

Supervised Learning

Decision Trees

Road Map

1. Basic Concepts of Classification
2. Decision Tree Induction
3. Attribute Selection Measures
4. Pruning Strategies

Definition

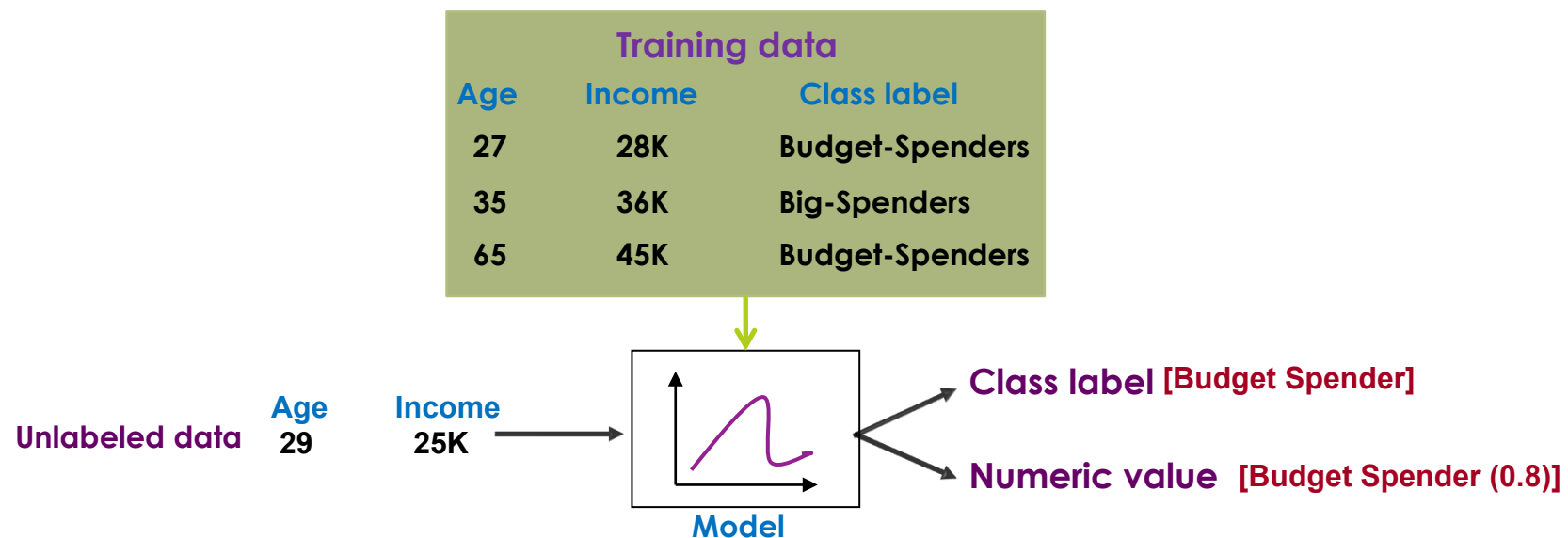
■ Supervised Learning is also called **Classification (or Prediction)**

■ **Principle**

■ Construct models (functions) based on training data

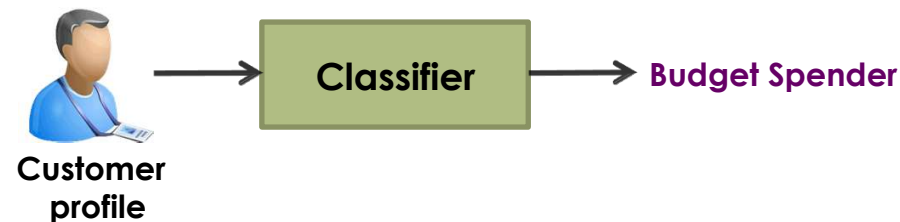
■ The training data are **labeled** data

■ New data (**unlabeled**) are classified using the training data

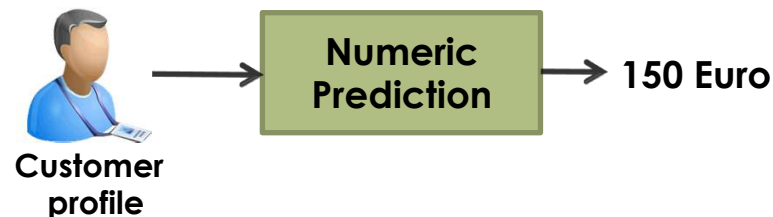


Classification vs Prediction

- ▣ **Classification** predicts categorical class labels (discrete or nominal)



- ▣ **Prediction** models continuous-valued functions, i.e., predicts unknown or missing values (ordered values)



- ▣ **Regression** analysis is used for prediction

Entropy: Bits

- You are watching a set of independent random samples of X
- X has 4 possible values: A, B, C, and D
- The probabilities of generating each value are given by:

$$P(X=A)=1/4, P(X=B)=1/4, P(X=C)=1/4, P(X=D)=1/4$$

- You get a string of symbols ACBABBBCDADDC...
- To transmit the data over binary link you can encode each symbol with bits (A=00, B=01, C=10, D=11)

Entropy: Bits

- Now someone tells you the probabilities are not equal

$$P(X=A)=1/2, P(X=B)=1/4, P(X=C)=1/8, P(X=D)=1/8$$

- In this case, it is possible to find coding that uses only 1.75 bits on the average
 - E.g., Huffman coding
- Compute the average number of bits needed per symbol

Entropy: General Case

- Suppose X takes n values, V_1, V_2, \dots, V_n , and

$$P(X=V_1)=p_1, P(X=V_2)=p_2, \dots, P(X=V_n)=p_n$$

- The smallest number of bits, on average, per symbol, needed to transmit the symbols drawn from distribution of X is given by:

