

COMP 345: Data Mining

Classification Basics

Slides Adapted From : Jiawei Han, Micheline Kamber & Jian Pei
Data Mining: Concepts and Techniques, 3rd ed.



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Supervised vs. Unsupervised Learning

- **Supervised learning (classification)**
 - Supervision: The training data (observations, measurements, etc.) are accompanied by **labels** indicating the class of the observations
 - New data is classified based on the training set
- **Unsupervised learning (clustering)**
 - The class labels of training data is unknown
 - Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

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Prediction Problems: Classification vs. Numeric Prediction

- **Classification**
 - predicts categorical class labels (discrete or nominal)
 - classifies data (constructs a model) based on the training set and the values (**class labels**) in a classifying attribute and uses it in classifying new data
- **Numeric Prediction**
 - models continuous-valued functions, i.e., predicts unknown or missing values
- Typical applications
 - Credit/loan approval:
 - Medical diagnosis: if a tumor is cancerous or benign
 - Fraud detection: if a transaction is fraudulent
 - Web page categorization: which category it is

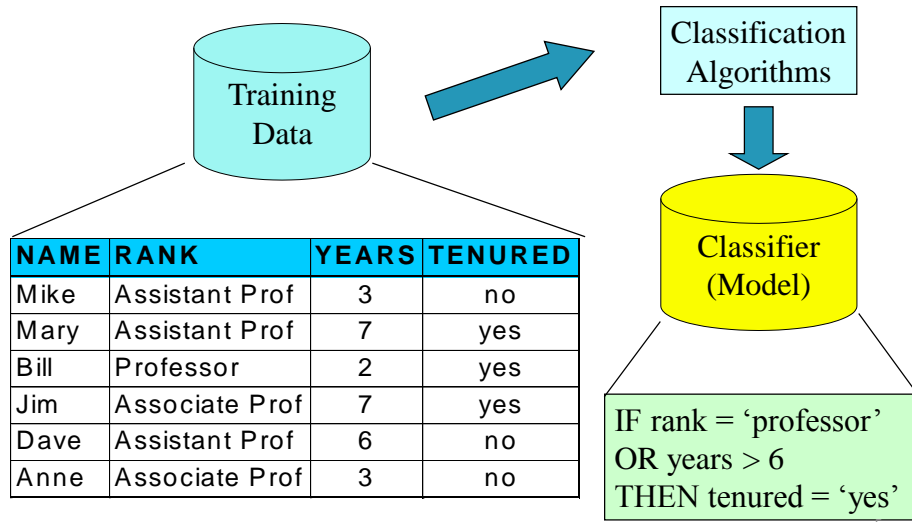
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Classification—A Two-Step Process

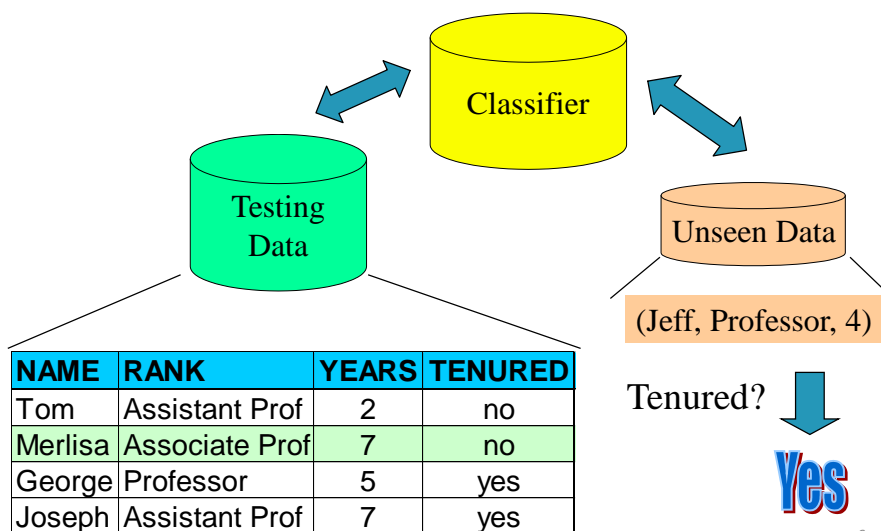
1. **Model construction**: describing a set of predetermined classes
 - Each tuple/sample is assumed to belong to a predefined class, as determined by the **class label attribute**
 - The set of tuples used for model construction is **training set**
 - The model is represented as classification rules, decision trees, or mathematical formulae
 2. **Model usage**: for classifying future or unknown objects
 - **Estimate accuracy** of the model
 - The known label of test sample is compared with the classified result from the model
 - **Accuracy** rate is the percentage of test set samples that are correctly classified by the model
 - **Test set** is independent of training set (otherwise overfitting)
 - If the accuracy is acceptable, use the model to **classify new data**
- Note: If *the test set* is used to select models, it is called **validation (test) set**

