Decision tree classifier

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Many slides are taken from Jiawei Han at UIUC

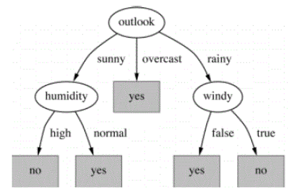
Decision Tree (1/2)

- Training set

feature vector (x_i) y_i: +1:Yes, -1: No

Outlook	Temperature	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	Normal	False	Yes
…	…	…	…	…

- Learned decision tree



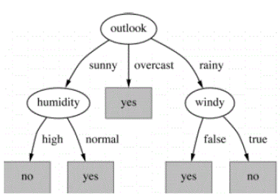
[Note]
Only one feature will be involved at a node

Decision Tree (2/2)

- Example:

(A test instance)

Outlook	Temperature	Humidity	Windy	Play
Rainy	Hot	High	True	?

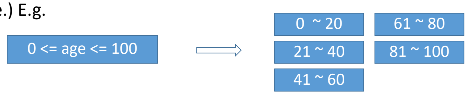


Ans: no

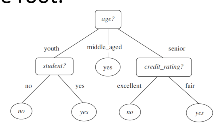
How to generate a classification tree?

Algorithm for Decision Tree Induction

- Basic algorithm (a **greedy algorithm**)
  - Tree is constructed in a top-down recursive divide-and-conquer manner.
  - Attributes are categorical.
    (if an attribute is a continuous number, it needs to be discretized in advance.) E.g.



  - At start, all the training examples are at the root.
  - Examples are partitioned recursively based on selected attributes.

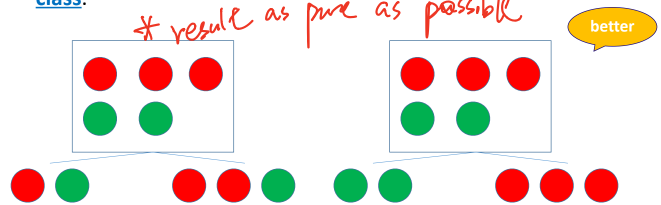


* which Q be first?
question

Algorithm for Decision Tree Induction

- Basic algorithm (a **greedy algorithm**)
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain): maximizing an information gain measure, i.e., **favoring the partitioning which makes the majority of examples belong to a single class**.

* result as pure as possible



Algorithm for Decision Tree Induction

- Basic algorithm (a **greedy algorithm**)
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain): maximizing an information gain measure, i.e., **favoring the partitioning which makes the majority of examples belong to a single class**.
- Examples of conditions for stopping partitioning:
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left

Primary Issues in Tree Construction (1/2)

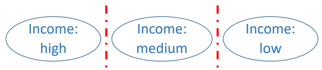
(多 pure)

- **Split criterion**: *Goodness function*
  - Used to select the attribute to be split at a tree node during the tree generation phase
  - Different algorithms may use different goodness functions:
    - Information gain (used in ID3)
    - Gain ratio (used in C4.5)
    - Gini index (used in CART)

not only

Primary Issues in Tree Construction (2/2)

- **Branching scheme**:
  - Determining the tree branch to which a sample belongs
  - Binary vs. *k-ary* splitting



- When to stop the further splitting of a node? e.g. impurity measure
- Labeling rule: a node is labeled as the class to which most samples at the node belongs.

How to Use a Tree?

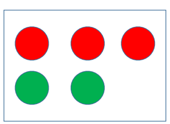
- Directly
  - Test the attribute value of unknown sample against the tree.
  - A path is traced from root to a leaf which holds the label.
- Indirectly
  - Decision tree is converted to classification rules.
  - One rule is created for each path from the root to a leaf.
  - **IF-THEN** might be easier for humans to understand .

Expected Information (Entropy)

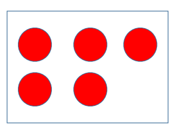
- Expected information (entropy) needed to classify a tuple in D:

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

(p_i: probability that a tuple in D belongs to class C_i, m: number of classes)



$$Info(D) = I(3,2) = -\frac{3}{5}\log_2(\frac{3}{5}) - \frac{2}{5}\log_2(\frac{2}{5})$$
$$\approx -\frac{3}{5}\times(-0.737) - \frac{2}{5}\times(-1.322)$$
$$\approx 0.971$$