$$H(X) = - \sum_{i=1}^m p_i \log_2(p_i)$$

- $H(X)$ = the **entropy** of X

Entropy Definition

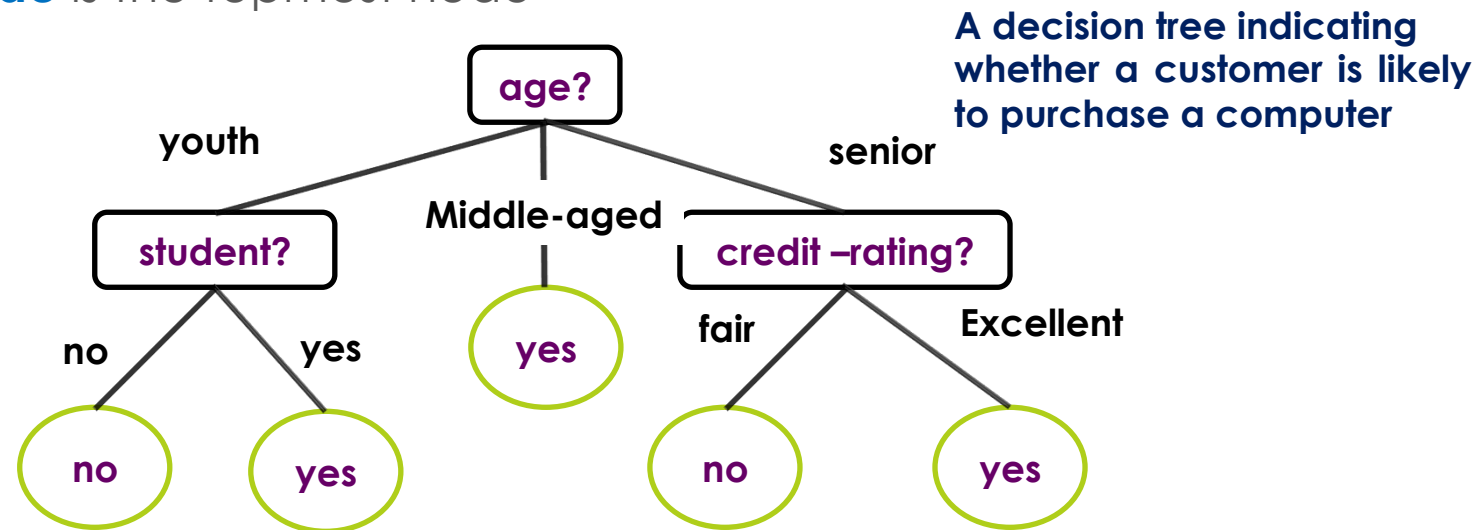
- Entropy is a measure of the average information content one is missing when one does not know the value of the random variable
- **High Entropy**
 - X is from a uniform like distribution
 - Flat histogram
 - Values sampled from it are less predictable
- **Low Entropy**
 - X is from a varied (peaks and valleys) distribution
 - Histogram has many lows and highs
 - Values sampled from it are more predictable

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Decision Tree Induction

- Decision tree induction is the learning of decision trees from class-labeled training tuples
- A decision tree is a flowchart-like tree structure
 - Internal nodes (non leaf node) denotes a test on an attribute
 - Branches represent outcomes of tests
 - Leaf nodes (terminal nodes) hold class labels
 - Root node is the topmost node



Class-label Yes: The customer is likely to buy a computer

Class-label no: The customer is unlikely to buy a computer

Decision Tree Induction

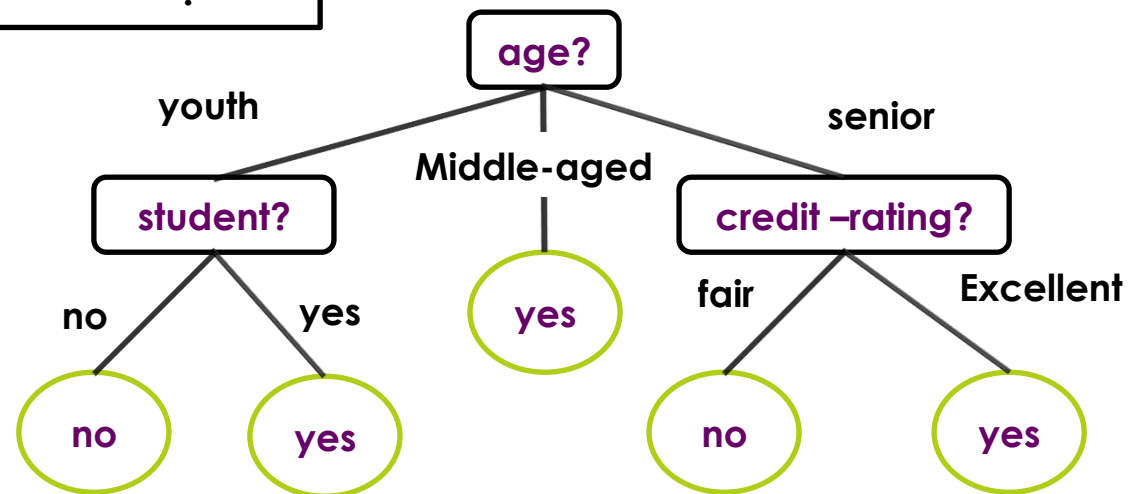
How are decision trees used for classification?

- The attributes of a tuple are tested against the decision tree
- A path is traced from the root to a leaf node which holds the prediction for that tuple

Example

RID	age	income	student	credit-rating	Class
1	youth	high	no	fair	?

- Test on age: youth
- Test of student: no
- Reach leaf node
- **Class NO:** the customer is unlikely to buy a computer



A decision tree indicating whether a customer is likely to purchase a computer

Decision Tree Induction

□ Why decision trees classifiers are so popular?

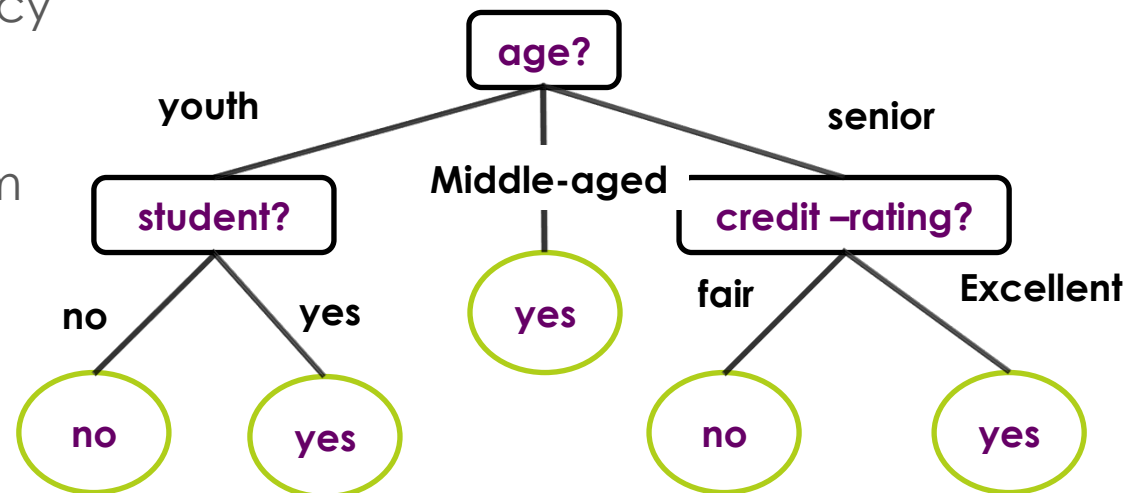
- The construction of a decision tree does not require any domain knowledge or parameter setting
- They can handle high dimensional data
- Intuitive representation that is easily understood by humans
- Learning and classification are simple and fast
- They have a good accuracy

□ Note

- Decision trees may perform Differently depending on the data set

□ Applications

- Medicine, astronomy
- Financial analysis, manufacturing
- Many other applications



