



CS 412 Intro. to Data Mining

Chapter 8. Classification: Basic Concepts

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Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Techniques to Improve Classification Accuracy: Ensemble Methods
- Additional Concepts on Classification
- Summary

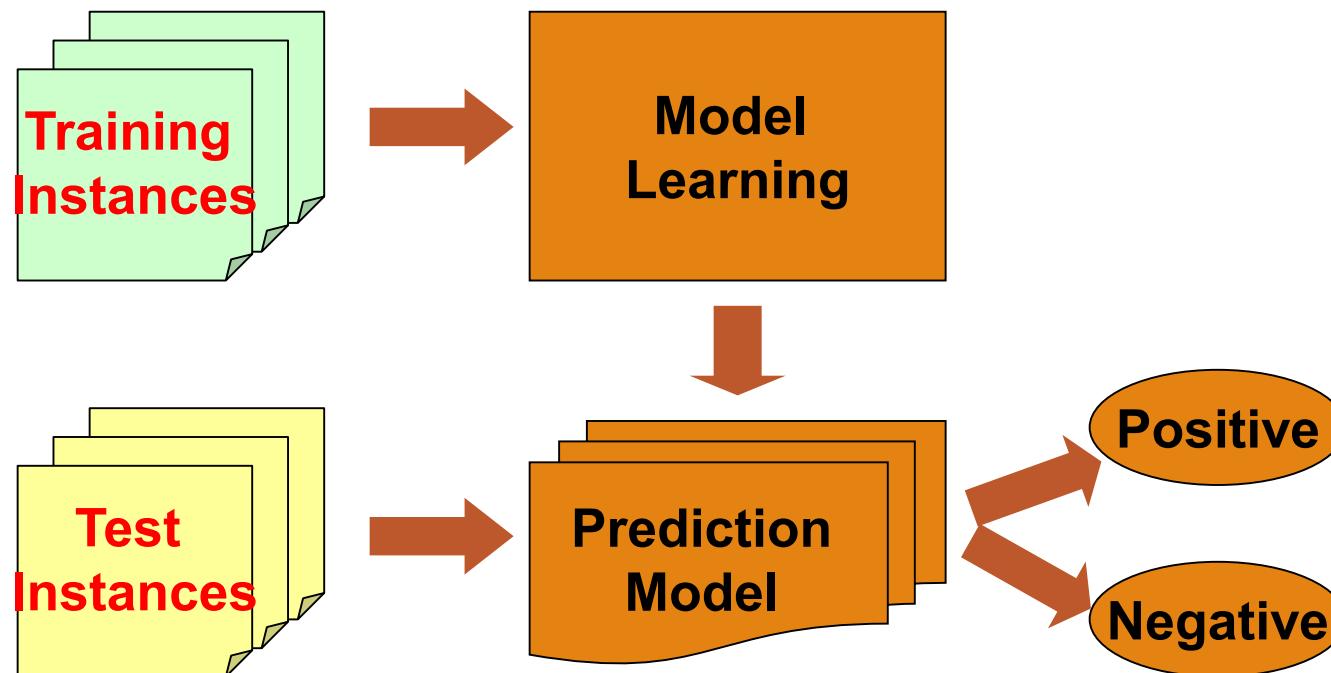


Supervised vs. Unsupervised Learning (1)

- Supervised learning (classification) គំរាល់ Model ទៅយើងពី Training
- Supervision: The training data such as observations or measurements are accompanied by **labels** indicating the classes which they belong to
- New data is classified based on the models built from the training set