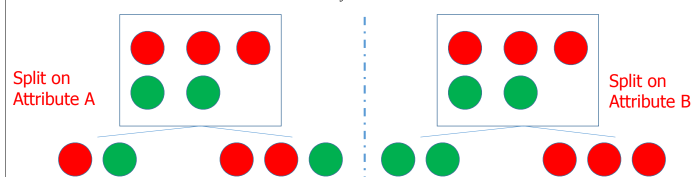


$$Info(D) = I(5,0) = -\frac{5}{5}\log_2(\frac{5}{5}) - \frac{0}{5}\log_2(\frac{0}{5})$$
$$= 0 - 0 = 0$$

Expected Information (Entropy)

- Information needed (after using A to split D into v partitions) to classify D:

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j)$$

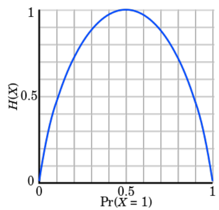


$$Info_A(D) = \frac{2}{5} Info(1,1) + \frac{3}{5} Info(2,1) = 0.918$$
$$Gain(A) = Info(D) - Info_A(D)$$
$$= 0.971 - 0.918 = 0.053$$

$$Info_B(D) = \frac{2}{5} Info(2,0) + \frac{3}{5} Info(3,0) = 0$$
$$Gain(B) = Info(D) - Info_B(D)$$
$$= 0.971 - 0 = 0.971$$

Expected Information (Entropy)

- Entropy is a measurement of uncertainty (or randomness, untidiness)
- Entropy H(X) of a coin flip
  - X: the probability of getting a head
- If the coin is fair, then entropy of the next flip is maximized
  - This is the situation of maximum uncertainty, since it is most difficult to predict the outcome
- If the coin is unfair, there is less uncertainty
  - One side is more likely to come up than the other
- Extreme case: a double-headed or a double-tailed coin
  - There is no uncertainty
  - The entropy is zero



Attribute Selection Measure: Information Gain (ID3)

- Select the attribute with the highest information gain
  - To minimize # of tests needed to classify a given tuple
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i; p_i is estimated by $|C_{i,D}|/|D|$
- Expected information (entropy) needed to classify a tuple in D:

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

- Information needed (after using A to split D into v partitions) to classify D:

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j)$$

- Information gained by branching on attribute A

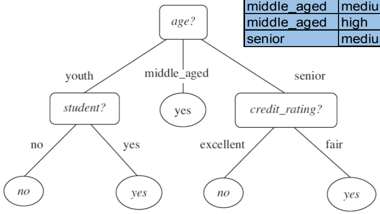
We'd like to maximize Gain(A), i.e., to minimize $Info_A(D)$, the information still required to finish classifying the tuples

$$Gain(A) = Info(D) - Info_A(D)$$

Decision Tree Induction: An Example

- Training data set: Buys_computer
- Resulting tree:

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no



Attribute Selection: Information Gain

ID
1
2
3
14

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

yes

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) = 0.940$$

no

Attribute Selection: Information Gain

age	p_i	n_i	$I(p_i, n_i)$
youth	2	3	0.971
middle_aged	4	0	0
senior	3	2	0.971

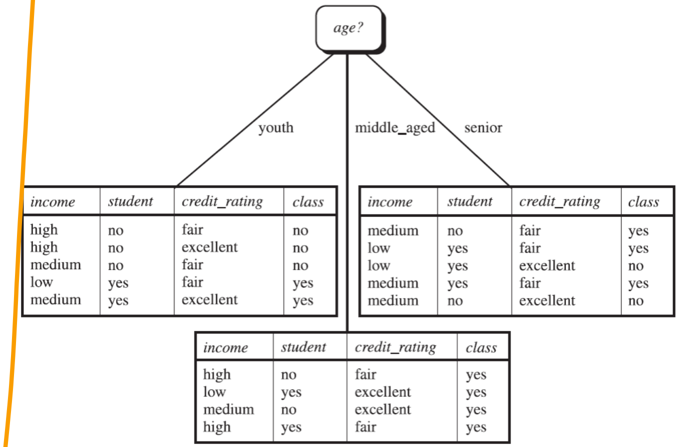
- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

- $Info_{age}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$
- $\frac{5}{14}I(2,3)$: age="youth" appears in 5 out of 14 samples, with 2 positive and 3 negative examples
- $Gain(age) = Info(D) - Info_{age}(D) = 0.246$
- Similarly, we can get
- $Gain(income) = 0.029$
- $Gain(student) = 0.151$

