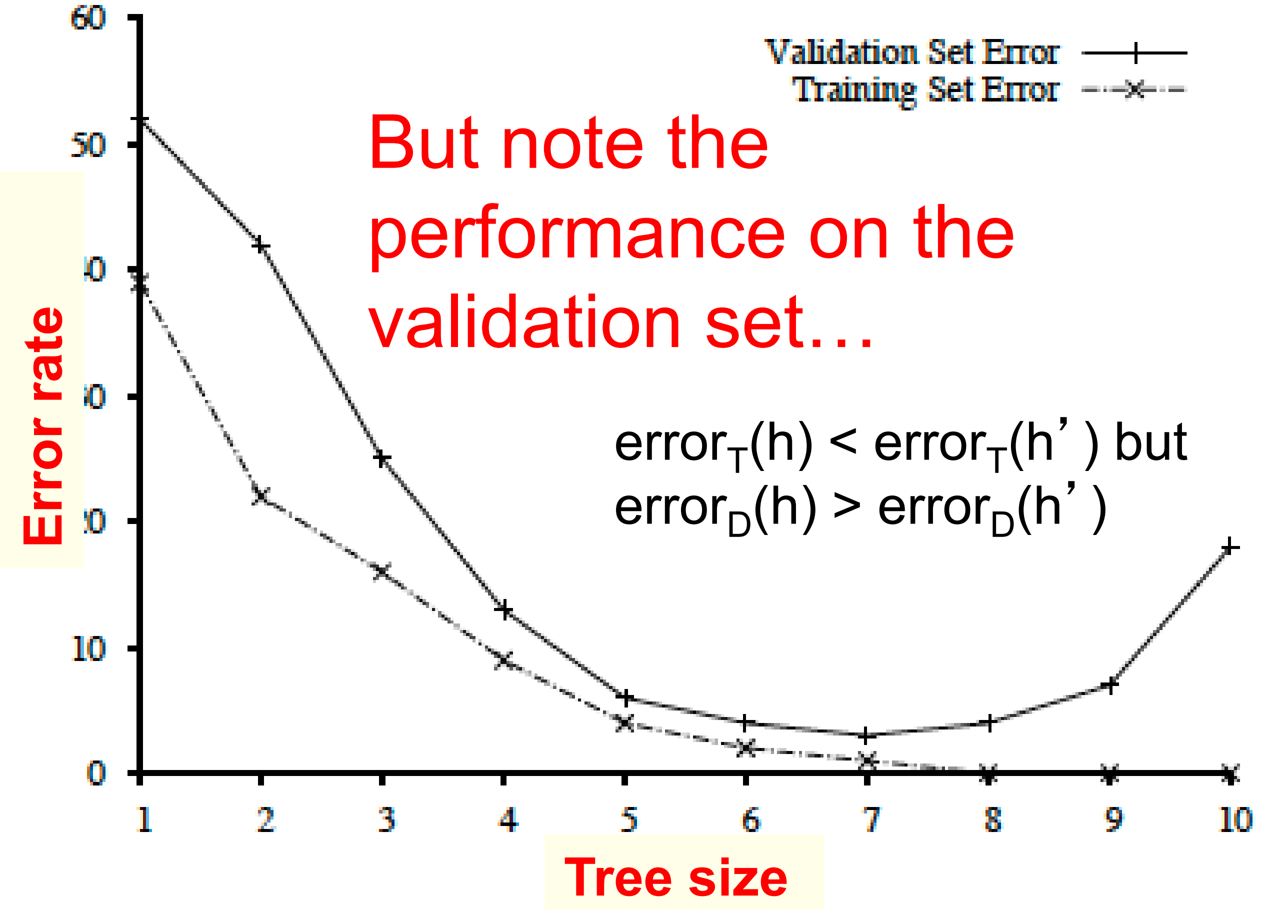
CART:
surrogate splits

树的大小
Tree size



We set tree size as a parameter in our DT learning algorithm
Note: with larger and larger trees,
we just do better and better on the training set!

树的大小
Tree size



But note the performance on the validation set…

$error_T(h) < error_T(h')$ but
$error_D(h) > error_D(h')$

Overfitting!