A decision tree indicating whether a customer is likely to purchase a computer

The Algorithm

Principle

- ▣ Basic algorithm (adopted by ID3, C4.5 and CART): a **greedy algorithm**
- ▣ Tree is constructed in a top-down recursive divide-and-conquer manner

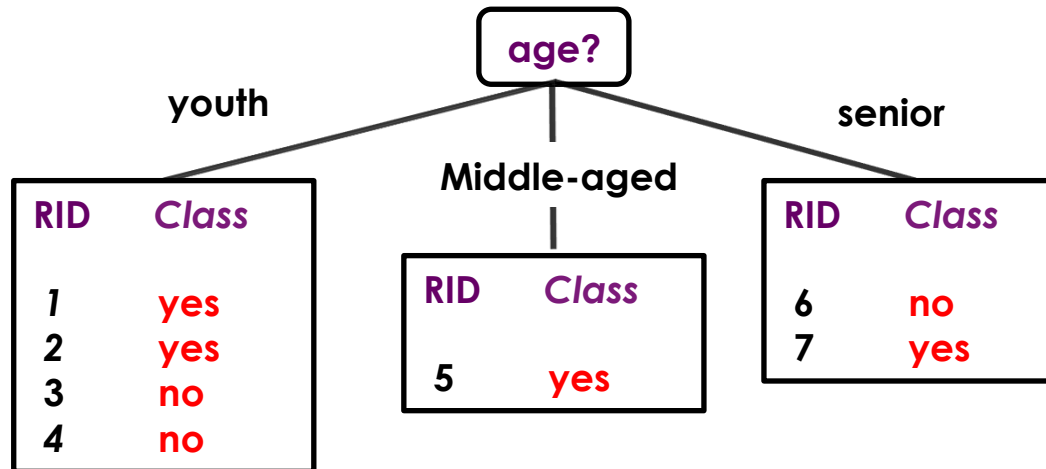
▣ Iterations

- ▣ At start, all the training tuples are at the root
- ▣ Tuples are partitioned recursively based on selected attributes
- ▣ Test attributes are selected on the basis of a heuristic or statistical measure (e.g., **information gain**)

▣ Stopping conditions

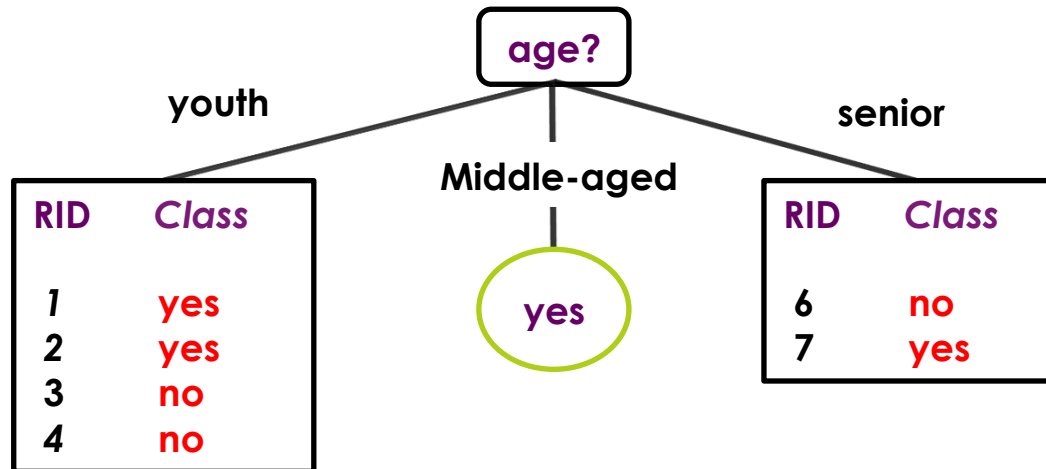
- ▣ All samples for a given node belong to the same class
- ▣ There are no remaining attributes for further partitioning – **majority voting** is employed for classifying the leaf
- ▣ There are no samples left

Example



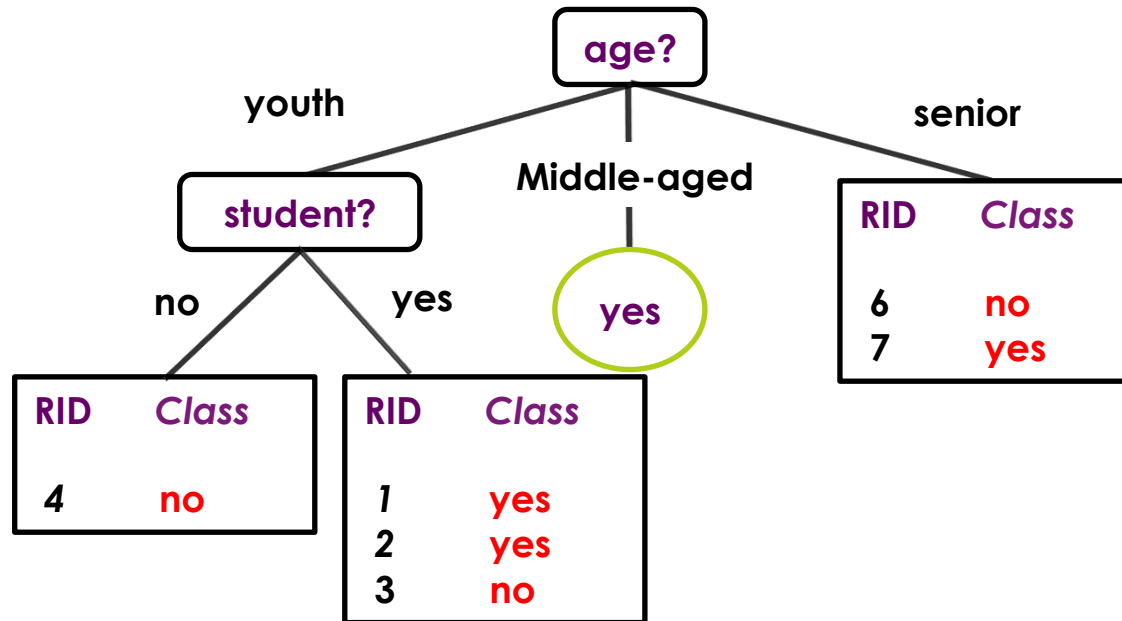
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Example