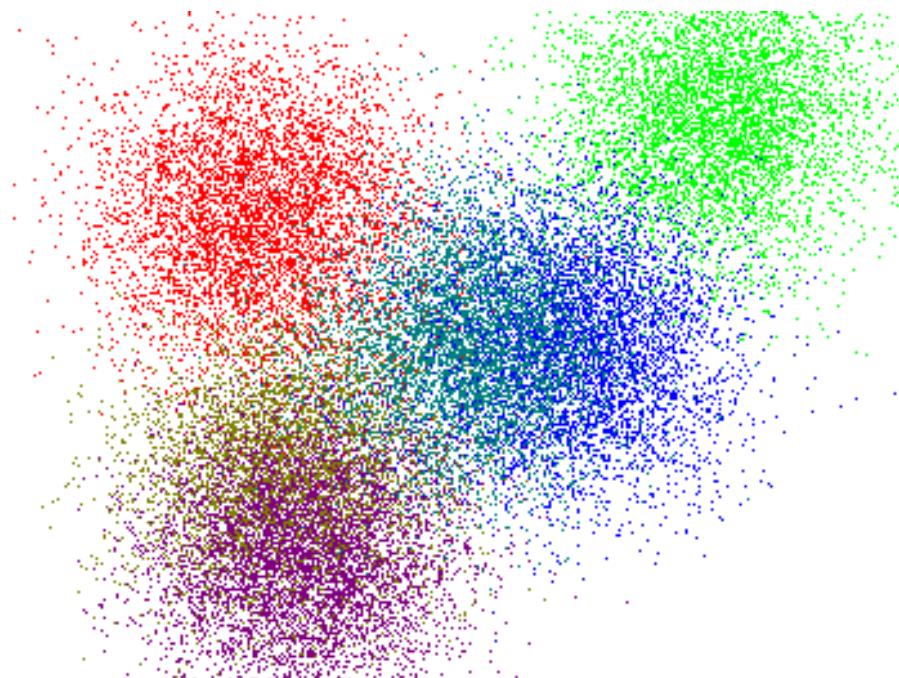
Training Data with class label:

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



Supervised vs. Unsupervised Learning (2)

- ❑ Unsupervised learning (clustering) សំរាប់ Model ដើម្បីមាន Training
- ❑ The class labels of training data are unknown សំណើលួចចែងក្នុង (clustering) នូវទីតាំង
- ❑ Given a set of observations or measurements, establish the possible existence of classes or clusters in the data



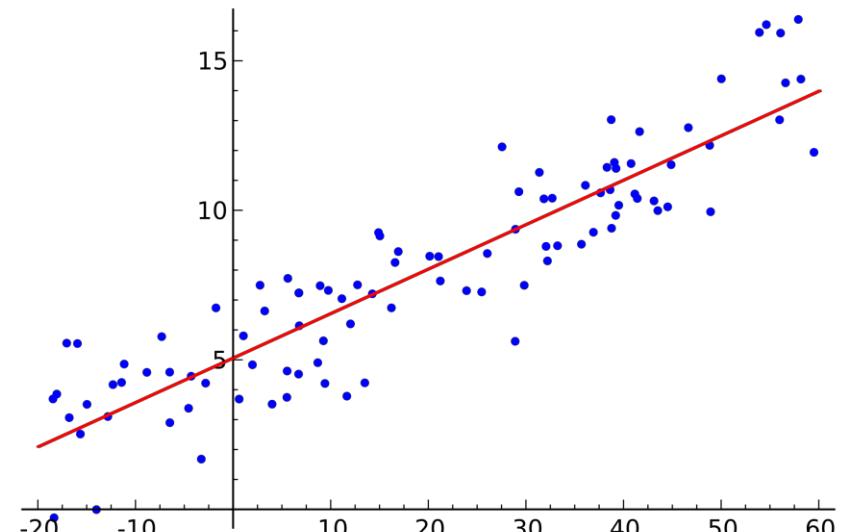
Prediction Problems: Classification vs. Numeric Prediction

□ Classification

- Predict categorical class labels (discrete or nominal)  ລວງເພີ້ນທຶນຍົດໄລວນ
- Construct a model based on the training set and the **class labels** (the values in a classifying attribute) and use it in classifying new data

□ Numeric prediction

- Model continuous-valued functions (i.e., predict unknown or missing values)
- Typical applications of classification
 - 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