We set tree size as a parameter in our DT learning algorithm
Note: with larger and larger trees,
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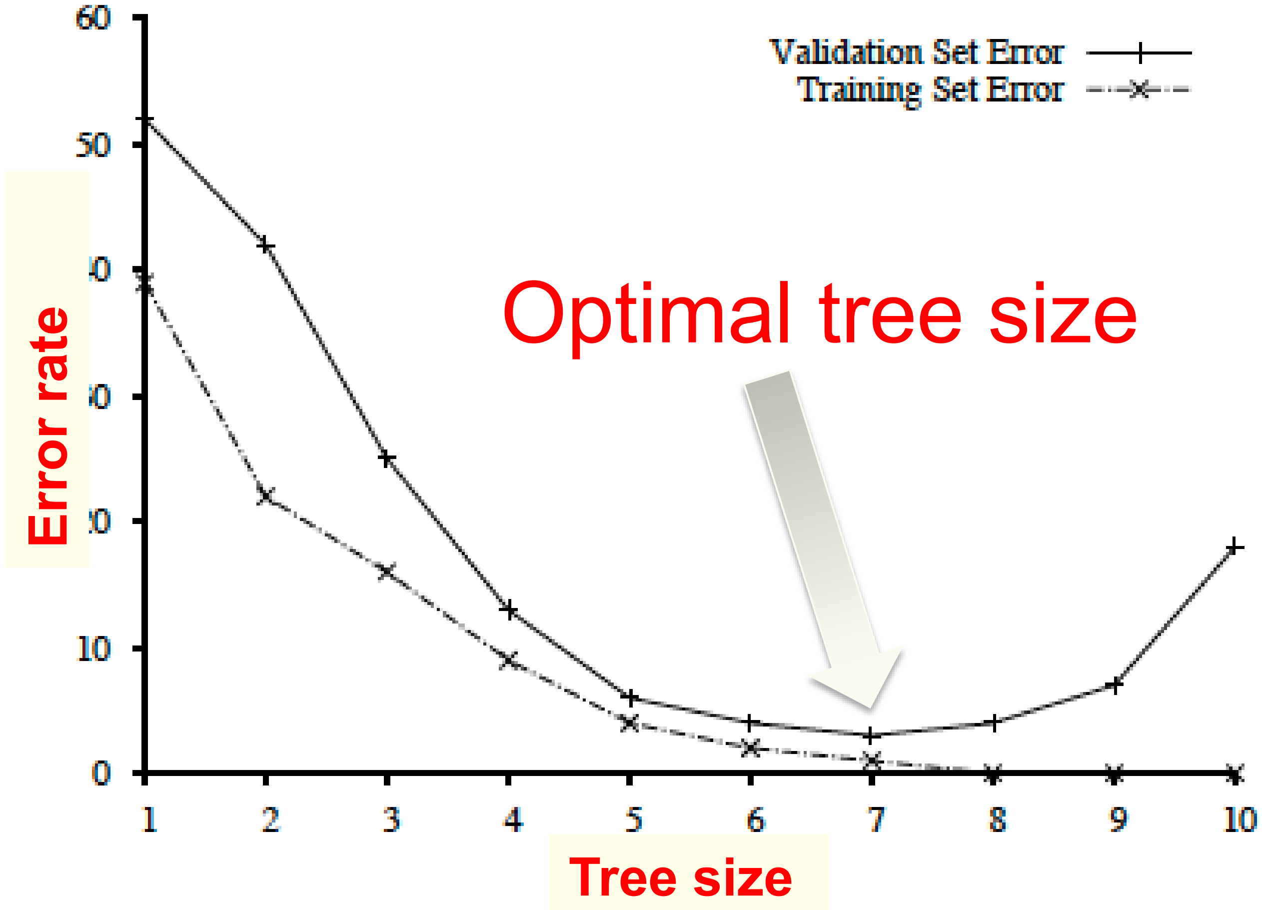
树的大小
Tree size



We set tree size as a parameter in our DT learning algorithm
Note: with larger and larger trees,
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确定树的最优大小
Find optimal tree size

- Procedure for finding the optimal tree size is called ‘model selection’.

  - To determine validation error for each tree size, use k-fold cross-validation.
  - Uses “all data - test set” --- k times splits that set into a training set and a validation set.
  - After right decision tree size is found from the error rate curve on validation data, train on all training data to get final decision tree (of the right size).
  - Finally, evaluate tree on the test data (not used before) to get true generalization error (to unseen examples).

树剪枝
Pruning Trees

- technique for reducing the number of attributes used in a tree – **pruning**

  – Remove subtrees for better generalization (requires a separate pruning set)

  – Two types of pruning:
    - Pre-pruning (forward pruning)
    - Post-pruning (backward pruning)

预剪枝
Prepruning

- In prepruning, we decide during the building process when to stop adding attributes
  - e.g., all attributes have been used; the number of instances in a node has less than a certain threshold; the accuracy can not been improved
  - reduce the risk of overfitting