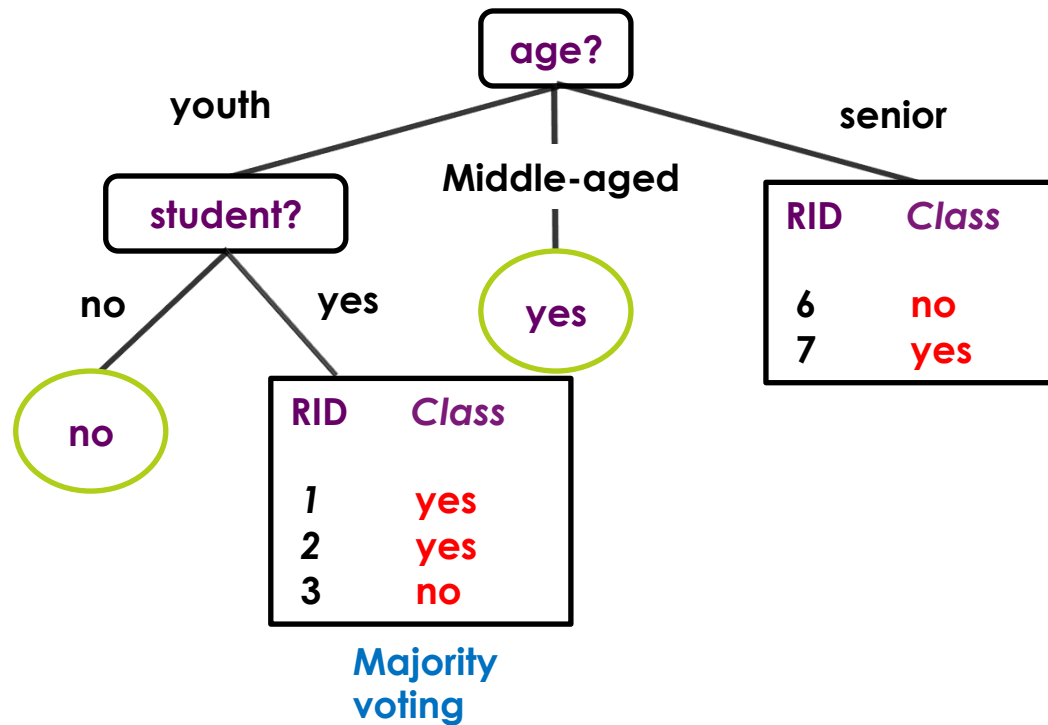
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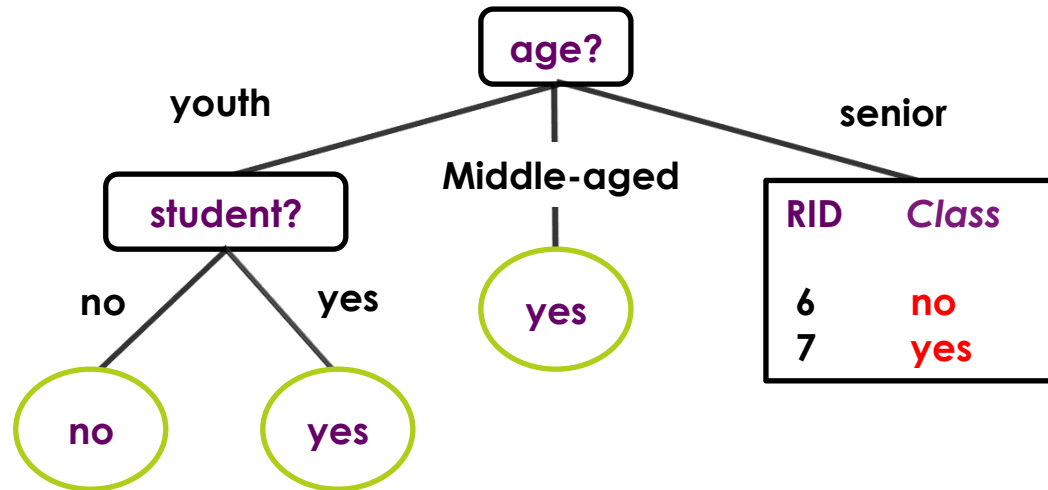
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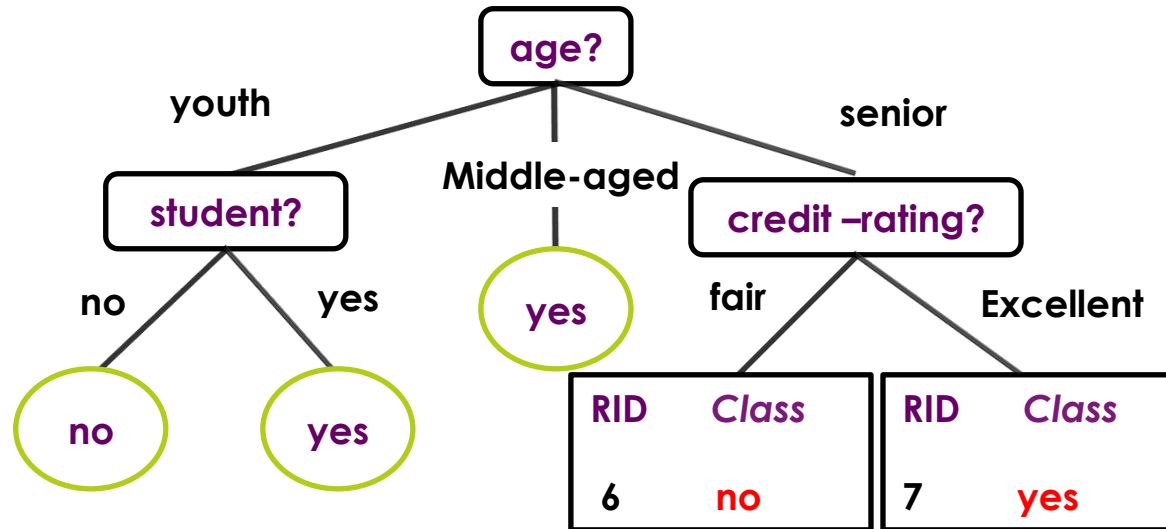
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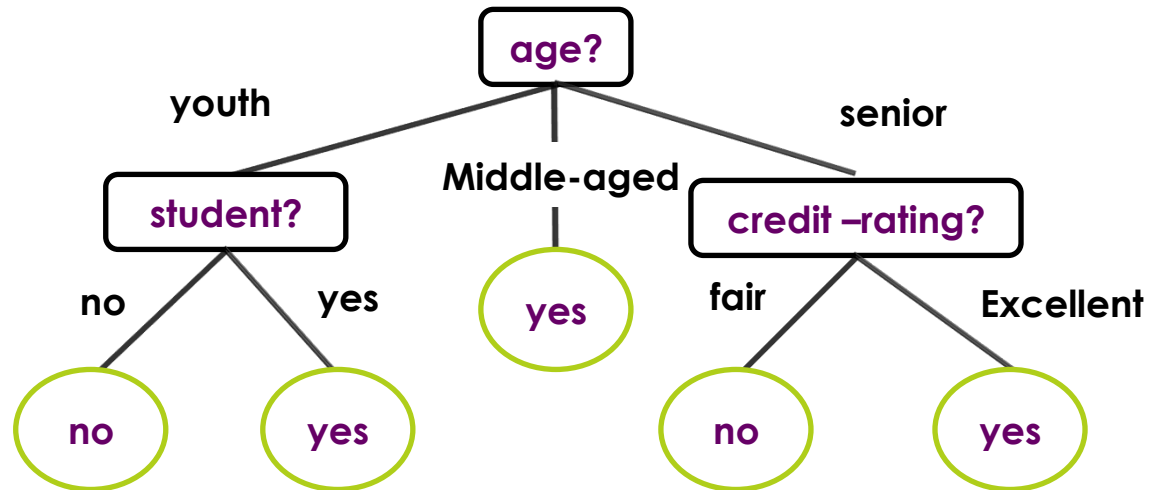
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Example