Classification—Model Construction, Validation and Testing

- **Model construction**
 - Each sample is assumed to belong to a predefined class (shown by the **class label**)
 - The set of samples used for model construction is **training set**
 - Model: Represented as decision trees, rules, mathematical formulas, or other forms
- **Model Validation and Testing:**
 - **Test:** Estimate accuracy of the model
 - The known label of test sample is compared with the classified result from the model
 - **Accuracy:** % of test set samples that are correctly classified by the model
 - Test set is independent of training set
 - **Validation:** If *the test set* is used to select or refine models, it is called **validation (or development) (test) set**
- **Model Deployment:** If the accuracy is acceptable, use the model to classify new data

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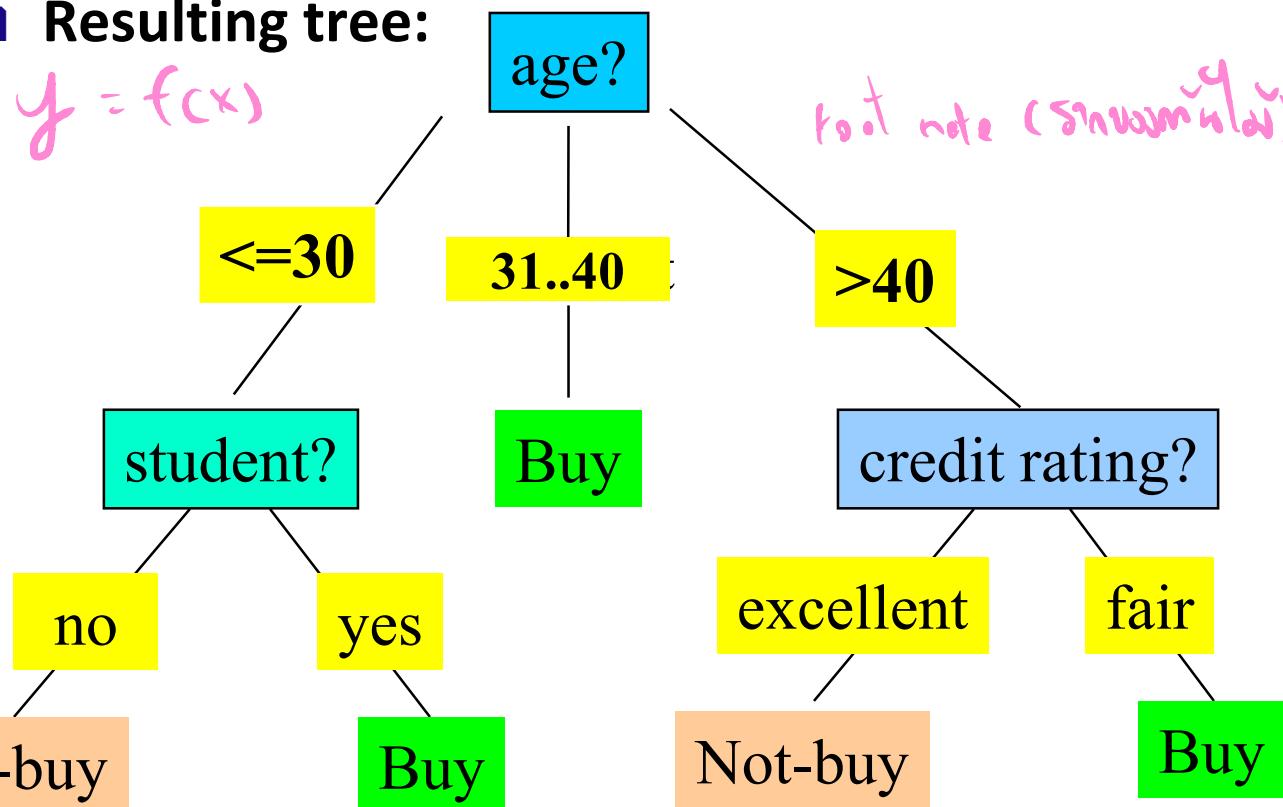


Decision Tree Induction: An Example

□ Decision tree construction:

- A top-down, recursive, divide-and-conquer process

□ Resulting tree:



សំណងចុច \times (feature)

Training data set: Who buys computer?