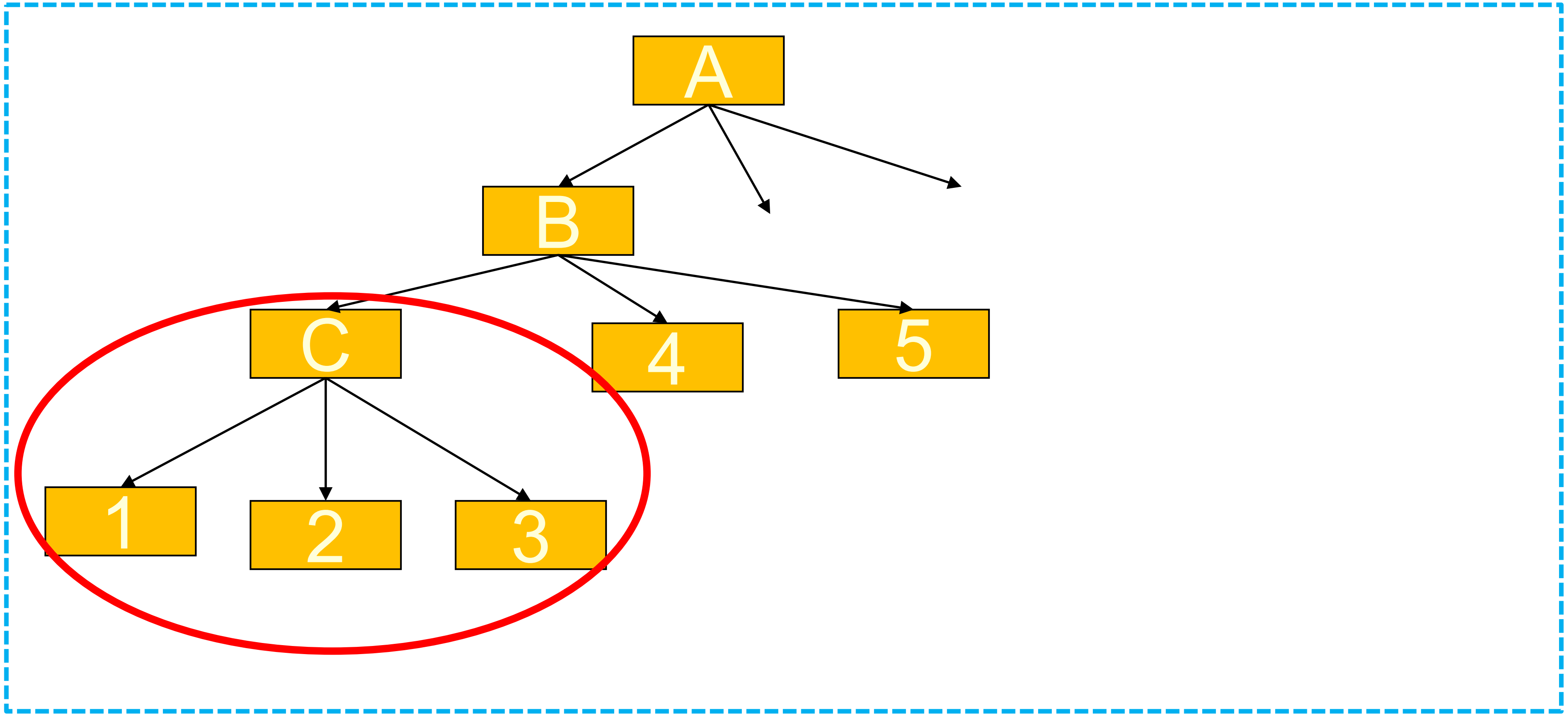
- However, this may be problematic – Why?
  - underfitting
  - Sometimes the current division of some branches can not improve the generalization performance, but the subsequent division on the basis of it may lead to a significant performance improvement

后剪枝
Postpruning

- Postpruning is a technique that waits until a full decision tree is built and then prunes it to remove unnecessary branches, thereby reducing overfitting.
  - Reduced-Error Pruning(REP) : Evaluates the pruning effect using a validation set and removes branches that do not improve validation set performance.
  - Pesimistic-Error Pruning(PEP) ： Commonly used in C4.5 algorithm， this method prunes based on a pessimistic estimation of error.
  - Cost-Complexity Pruning(CCP)： Commonly used in the CART algorithm, this method prunes the tree by minimizing a cost function that balances model complexity and error rate.
- Postpruning techniques:
  - Direct Leaf Pruning, Node Merging, Sibling Merging, Level-Based Pruning
  - Subtree Replacement, Subtree Raising
- Advantages and Disadvantages:
  - Low risk of underfitting
  - Better generalization
  - Longer training time