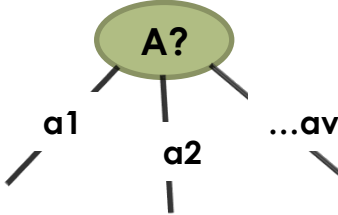
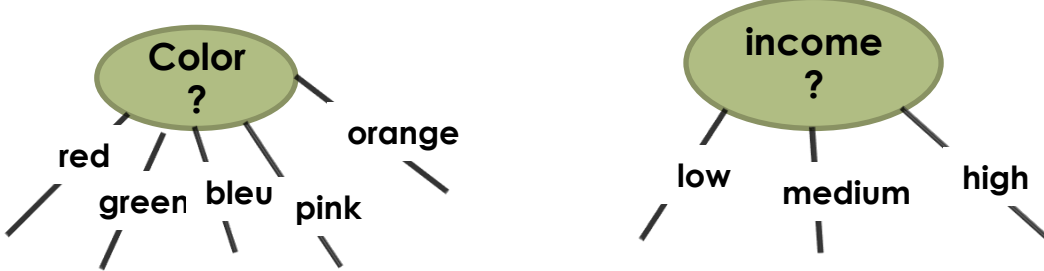
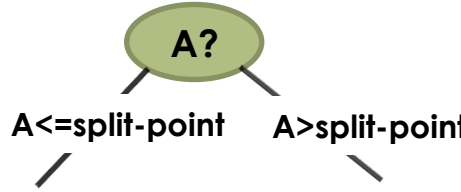
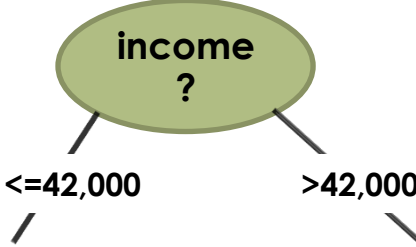
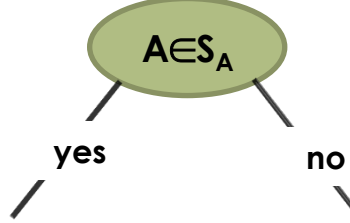
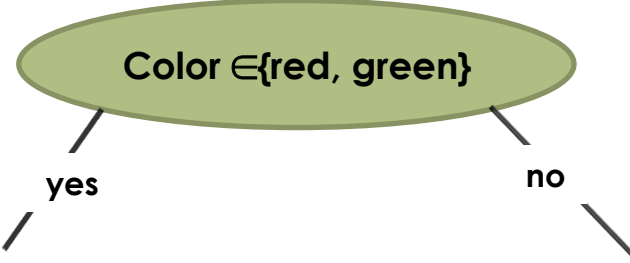
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Three Possible Partition Scenarios

Partitioning scenarios	Examples
<p>Discrete-valued</p>  <pre> graph TD A((A?)) --> a1[a1] A --> a2[a2] A --> av["...av"] </pre>	 <pre> graph TD Color((Color ?)) --> red[red] Color --> green[green] Color --> bleu[bleu] Color --> pink[pink] Color --> orange[orange] income1((income ?)) --> low[low] income1 --> medium[medium] income1 --> high[high] </pre>
<p>Continuous-valued</p>  <pre> graph TD A((A?)) --> left["A <= split-point"] A --> right["A > split-point"] </pre>	 <pre> graph TD income2((income ?)) --> left["<=42,000"] income2 --> right[">42,000"] </pre>
<p>Discrete-valued+ binary tree</p>  <pre> graph TD A3((A ∈ S_A)) --> yes[yes] A3 --> no[no] </pre>	 <pre> graph TD Color3((Color ∈ {red, green})) --> yes3[yes] Color3 --> no3[no] </pre>

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Attribute Selection Measures

- An **attribute selection measure** is a heuristic for selecting the splitting criterion that “best” separates a given data partition **D**

Ideally

- Each resulting partition would be pure
- A **pure** partition is a partition containing tuples that all belong to the same class
- Attribute selection measures (splitting rules)
 - Determine how the tuples at a given node are to be split
 - Provide ranking for each attribute describing the tuples
 - The attribute with highest score is chosen
 - Determine a **split point** or a **splitting subset**
- **Methods**
 - Information gain
 - Gain ratio
 - Gini Index

Quiz

- In both pictures **A** and **B** the child is eating a soup

Low Entropy



A

The values (locations of the soup) sampled entirely from within the soup ball

High Entropy



The values (locations of the soup) almost unpredictable...almost uniformly sampled throughout the living room

- Which situation (A or B) has a high/low entropy in terms of the locations of the soup?

Information Gain Approach

- **D**: the current partition
- **N**: represent the tuples of partition D
- Select the attribute with the highest information gain (based on the work by Shannon on information theory)
- This attribute
 - minimizes the information needed to classify the tuples in the resulting partitions
 - reflects the least randomness or “impurity” in these partitions
- **Information gain** approach minimizes the expected number of tests needed to classify a given tuple and guarantee a simple tree

First Step

- Compute **Expected information** (entropy) needed to classify a tuple in partition **D**

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

- **m**: the number of classes
 - **p_i**: the probability that an arbitrary tuple in **D** belongs to class **C_i**
estimated by: $|C_i, D| / |D|$ (proportion of tuples of each class)
 - A **log** function to the base 2 is used because the information is encoded in bits
- **Info(D)**
 - The average amount of information needed to identify the class label of a tuple in D
 - It is the **entropy**

Example

RID	age	income	student	credit-rating	class:buy_computer
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle-aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle-aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle-aged	medium	no	excellent	yes
13	middle-aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

In partition D

m=2 (the number of classes)

N= 14 (number of tuples)

9 tuples in class yes

5 tuples in class no

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

Second Step

- For each attribute, compute the amount of information needed to arrive at an exact classification after portioning using that attribute
- Suppose that we were to partition the tuples in D on some attribute A $\{a_1, \dots, a_v\}$
 - Split D into v partitions $\{D_1, D_2, \dots, D_v\}$
 - Ideally D_i partitions are pure but it is unlikely
- The amount of information needed to arrive at an exact classification is measured by:

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

- $|D_j| / |D|$: the weight of the j th partition
- $Info(D_j)$: the entropy of partition D_j
- The smaller the expected information still required, the greater the purity of the partitions