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

Note: The data set is adapted from "Playing Tennis" example of R. Quinlan

ថា
y (label)

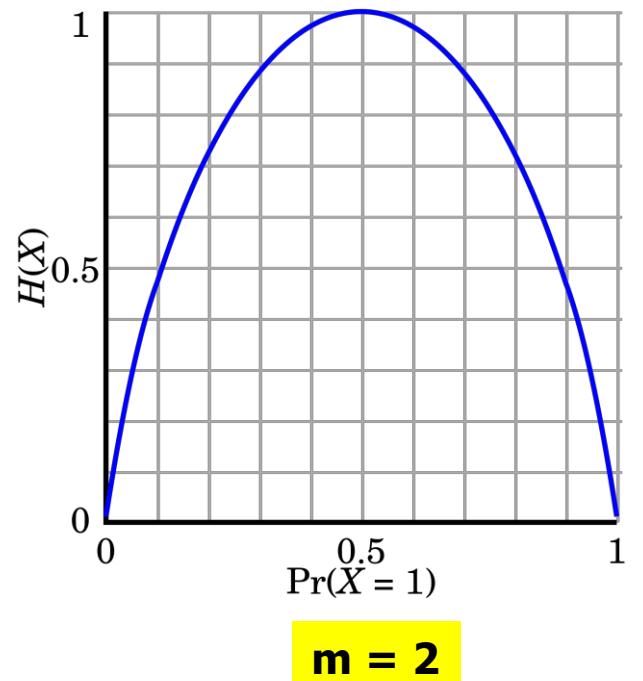
From Entropy to Info Gain: A Brief Review of Entropy

- Entropy (Information Theory)
 - A measure of uncertainty associated with a random number
 - Calculation: For a discrete random variable Y taking m distinct values $\{y_1, y_2, \dots, y_m\}$

$$H(Y) = - \sum_{i=1}^m p_i \log(p_i) \text{ where } p_i = P(Y = y_i)$$

- Interpretation
 - Higher entropy \rightarrow higher uncertainty
 - Lower entropy \rightarrow lower uncertainty
- Conditional entropy

$$H(Y|X) = \sum_x p(x) H(Y|X = x)$$



Information Gain: An Attribute Selection Measure

- Select the attribute with the highest information gain (used in typical decision tree induction algorithm: ID3/C4.5)
- 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

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

ນາ node ກົດກໍສູດ

Example: Attribute Selection with 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
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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'es and 3 no's.

Hence

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

Similarly, we can get

$$Gain(income) = 0.029$$

$$Gain(student) = 0.151$$

$$Gain(credit_rating) = 0.048$$

Decision Tree Induction: Algorithm

- Basic algorithm
 - Tree is constructed in a **top-down, recursive, divide-and-conquer manner**
 - At start, all the training examples are at the root
 - Examples are partitioned recursively based on selected attributes
 - On each node, attributes are selected based on the training examples on that node, and 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
 - There are no samples left
- Prediction
 - **Majority voting** is employed for classifying the leaf

How to Handle Continuous-Valued Attributes?