比較如果用其它分的 gain

Gain(student) = 0.151

Gain(credit_rating) = 0.048



income	student	credit_rating	class
high	no	fair	no
high	no	excellent	no
medium	no	fair	no
low	yes	fair	yes
medium	yes	excellent	yes

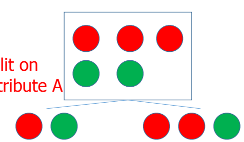
income	student	credit_rating	class
high	no	fair	yes
low	yes	excellent	yes
medium	no	excellent	yes
high	yes	fair	yes

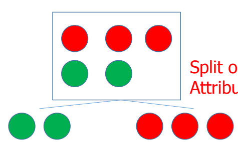
income	student	credit_rating	class
medium	no	fair	yes
low	yes	fair	yes
low	yes	excellent	no
medium	yes	fair	yes
medium	no	excellent	no

Quiz

- Which of the following has a higher entropy?
  - (O,O,X,X) vs (O,O,X,X,X) vs (O,O,O)
- Which attribute (A or B) will be selected by a decision tree classifier based on information gain?

Split on Attribute A





Split on Attribute B

※ 若用 Info gain 分類, feature 如有 ID 会很没用

Gain Ratio for Attribute Selection (C4.5)

- Information gain measure is biased towards attributes with a large number of values
  - E.g., unique pID -> split on pID results in large number of partitions, each containing just one tuple => each partition is pure => information required to classify this partition would be ***$Info_{pID}(D)=0$***, i.e., the information gain is maximal!!
- C4.5 (a successor of ID3) uses gain ratio to overcome the problem (normalization to information gain)

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right)$$

, If A has many 不同 value, splitinfo tend to high

  - GainRatio(A) = Gain(A)/SplitInfo(A)
- The attribute with the maximum gain ratio is selected as the splitting attribute

Example of Gain Ratio

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no

income=high: 4
income=medium: 6
income=low: 4

- $SplitInfo_{income}(D) = -\frac{4}{14}\log_2\left(\frac{4}{14}\right) - \frac{6}{14}\log_2\left(\frac{6}{14}\right) - \frac{4}{14}\log_2\left(\frac{4}{14}\right) \approx 1.557$
- $GainRatio(income) = Gain(income)/SplitInfo_A(D) = \frac{0.029}{1.557} \approx 0.019$

* If ID, $SplitInfo_{ID}(D) = \sum_{i=1}^{14} \frac{1}{14} \log 14 \rightarrow GainRatio = \frac{0.029}{\log 14}$ 很低

Quiz

- Given students' ID, height, weight, and gender as the training data, you are asked to build a decision tree classifier to predict a student's gender based on her/his ID, height, and weight
  - Which attribute (ID, height, or weight) is likely to be selected first if you use information gain as the attribute selection method?

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Gini Index (CART, IBM IntelligentMiner)

expect higher　　　lower

- If a data set D contains examples from n classes, impurity measure is calculated by Gini index, $Gini(D)$

ex: $p_1 = p_2 = \frac{1}{2}$　　$p_1 = \frac{1}{4}$ $p_2 = \frac{3}{4}$

$1-(\frac{1}{2})^2-(\frac{1}{2})^2 = \frac{1}{2}$　　$1-(\frac{1}{4})^2-(\frac{3}{4})^2 = \frac{6}{16}$

$$Gini(D) = 1 - \sum_{i=1}^{m} p_i^2$$

where p_i is the probability of class C_i in D, estimated by $|C_{i,D}|/|D|$

- If a data set D is split on A into subsets D_i, the *Gini* index $Gini_A(D)$ given the split on A is:

$$Gini_A(D) = \sum_i \frac{|D_i|}{|D|} Gini(D_i)$$

- Reduction in Impurity:

$\Delta Gini(A) = Gini(D) - Gini_A(D)$

- The attribute provides the largest reduction in impurity, i.e., maximized $\Delta Gini(A)$, is chosen to split the node (*need to enumerate all the possible cut-point for each attribute*)

Example of Gini index

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no

- D has **9** tuples in **buys_computer = "yes"** and **5** in **"no"**
- $Gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$

Example of Gini index

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no

When income = “high”
➔ 2 “yes” and 2 “no”

When income = “medium”
➔ 4 “yes” and 2 “no”

When income = “low”
➔ 3 “yes” and 1 “no”

- $Gini_{income}(D) = \frac{4}{14}\left(1-\left(\frac{2}{4}\right)^2-\left(\frac{2}{4}\right)^2\right)+\frac{6}{14}\left(1-\left(\frac{4}{6}\right)^2-\left(\frac{2}{6}\right)^2\right)$

$$+\frac{4}{14}\left(1-\left(\frac{3}{4}\right)^2-\left(\frac{1}{4}\right)^2\right)=0.325$$

- $\Delta Gini(income) = Gini(D) - Gini_{income}(D) = 0.134$

Quiz

- Can we apply Decision Tree Classifier on the datasets with only numerical attributes?