Example

RID	age	income	student	credit-rating	class:buy_computer
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Using attribute age

Part1 (youth) **D1** has **2 yes** and **3 no**

Part2 (middle-aged) **D2** has **4 yes** and **0 no**

Part3 (senior) **D3** has **3 yes** and **2 no**

$$Info_{age}(D) = \frac{5}{14} Info(D_1) + \frac{4}{14} Info(D_2) + \frac{5}{14} Info(D_3) = 0.694$$

Third Step

- Compute Information Gain
- Information gain by branching on A is:

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

- Information gain is the expected reduction in the information requirements caused by knowing the value of A
- The attribute **A** with the **highest information gain** ($Gain(A)$), is **chosen** as the splitting attribute at node N

Example

RID	age	income	student	credit-rating	class:buy_computer
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$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Gain(income)=0.029,

Gain(student)=0.151

Gain(credit_rating)=0.048

“Age” has the highest gain \Rightarrow It is chosen as the splitting attribute

Note on Continuous Valued Attributes

- Let attribute **A** be a continuous-valued attribute
- Must determine the **best split point** for A
 - Sort the values of 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
- **Split**
 - **D1** is the set of tuples in D satisfying **$A \leq \text{split-point}$**
 - **D2** is the set of tuples in D satisfying **$A > \text{split-point}$**

Gain Ratio Approach

- Problem of Information Gain
 - Biased towards tests with many outcomes (attributes having a large number of values)
 - E.g: attribute acting as a unique identifier
 - Produce a **large number of partitions** (1 tuple per partition)
 - Each resulting partition D is **pure** $\text{Info}(D)=0$
 - The **information gain** is **maximized**
- Extension to Information Gain
 - Use **gain ratio**
 - Overcomes the bias of Information gain
 - Applies a kind of normalization to information gain using a **split information** value

Split Information

- The **split information value** represents the potential information generated by splitting the training data set **D** into **v** partitions, corresponding to v outcomes on attribute **A**

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

- **High split Info**: partitions have more or less the same size (uniform)
- **Low split Info**: few partitions hold most of the tuples (peaks)
- The gain ratio is defined as:

$$GainRatio(A) = \frac{Gain(A)}{SplitInfo(A)}$$

- The attribute with the maximum gain ratio is selected as the splitting attribute

Example

RID	age	income	student	credit-rating	class:buy_computer
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Using attribute income

Part1 (low) : **4 tuples** , Part2 (medium): **6 tuples**, Part3 (high): **4 tuples**

$$SplitInfo_{income}(D) = -\frac{4}{14}\log_2\left(\frac{4}{14}\right) - \frac{6}{14}\log_2\left(\frac{6}{14}\right) - \frac{4}{14}\log_2\left(\frac{4}{14}\right) = 0.926$$

$$Gain(income) = 0.029$$

$$GainRatio(income) = \frac{0.029}{0.926} = 0.031$$

Gini Index Approach

- Measures the impurity of a data partition D

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

- m : the number of classes
- p_i : the probability that a tuple in D belongs to class C_i
- The Gini Index considers a **binary split** for each attribute A , say D_1 and D_2 . The Gini index of D given that partitioning is:

$$Gini_A(D) = \frac{|D_1|}{|D|} Gini(D_1) + \frac{|D_2|}{|D|} Gini(D_2)$$

- The reduction in impurity is given by:

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

- The attribute that maximizes the reduction in impurity is chosen as the splitting attribute

Binary Split

■ Continuous Values Attributes

- Examine each possible split point. The midpoint between each pair of (sorted) adjacent values is taken as a possible split-point
- For each split-point, compute the weighted sum of the impurity of each of the two resulting partitions ($D_1: A \leq \text{split-point}$, $D_2: A > \text{split-point}$)
- The point that gives the minimum Gini index for attribute A is selected as its split-point

■ Discrete Attributes

- Examine the partitions resulting from all possible subsets of $\{a_1, \dots, a_v\}$
- Each subset S_A is a binary test of attribute A of the form " $A \in S_A?$ "
- 2^v possible subsets. We exclude the power set and the empty set, then we have $2^v - 2$ subsets
- The subset that gives the minimum Gini index for attribute A is selected as its splitting subset

Example

RID	age	income	student	credit-rating	class:buy_computer
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Compute the Gini index of the training set D: 9 tuples in class yes and 5 in class no

$$Gini(D) = 1 - \left[\left(\frac{9}{14} \right)^2 + \left(\frac{5}{14} \right)^2 \right] = 0.459$$

Using attribute income: there are three values: low, medium and high

Choosing the subset {low, medium} results in two partitions:

D1 (income ∈ {low, medium}): 10 tuples

D2 (income ∈ {high}): 4 tuples

Example

$$\begin{aligned} Gini_{income \in \{low, medium\}}(D) &= \frac{10}{14} Gini(D_1) + \frac{4}{14} Gini(D_2) \\ &= \frac{10}{14} \left(1 - \left(\frac{6}{10} \right)^2 - \left(\frac{4}{10} \right)^2 \right) + \frac{4}{14} \left(1 - \left(\frac{1}{4} \right)^2 - \left(\frac{3}{4} \right)^2 \right) \\ &= 0.450 \\ &= Gini_{income \in \{high\}}(D) \end{aligned}$$

The Gini Index measures of the remaining partitions are:

$$Gini_{\{low, high\} \text{ and } \{medium\}}(D) = 0.315$$

$$Gini_{\{medium, high\} \text{ and } \{low\}}(D) = 0.300$$

The best binary split for attribute income is on **{medium, high}** and **{low}**

Comparing Attribute Selection Measures

■ Information Gain

- Biased towards multivalued attributes

■ Gain Ratio

- Tends to prefer unbalanced splits in which one partition is much smaller than the other

■ Gini Index

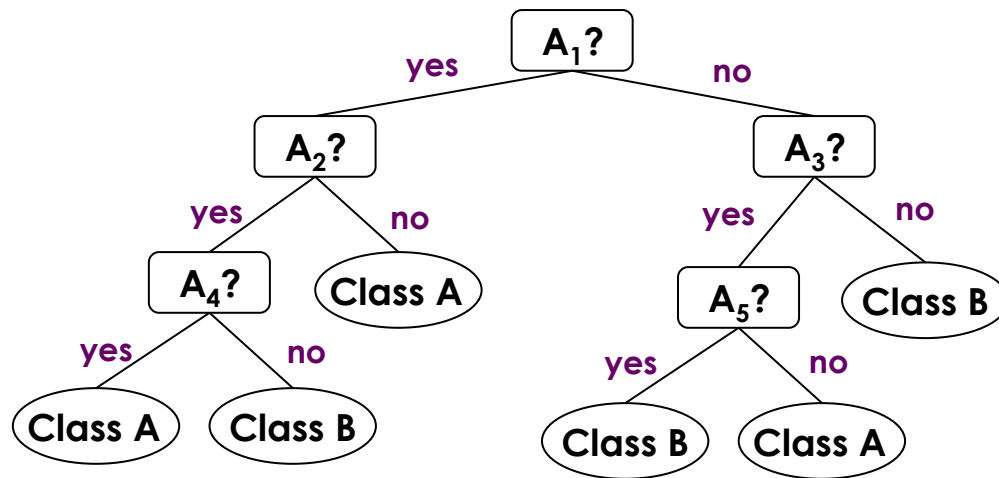
- Biased towards multivalued attributes
- Has difficulties when the number of classes is large
- Tends to favor tests that result in equal-sized partitions and purity in both partitions