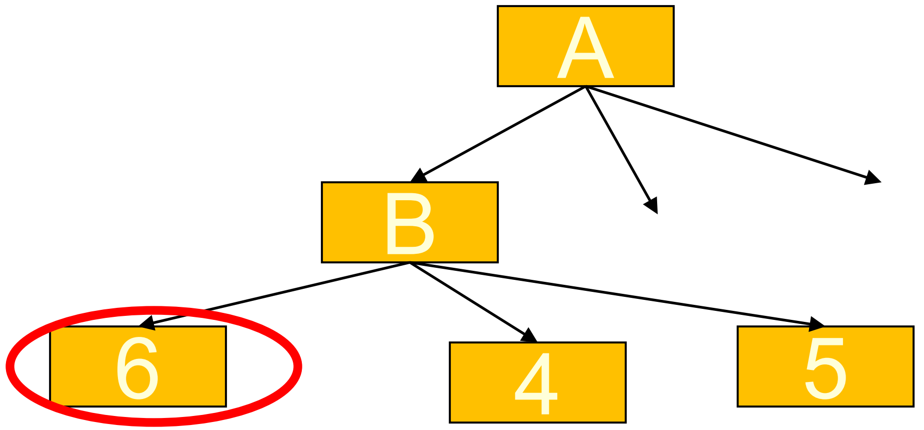
子树代替
Subtree Replacement

- Entire subtree is replaced by a single leaf node



子树代替
Subtree Replacement

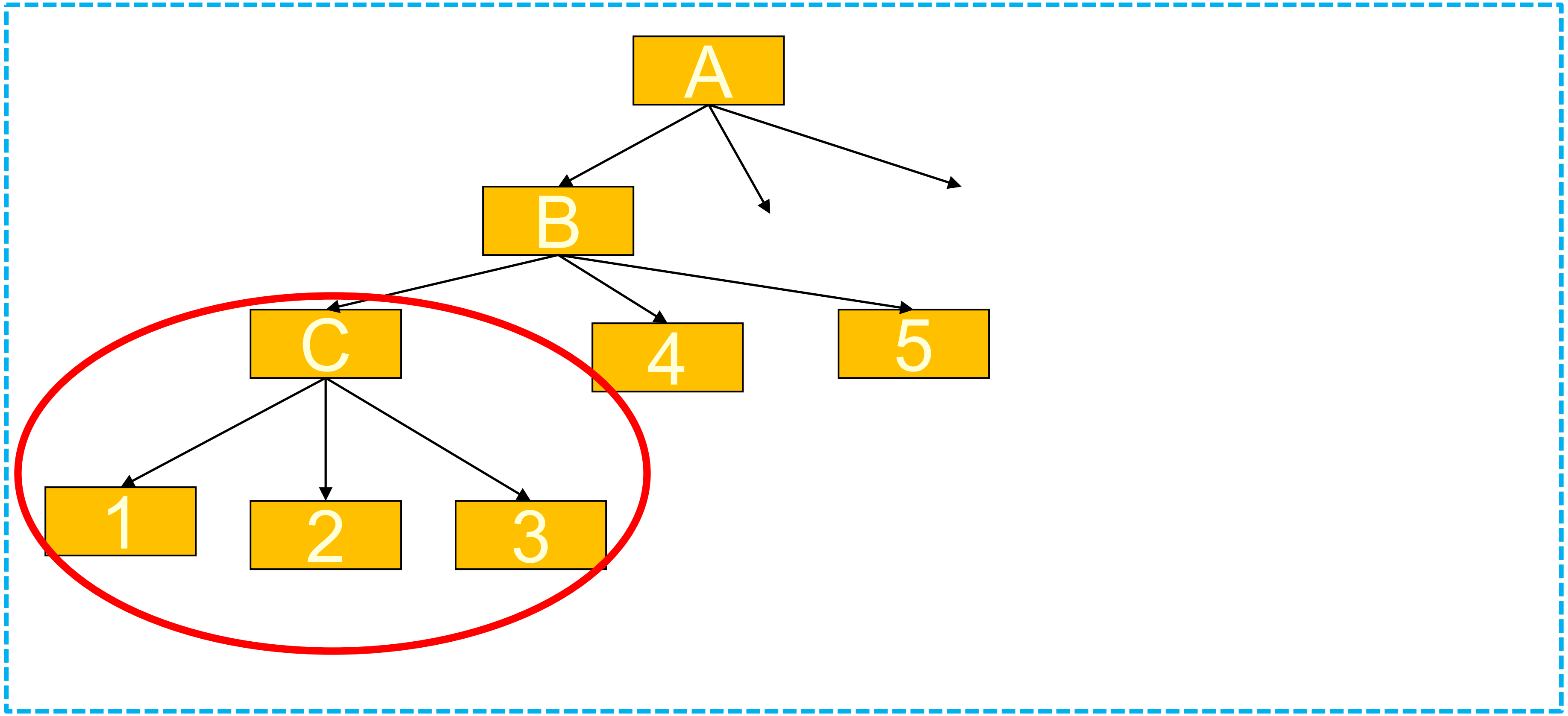
- Entire subtree is replaced by a single leaf node



Generalizes tree a little more,
but may increase accuracy!