HW

Computing Information-Gain for Continuous-Valued Attributes

- Let attribute A be a continuous-valued attribute
- Must determine the *best split point* for A
  - Sort the value A in increasing order
  - Typically, the midpoint between each pair of adjacent values is considered as a possible *split point*
    - $(a_i+a_{i+1})/2$ is the midpoint between the values of a_i and a_{i+1}
  - The point with the *minimum expected information requirement* for A is selected as the split-point for A
- Split:
  - D1 is the set of tuples in D satisfying A ≤ split-point, and D2 is the set of tuples in D satisfying A > split-point

Example of Information-Gain for Continuous-Valued Attributes

Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

看怎分 purity 最高

- Sort the continuous-valued attributes
- Determine the classifier’s changing points
  - E.g., (48-60) and (80-90) in the above example
- Take the mid-points of the changing points as the candidates for discretization
  - E.g., (48+60)/2, (80+90)/2
- Use “54” to split
  - If Temperature <= 54 ➔ No; Else ➔ Yes
  - Gain(T=54) = Info(D) – $Info_{T=54}$(D) = 1 – 0.811 = 0.189
- Use “85” to split
  - If Temperature <= 85 ➔ Yes; Else ➔ No
  - Gain(T=85) = Info(D) – $Info_{T=85}$(D) = 1 – 0.696 = 0.304

Comparing Attribute Selection Measures

- The three measures, in general, return good results but
  - **Information gain**:
    - biased towards multivalued attributes
  - **Gain ratio**:
    - tends to prefer unbalanced splits in which one partition is much smaller than the others
  - **Gini index**:
    - biased to multivalued attributes
    - Usually faster than information gain (because information gain requires logarithm computation)

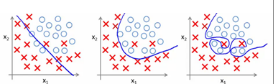
Why 很多人用 Gini? ∵ $O(\text{Gini}) = n^2 > O(\text{Gain, IG}) = \log n$?

Many Attribute Selection Measures

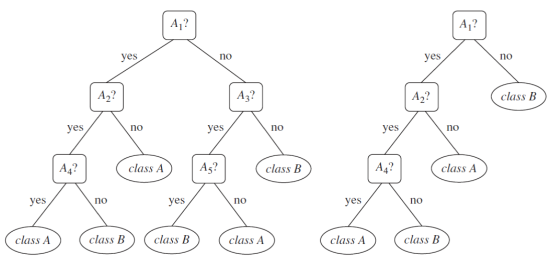
- **Which attribute selection measure is the best?**
  - **Most give good results, none is significantly superior than others**

Overfitting and Tree Pruning

- Overfitting: An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples, i.e., lose the ability of generalization



underfitting overfitting



Overfitting and Tree Pruning

- Perfect decision tree performs 100% accuracy on the training data
  - Assuming that in the training data if two instances have the same feature sets then they must have the same label
- Prevent overfitting
  - Pre-prune the tree
    - Stop before a tree is fully grown
      - E.g., limit the tree height; stop when the number of instances in a node is small; when misclassification rate is low enough
    - The method is short-sighted
      - A seemly worthless early split may be followed by a very good split
  - Post-prune the tree
    - Grow a perfect tree and prune the nodes from bottom up
    - $R_\alpha(T) = R(T) + \alpha \cdot |f(T)|$

Training error # leaves

small small

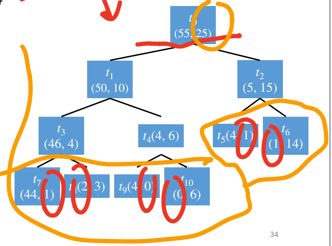
Post-pruning considerations

- Goal: cut a large portion of a tree, but only increase few error rate
- The two requests are usually against each other
- We may define the goodness of a cut by
  - $\alpha(t_i) = \dfrac{\#\text{ error after cut} - \#\text{ error before cut}}{\#\text{ leaves been cut} - 1}$ (小) (大)