Road Map

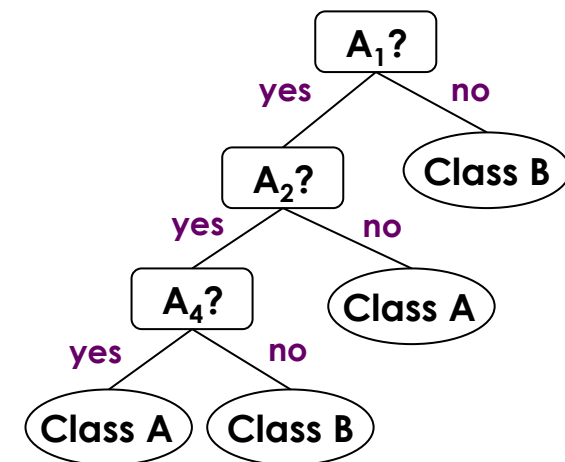
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Overfitting

- Many branches of the decision tree will reflect anomalies in the training data due to noise or outliers
- Poor accuracy for unseen samples
- Solution: **Pruning**
 - Remove the least reliable branches



Before Pruning



After Pruning

Tree Pruning Strategies

■ Prepruning

- Halt tree construction early—do not split a node if this would result in the goodness measure falling below a threshold
- Statistical significance, information gain, Gini index are used to assess the goodness of a split
- Upon halting, the node becomes a leaf
- The leaf may hold the most frequent class among the subset tuples

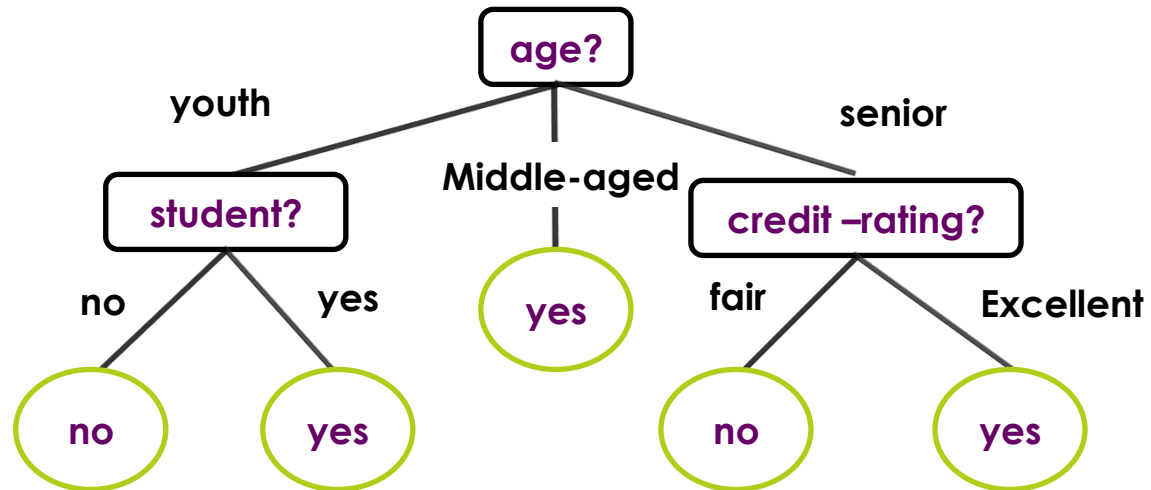
■ Postpruning

- Remove branches from a “fully grown” tree:
- A subtree at a given node is pruned by replacing it by a leaf
- The leaf is labeled with the most frequent class

Cost Complexity Pruning Algorithm

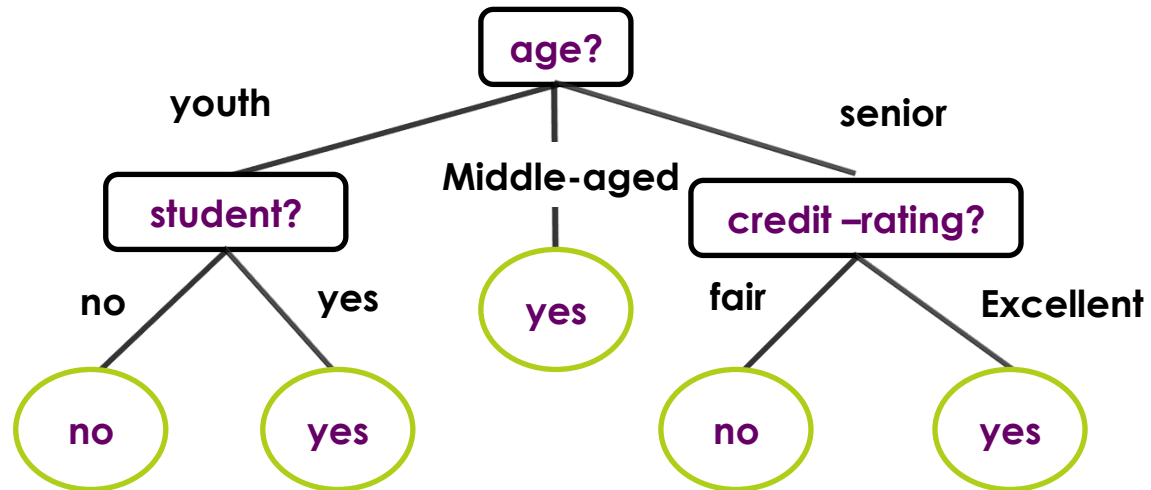
- Cost complexity of a tree is a function of the the number of leaves and the error rate (percentage of tuples misclassified by the tree)
- At each node N compute
 - The cost complexity of the subtree at N
 - The cost complexity of the subtree at N if it were to be pruned
- If pruning results in smaller cost, then prune the subtree at N
- Use a set of data different from the training data to decide which is the “best pruned tree”