子树提升
Subtree Raising

- Entire subtree is raised onto another node



子树提升
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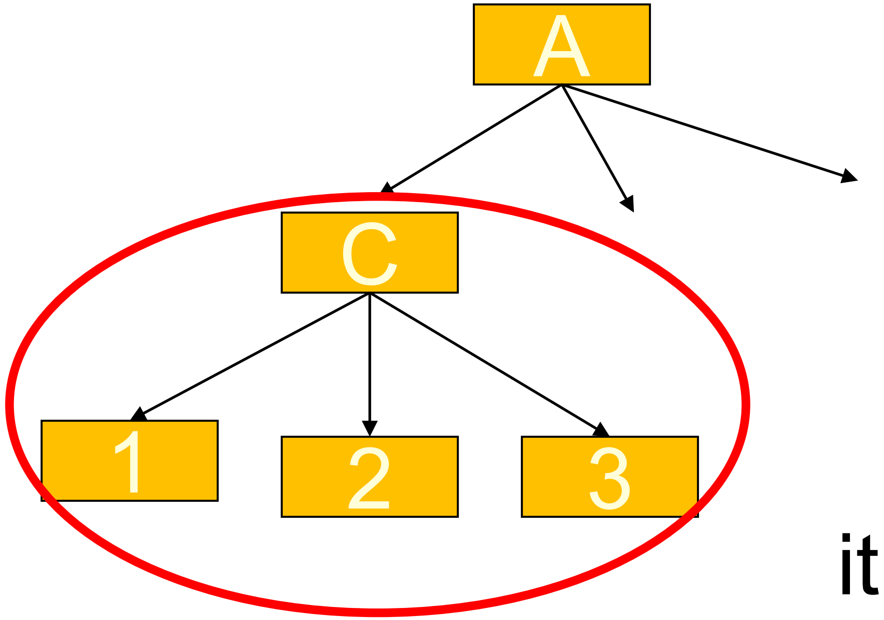
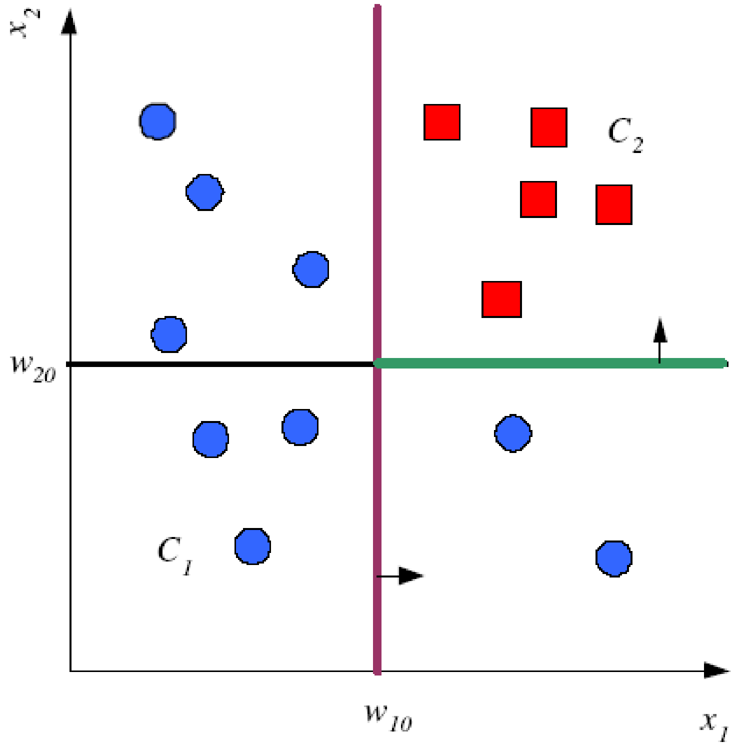


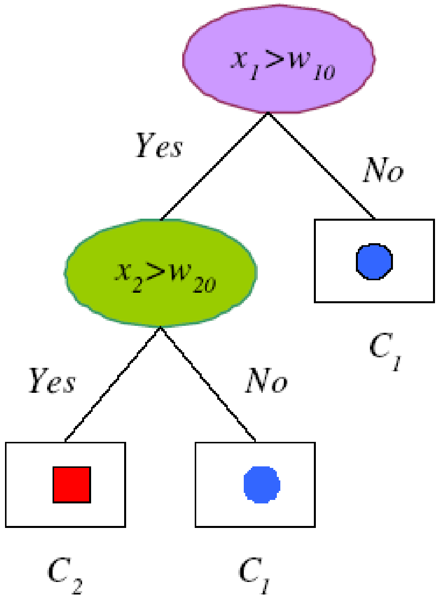
it is very time consuming！

If the subtree provides a good generalization of the ancestor's decisions, the intermediate nodes are pruned away.

决策树分类界面
Decision Boundary

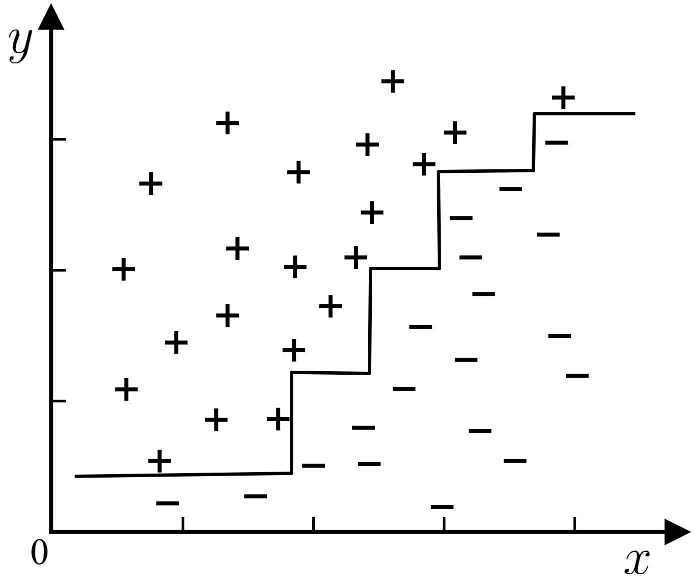
- Decision trees divide the feature space into axis-parallel(hyper-)rectangles
- Each rectangular region is labeled with one label