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Process (1): Model Construction

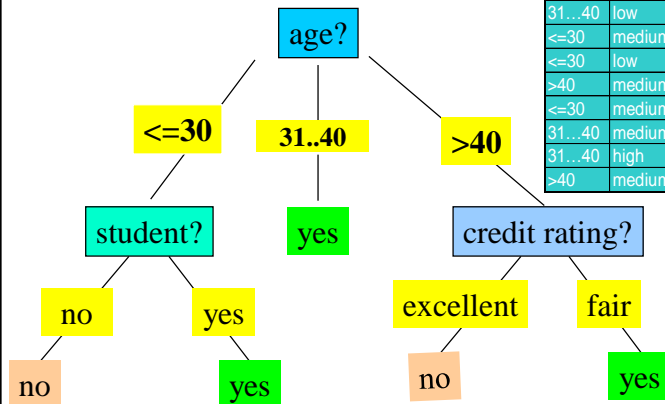


Process (2): Using the Model in Prediction



Decision Tree Induction: An Example

- Training data set: Buys_computer
- Resulting tree:



age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31...40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31...40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31...40	medium	no	excellent	yes
31...40	high	yes	fair	yes
>40	medium	no	excellent	no

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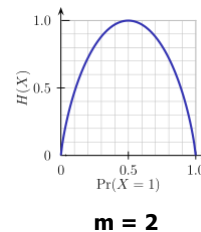
Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
 - Tree is constructed in a **top-down recursive divide-and-conquer manner**
 - At start, all the training examples are at the root
 - Attributes are categorical (if continuous-valued, they are discretized in advance)
 - Examples are partitioned recursively based on selected attributes
 - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., **information gain**)
- 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

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Entropy

- Entropy (Information Theory)
 - A measure of uncertainty associated with a random variable
 - Calculation: For a discrete random variable Y taking m distinct values $\{y_1, \dots, y_m\}$,
 - $H(Y) = -\sum_{i=1}^m p_i \log(p_i)$, where $p_i = P(Y = y_i)$
 - Interpretation:
 - Higher entropy \Rightarrow higher uncertainty
 - Lower entropy \Rightarrow lower uncertainty
- Conditional Entropy
 - $H(Y|X) = \sum_x p(x) H(Y|X = x)$



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Attribute Selection Measure: Information Gain (ID3/C4.5)

- Select the attribute with the highest information gain
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i , 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

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

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Example Data

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31...40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
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31...40	low	yes	excellent	yes
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Attribute Selection: Information Gain

■ Class P: buys_computer = "yes"

■ Class N: buys_computer = "no"

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

age	p _i	n _i	I(p _i , n _i)
<=30	2	3	0.971
31...40	4	0	0
>40	3	2	0.971

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31...40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31...40	low	yes	excellent	yes
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<=30	medium	yes	excellent	yes
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31...40	high	yes	fair	yes
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$$Info_{age}(D) = \frac{5}{14} I(2,3) + \frac{4}{14} I(4,0) + \frac{5}{14} I(3,2) = 0.694$$

$\frac{5}{14} I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes and 3 no.

Hence

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Similarly,

$$Gain(income) = 0.029$$

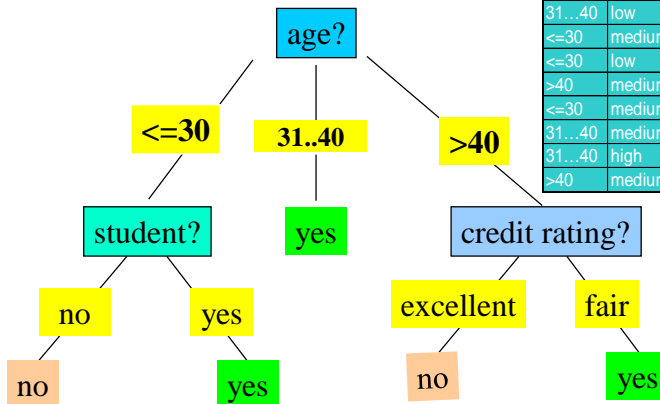
$$Gain(student) = 0.151$$

$$Gain(credit_rating) = 0.048$$

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Decision Tree

- Training data set: Buys_computer
- Resulting tree:



age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
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31...40	high	no	fair	yes
>40	medium	no	fair	yes
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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 $A \leq \text{split-point}$, and D2 is the set of tuples in D satisfying $A > \text{split-point}$