Pruning Example



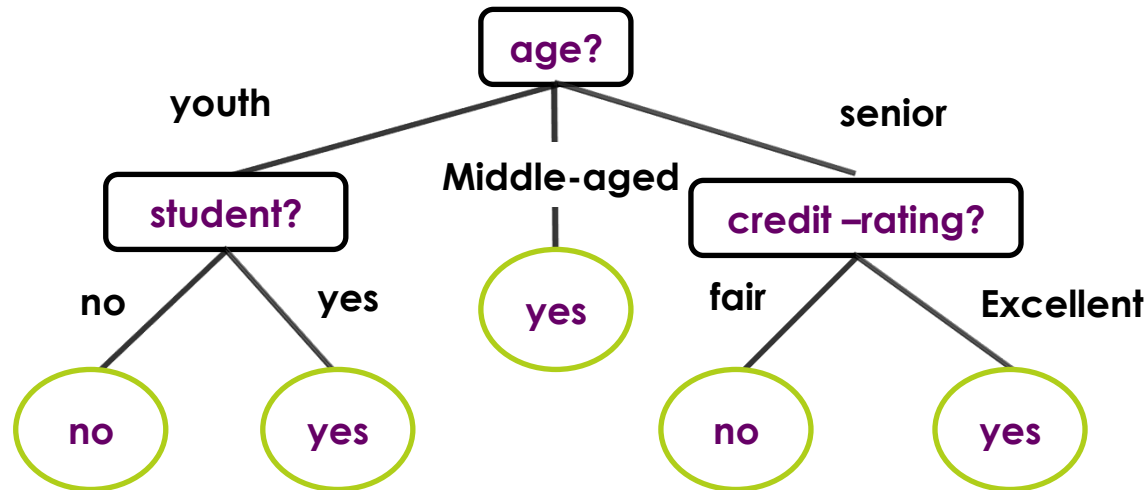
RID	age	student	credit-rating	Class: buys_computer
1	youth	yes	fair	yes
2	youth	yes	fair	yes
3	youth	yes	fair	no
4	youth	no	fair	no
5	middle-aged	no	excellent	yes
6	senior	yes	fair	no
7	senior	yes	excellent	yes

Optimistic Evaluation (Error = 1/7)



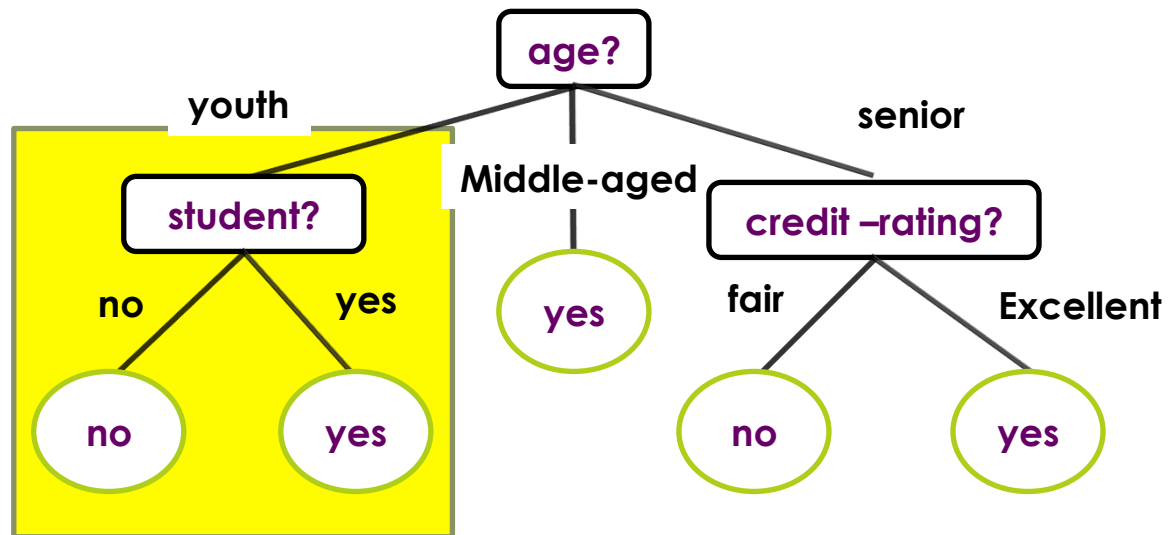
RID	age	student	credit-rating	Class: buys_computer
1	youth	yes	fair	yes
2	youth	yes	fair	yes
3	youth	yes	fair	no
4	youth	no	fair	no
5	middle-aged	no	excellent	yes
6	senior	yes	fair	no
7	senior	yes	excellent	yes

Evaluation using Validation Set (Error=3/7)



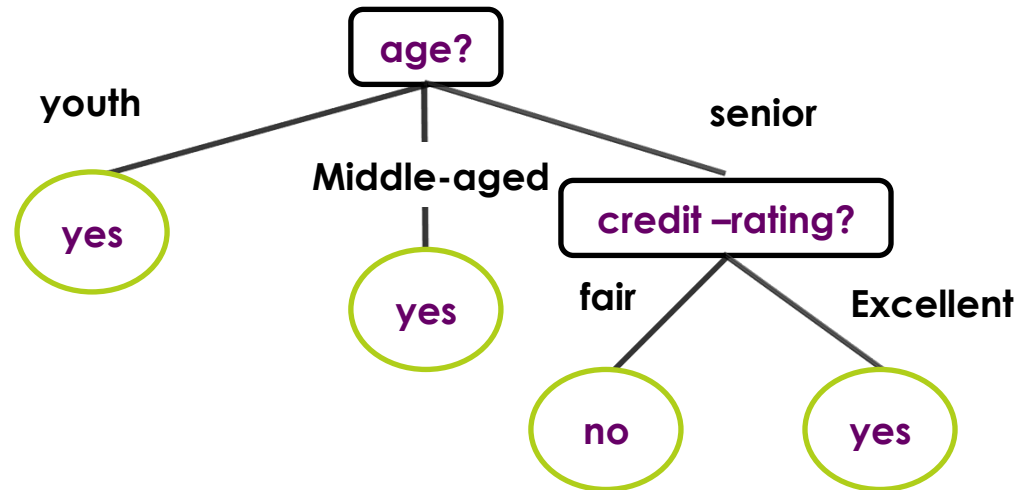
RID	age	student	credit-rating	Class: buys_computer
1	youth	no	excellent	yes
2	youth	yes	fair	yes
3	youth	yes	fair	no
4	youth	no	fair	yes
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Pruning



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After Pruning (Error=1/7)



RID	age	student	credit-rating	Class: buys_computer
1	youth	no	excellent	yes
2	youth	yes	fair	yes
3	youth	yes	fair	no
4	youth	no	fair	yes
5	youth	no	fair	yes
6	middle-aged	no	excellent	yes
7	senior	yes	excellent	no

Summary

- Decision Trees have relatively **faster learning** speed than other methods
- Conversable to simple and **easy to understand** classification rules
- Information Gain, Ratio Gain and Gini Index are the most common methods of **attribute selection**
- **Tree pruning** is necessary to remove unreliable branches

Question

Given dataset D and the number of attributes n , show that the computational cost of growing a binary decision tree is at most

$$n \times |D| \times \log(|D|)$$