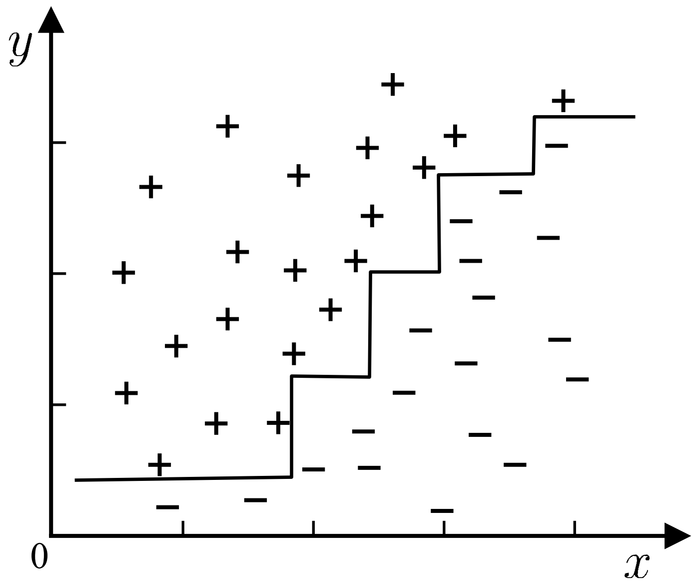
决策树分类界面
Decision Boundary

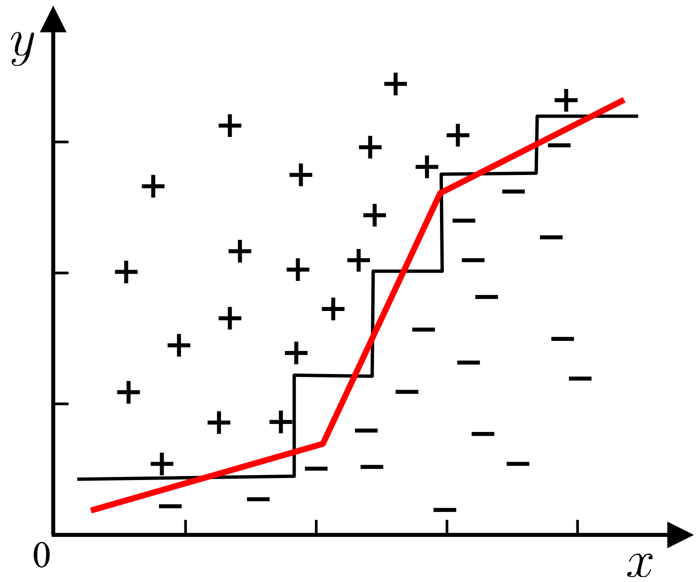
- Many segments must be used to get better approximations when the learning tasks are complex



决策树分类界面
Decision Boundary

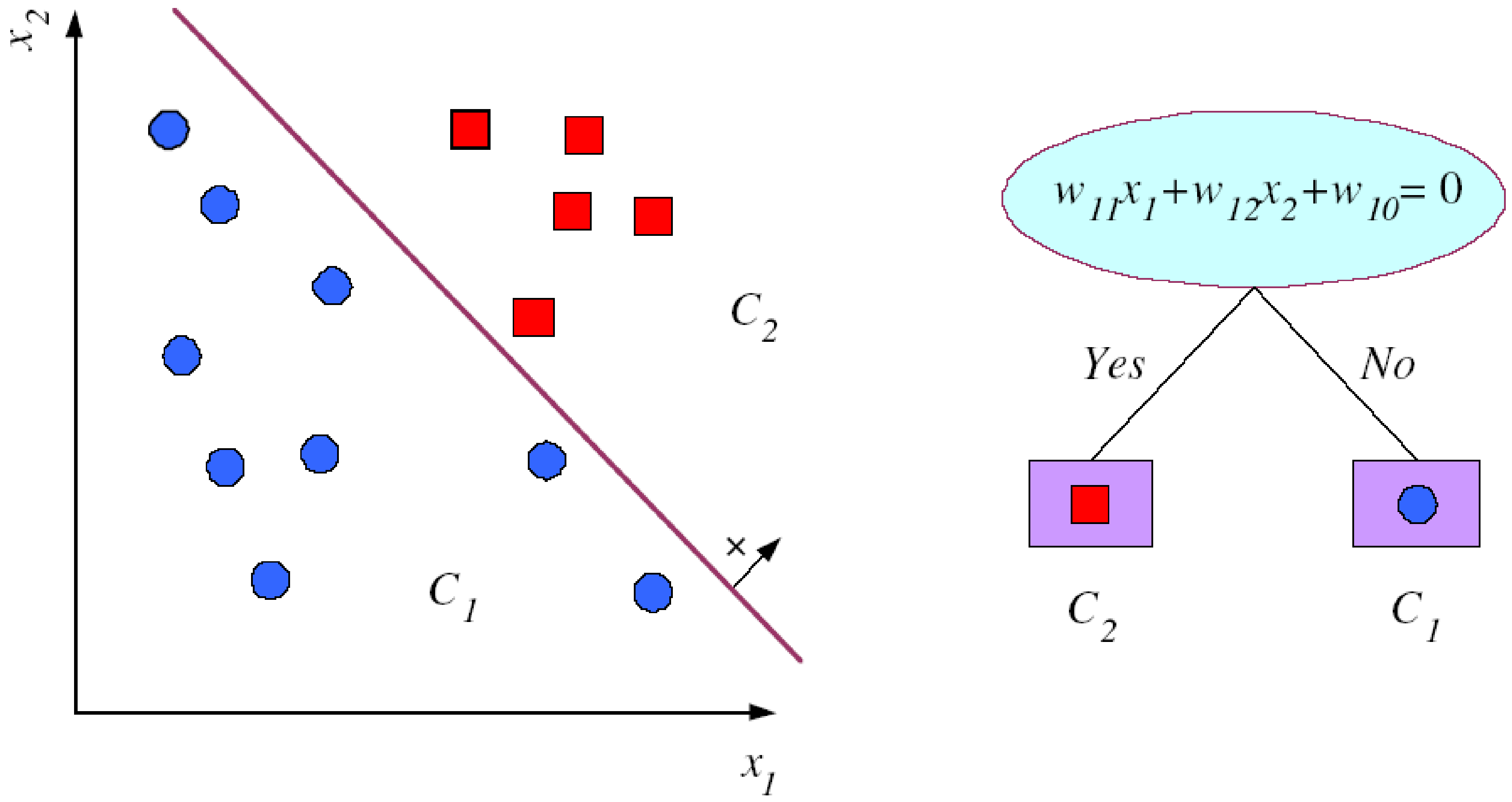
- many segments must be used to get better approximations when the learning tasks are complex