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Gain Ratio for Attribute Selection (C4.5)

- Information gain measure is biased towards attributes with a large number of values
- C4.5 (a successor of ID3) uses gain ratio to overcome the problem (normalization to information gain)

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

– $GainRatio(A) = Gain(A)/SplitInfo(A)$

- Ex. $SplitInfo_{income}(D) = -\frac{4}{14} \times \log_2 \left(\frac{4}{14} \right) - \frac{6}{14} \times \log_2 \left(\frac{6}{14} \right) - \frac{4}{14} \times \log_2 \left(\frac{4}{14} \right) = 1.557$
- $gain_ratio(income) = 0.029/1.557 = 0.019$
- The attribute with the maximum gain ratio is selected as the splitting attribute

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Gini Index (CART, IBM IntelligentMiner)

- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as

$$gini(D) = 1 - \sum_{j=1}^n p_j^2$$

where p_j is the relative frequency of class j in D

- If a data set D is split on A into two subsets D_1 and D_2 , the $gini$ index $gini_A(D)$ is defined as

$$gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$$

- Reduction in Impurity:

$$\Delta gini(A) = gini(D) - gini_A(D)$$

- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (**need to enumerate all the possible splitting points for each attribute**)

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Computation of Gini Index

Example: D has 9 tuples in buys_computer = "yes" and 5 in "no"

$$gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

- Suppose the attribute income partitions D into 10 in D_1 : {low, medium} and 4 in D_2

$$\begin{aligned} gini_{income \in \{low, medium\}}(D) &= \left(\frac{10}{14}\right) Gini(D_1) + \left(\frac{4}{14}\right) Gini(D_2) \\ &= \frac{10}{14} \left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14} \left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right) \\ &= 0.443 \\ &= Gini_{income \in \{high\}}(D). \end{aligned}$$

$Gini_{\{low, high\}}$ is 0.458; $Gini_{\{medium, high\}}$ is 0.450. Thus, split on the {low, medium} (and {high}) since it has the lowest Gini index

- All attributes are assumed continuous-valued
- May need other tools, e.g., clustering, to get the possible split values
- Can be modified for categorical attributes

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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
 - has difficulty when # of classes is large
 - tends to favor tests that result in equal-sized partitions and purity in both partitions

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Other Attribute Selection Measures

- CHAID: a popular decision tree algorithm, measure based on χ^2 test for independence
- C-SEP: performs better than info. gain and gini index in certain cases
- G-statistic: has a close approximation to χ^2 distribution
- MDL (Minimal Description Length) principle (i.e., the simplest solution is preferred):
 - The best tree as the one that requires the fewest # of bits to both (1) encode the tree, and (2) encode the exceptions to the tree
- Multivariate splits (partition based on multiple variable combinations)
 - CART: finds multivariate splits based on a linear comb. of attrs.
- Which attribute selection measure is the best?
 - Most give good results, none is significantly superior than others

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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
- Two approaches to avoid overfitting
 - Prepruning: *Halt tree construction early*-do not split a node if this would result in the goodness measure falling below a threshold
 - Difficult to choose an appropriate threshold
 - Postpruning: *Remove branches* from a “fully grown” tree—get a sequence of progressively pruned trees
 - Use a set of data different from the training data to decide which is the “best pruned tree”

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Enhancements to Basic Decision Tree Induction

- Allow for **continuous-valued attributes**
 - Dynamically define new discrete-valued attributes that partition the continuous attribute value into a discrete set of intervals
- Handle **missing attribute values**
 - Assign the most common value of the attribute
 - Assign probability to each of the possible values
- **Attribute construction**
 - Create new attributes based on existing ones that are sparsely represented
 - This reduces fragmentation, repetition, and replication

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Classification in Large Databases

- Classification—a classical problem extensively studied by statisticians and machine learning researchers
- Scalability: Classifying data sets with millions of examples and hundreds of attributes with reasonable speed
- Why is decision tree induction popular?
 - relatively faster learning speed (than other classification methods)
 - convertible to simple and easy to understand classification rules
 - can use SQL queries for accessing databases
 - comparable classification accuracy with other methods

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Summary

- **Classification** is a form of data analysis that extracts **models** describing important data classes.
- Effective and scalable methods have been developed for **decision tree induction**
- Coming up:
 - **More classification algorithms.**
 - **More evaluation metrics** include: accuracy, sensitivity, specificity, precision, recall, F measure, and F_β measure.
 - **Stratified k-fold cross-validation**
 - **Bagging** and **boosting**

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