(小)

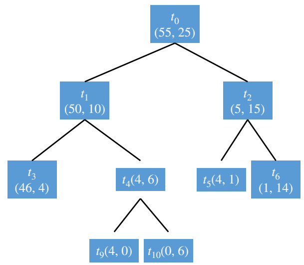
Example

- $\alpha(t_i) = \dfrac{\#\text{ error after cut} - \#\text{ error before cut}}{\#\text{ leaves been cut} - 1}$
- $\alpha(t_0) = ?$
  - If we cut the tree and leave only t_0, # errors = 25
  - If we don't cut the tree, # errors = 1+2+0+0+1+1=5
  - If we cut the tree, 6 leaves are cut
  - $\alpha(t_0) = \dfrac{25 - (1+2+0+0+1+1)}{6-1} = 4$
- By a similar manner, we may obtain
  - $\alpha(t_1) = \dfrac{10 - (1+2+0+0)}{4-1} = 2.33$
  - $\alpha(t_2) = \dfrac{5 - (1+1)}{2-1} = 3$
  - $\alpha(t_3) = \dfrac{4 - (1+2)}{2-1} = 1$ ➔ Cut here!
  - $\alpha(t_4) = \dfrac{4 - (0+0)}{2-1} = 4$



Example

- $\alpha(t_0) = \dfrac{25 - (4+0+0+1+1)}{5-1} = 4.75$
- $\alpha(t_1) = \dfrac{10 - (4+0+0)}{3-1} = 3$ ➔ Cut here!
- $\alpha(t_2) = \dfrac{5 - (1+1)}{2-1} = 3$
- $\alpha(t_4) = \dfrac{4 - (0+0)}{2-1} = 4$



Classification tree is constructed in a "greedy" manner

- Greedy: pick a feature to split the data best on the ***current*** information
  - This may lead to a local optimal

Example

A	B	C	label
1	0	1	1
0	1	0	1
0	1	1	1
0	0	0	0
1	1	1	0
…			

We build an imaginary dataset as follows

- The dataset has three binary features A, B, and C
- The label is constructed by A xor B
- C is set to label for 80% of the time and the inverse of the label for 20% of the time

On average, $Info_A(D) = 1$ entropy

- When A=1, 50% of the labels are 1 and 50% of the labels are 0
- When A=0, 50% of the labels are 1 and 50% of the labels are 0

Similarly, $Info_B(D) = 1$

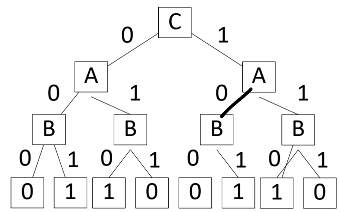
On average, $Info_C(D) = 0.722$

- When C=1, 80% of the labels are 1; 20% of the labels are 0
- When C=0, 80% of the labels are 0; 20% of the labels are 1

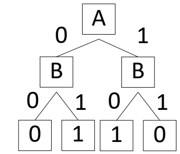
In the case, we will choose feature *C* as the feature to split data

However, an oracle should first select one feature from A or from B, and select the other feature as the second feature

Which one is better?



✓

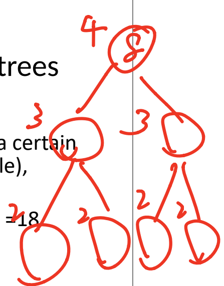


- Occam's razor
  - Among competing hypotheses, the one with the fewest assumptions should be selected.

Why not try all possible attribute splitting sequences?

- The best tree requires to test all possible sequences
  - Very large search space
  - If the training data have *d* binary features, consider one path from root to one leaf:
    - *d* possible roots
    - *d*-1 possible level-1 nodes
    - *d*-2 possible level-2 nodes
    - …
    - This is just one path from root to one leaf, there are *d* different leaves
  - If there are numerical attributes, the number of trees is even larger
    - Why?