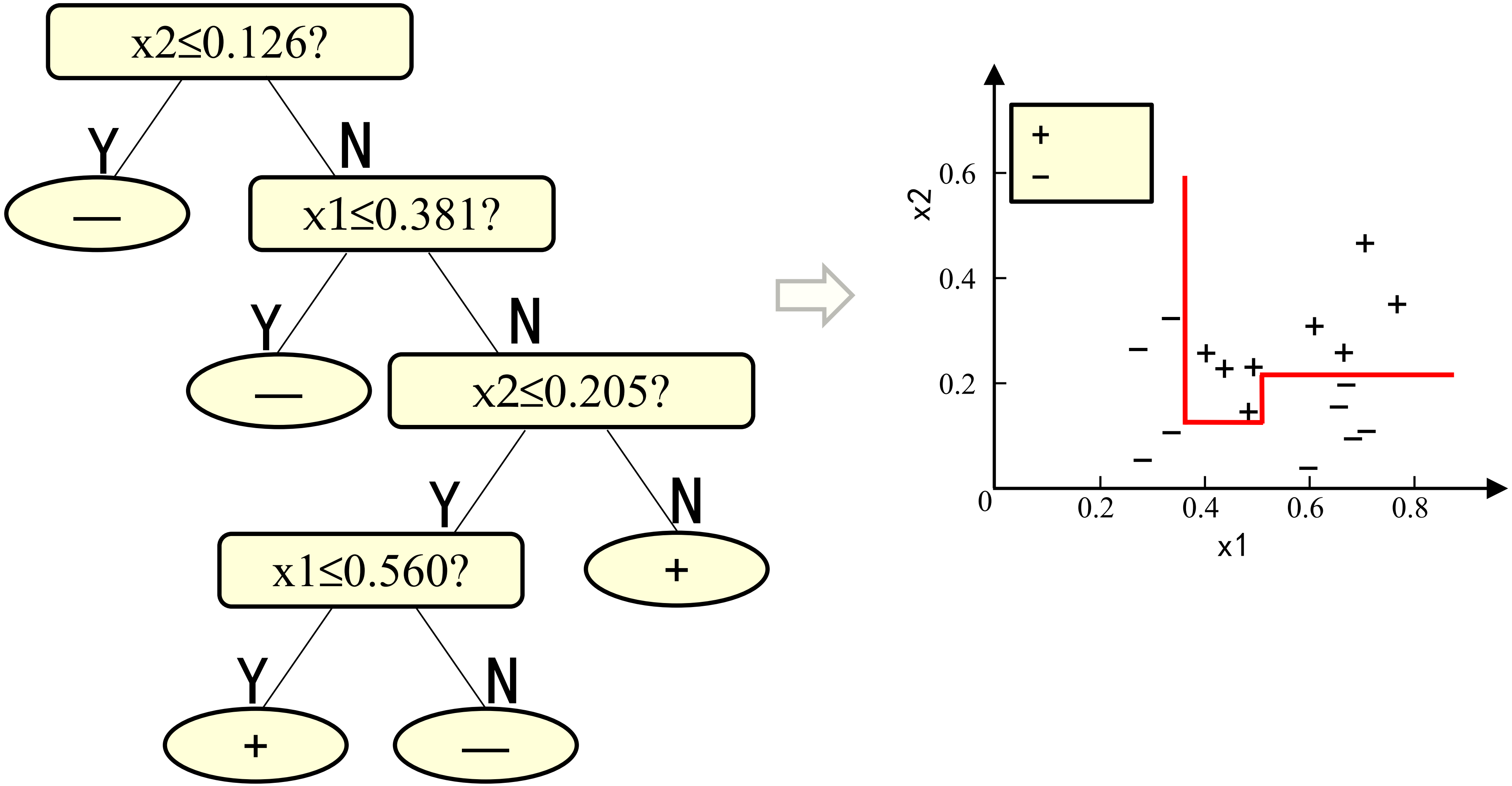


多变量决策树
Multivariate Trees

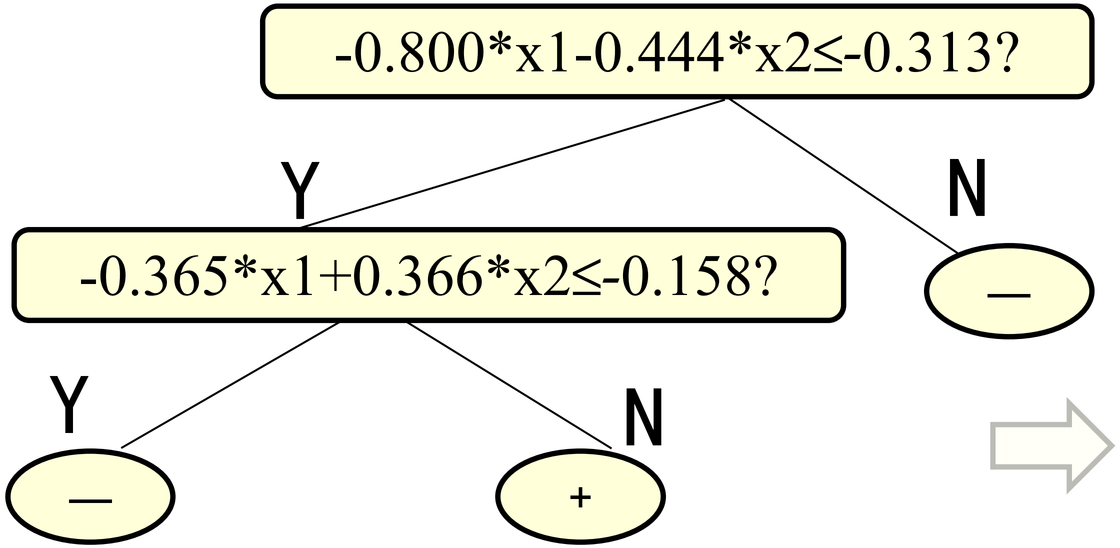
- Internal nodes can test linear combination of attributes

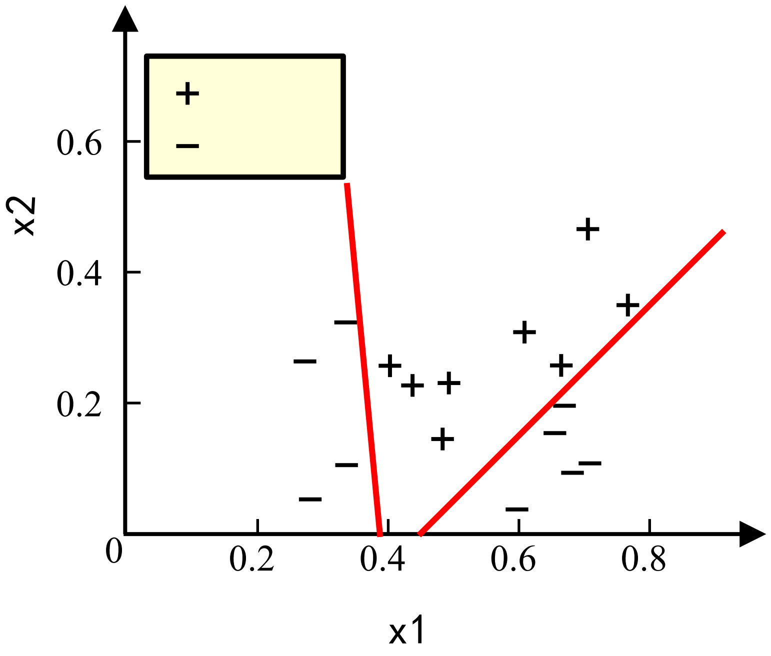


单变量决策树
Univariate Trees



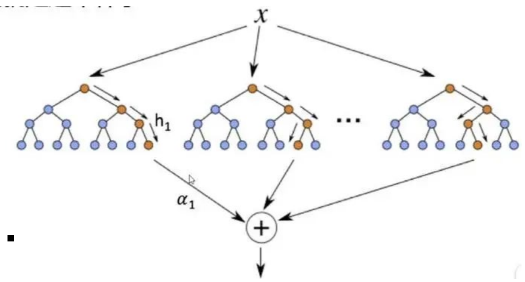
多变量决策树
Multivariate Trees





OC1 [Murthy et al., 1994] [Brodley and Utgoff,1995]

集成模型
Ensemble model



Multiple decision trees are combined to improve the overall performance.

- Random Forest

Each tree is built using a random subset of the data and a random subset of the feature.

Each tree is constructed independently and trained in parallel, with no dependence between them.

- Boosted Tree

Each new tree tries to correct the errors of the previous ones (trained on the residuals)

Trees are built sequentially, with each tree dependent on the previous ones.

  - XGBoost： An efficient and fast gradient boosting algorithm known for its high performance.
  - LightGBM： A lightweight gradient boosting framework optimized for speed and memory efficiency, especially suitable for large datasets.
  - CatBoost : A gradient boosting library designed to handle categorical features efficiently, with automatic handling of categorical data and robust performance even with default parameters.

决策树经典算法小结
Summary of DT algorithms

	support task	criterion structure	tree structure	continuous attribute value	missing attribute value	pruning	attribute multiple use
ID3	classification	Gain information	multiple Tree	No support	No support	No support	No support
C4.5	classification	Gain information rate	multiple Tree	support	support	support	No support
CART	Classification; regression	Gini index; mean square error	binary tree	support	support	support	support

思考题

- 决策树算法是否要做特征缩放？