An example of testing all trees vs decision trees

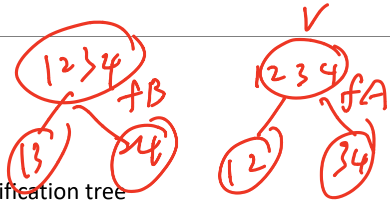


level-1

- Suppose we want to predict whether an individual has a certain disease based on 4 binary features: gender (male/female), height (tall/short), weight (fat/thin), age (young/old)
- Decision tree: need to test approximately 4 + 3*2 + 2*4 =18 splits
  - 4: root split test 4 features
  - 3*2: each level-1 node test 3 features; 2 level-1 nodes
  - 2*4: each level-1 node test 2 features; 4 level-1 nodes

level-2

- List all tress: need to test approximately 4 * 3*2 * 2*4 = 192
  - 4: root split test 4 features
  - 3*2: each level-1 node test 3 features; 2 level-1 nodes
  - 2*4: each level-1 node test 2 features; 4 level-1 nodes

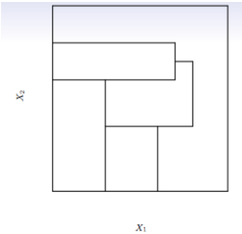


Regression tree

- A brief review of classification tree
  - Select a feature *A* and a cut-point *v* to split the original dataset *D* into sub-groups such that **the labels** in each sub-group are as pure as possible
  - Repeat the above step
- Regression tree
  - Select a feature *A* and a cut-point *v* to split the original dataset *D* into sub-groups such that **the target values** in each group is as pure as possible
    - There could be multiple ways to define "purity"
    - Possible choices: RSS (residual sum of squares), max-min, variance
  - Repeat the above step

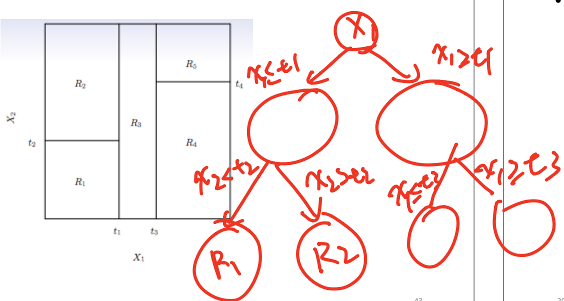
Quiz

- You are asked to build a decision tree classifier based on two features x1 and x2. How to partition the space into the following figure?



Quiz

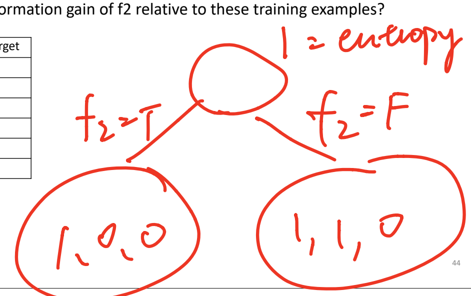
- You are asked to build a decision tree classifier based on two features x1 and x2. How to separate the space into the following figure?



Quiz

- True or false: if decision tree T2 is a pruned tree of tree T1, then T1 is less likely to overfit the training data
- Consider the following training data
  - What is the entropy of the training examples? one
  - What is the information gain of f2 relative to these training examples?

f1	f2	Target
T	T	1
T	F	1
T	T	0
F	F	1
F	T	0
F	F	0



$\frac{3}{6}\left(-\frac{1}{3}\log\frac{1}{3}-\frac{2}{3}\log\frac{2}{3}\right)+\frac{3}{6}\left(-\frac{1}{3}\log\frac{1}{3}-\frac{2}{3}\log\frac{2}{3}\right)$

Random forest

- A random forest is a **meta estimator** that fits numerous decision tree classifiers on various sub-samples of the dataset
  - Each tree can use only part of the available features
    - A common practice is using sqrt(n_features)
  - Sub-sampling the training data for each tree
    - A common practice: the sub-sample size is always the same as the original input sample size, but the samples are ***<u>drawn with replacement</u>***
- The prediction is based on the majority voting of all the generated decision trees
  - Prevent overfitting
  - Usually yield higher test accuracy
- Highly parallelizable during training and testing
- One of the best predictor in many applications and competitions

Info gain = entropy 1 − entropy 2

分前 − 分後

Summary

- Decision tree generates a set of classification/ regression rules based on the training data
- "Interpretable" prediction

* P.12

$= 0.918$

$Info_A(D) = \frac{2}{5} Info(1,1) + \frac{3}{5} Info(2,1)$ $\quad Info_B(D) = \frac{2}{5} Info(2,0) + \frac{3}{5} Info(3,0) = 0$

$Gain(A) = Info(D) - Info_A(D) = \cancel{0.918}$

$= 0.971 - 0.918 = 0.053$

$Gain(B) = Info(D) - Info_B(D)$

$= 0.971 - 0 = 0.971$

befor分 − afeer分 = Improvement of puriey