- Method 1: Discretize continuous values and treat them as categorical values
 - E.g., age: < 20, 20..30, 30..40, 40..50, > 50
- Method 2: Determine the *best split point* for continuous-valued attribute A
 - Sort the value A in increasing order: e.g. 15, 18, 21, 22, 24, 25, 29, 31, ...
 - *Possible split point*: the midpoint between *each pair of adjacent values*
 - $(a_i + a_{i+1})/2$ is the midpoint between the values of a_i and a_{i+1}
 - e.g., $(15+18)/2 = 16.5, 19.5, 21.5, 23, 24.5, 27, 30, \dots$
 - The point with the *maximum information gain* for A is selected as the **split-point** for A
- Split: Based on split point P
 - The set of tuples in D satisfying $A \leq P$ vs. those with $A > P$

Gain Ratio: A Refined Measure for Attribute Selection

- Information gain measure is biased towards attributes with a large number of values
- Gain ratio: Overcomes the problem (as a normalization to information gain)

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

- $\text{GainRatio}(A) = \text{Gain}(A)/\text{SplitInfo}(A)$
- The attribute with the maximum gain ratio is selected as the splitting attribute
- Gain ratio is used in a popular algorithm C4.5 (a successor of ID3) by R. Quinlan
- Example
 - $\text{SplitInfo}_{\text{income}}(D) = -\frac{4}{14} \log_2 \frac{4}{14} - \frac{6}{14} \log_2 \frac{6}{14} - \frac{4}{14} \log_2 \frac{4}{14} = 1.557$
 - $\text{GainRatio}(\text{income}) = 0.029/1.557 = 0.019$

Another Measure: Gini Index

- Gini index: Used in CART, and also in IBM IntelligentMiner
- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as
 - $$gini(D) = 1 - \sum_{j=1}^n p_j^2$$
 - 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 $gini(D)$ 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*)

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

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

- 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

Comparing Three Attribute Selection Measures

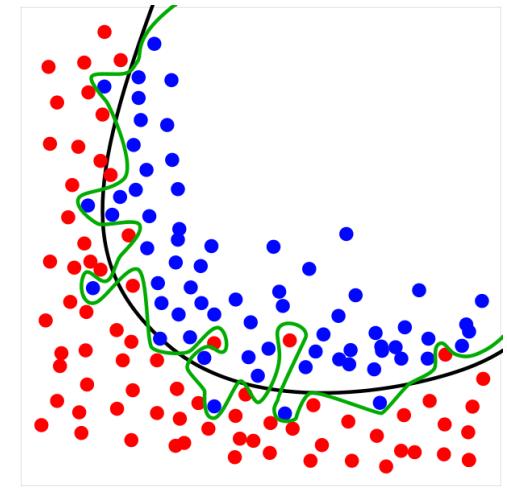
- ❑ The three measures, in general, return good results but
 - ❑ **Information gain:**
 - ❑ biased towards multivalued attributes
- ❑ **Gain ratio:**
 - ❑ tends to prefer unbalanced splits in which one partition is much smaller than the others
- ❑ **Gini index:**
 - ❑ biased to multivalued attributes
 - ❑ has difficulty when # of classes is large
 - ❑ tends to favor tests that result in equal-sized partitions and purity in both partitions

Other Attribute Selection Measures

- Minimal Description Length (MDL) principle
 - Philosophy: 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
- CHAID: a popular decision tree algorithm, measure based on χ^2 test for independence
- Multivariate splits (partition based on multiple variable combinations)
 - CART: finds multivariate splits based on a linear combination of attributes
- There are many other measures proposed in research and applications
 - E.g., G-statistics, C-SEP
- 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
- ❑ 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”



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 fast learning speed
 - Convertible to simple and easy to understand classification rules
 - Easy to be adapted to database system implementations (e.g., using SQL)
 - Comparable classification accuracy with other methods
- **RainForest** (VLDB'98 — Gehrke, Ramakrishnan & Ganti)
 - Builds an AVC-list (attribute, value, class label)

RainForest: A Scalable Classification Framework

- The criteria that determine the quality of the tree can be computed separately
 - Builds an AVC-list: **AVC (Attribute, Value, Class_label)**
- **AVC-set** (of an attribute X)
 - Projection of training dataset onto the attribute X and class label where counts of individual class label are aggregated
- **AVC-group** (of a node n)
 - Set of AVC-sets of all predictor attributes at the node n

age	income	student	credit_rating	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
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>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

The Training Data

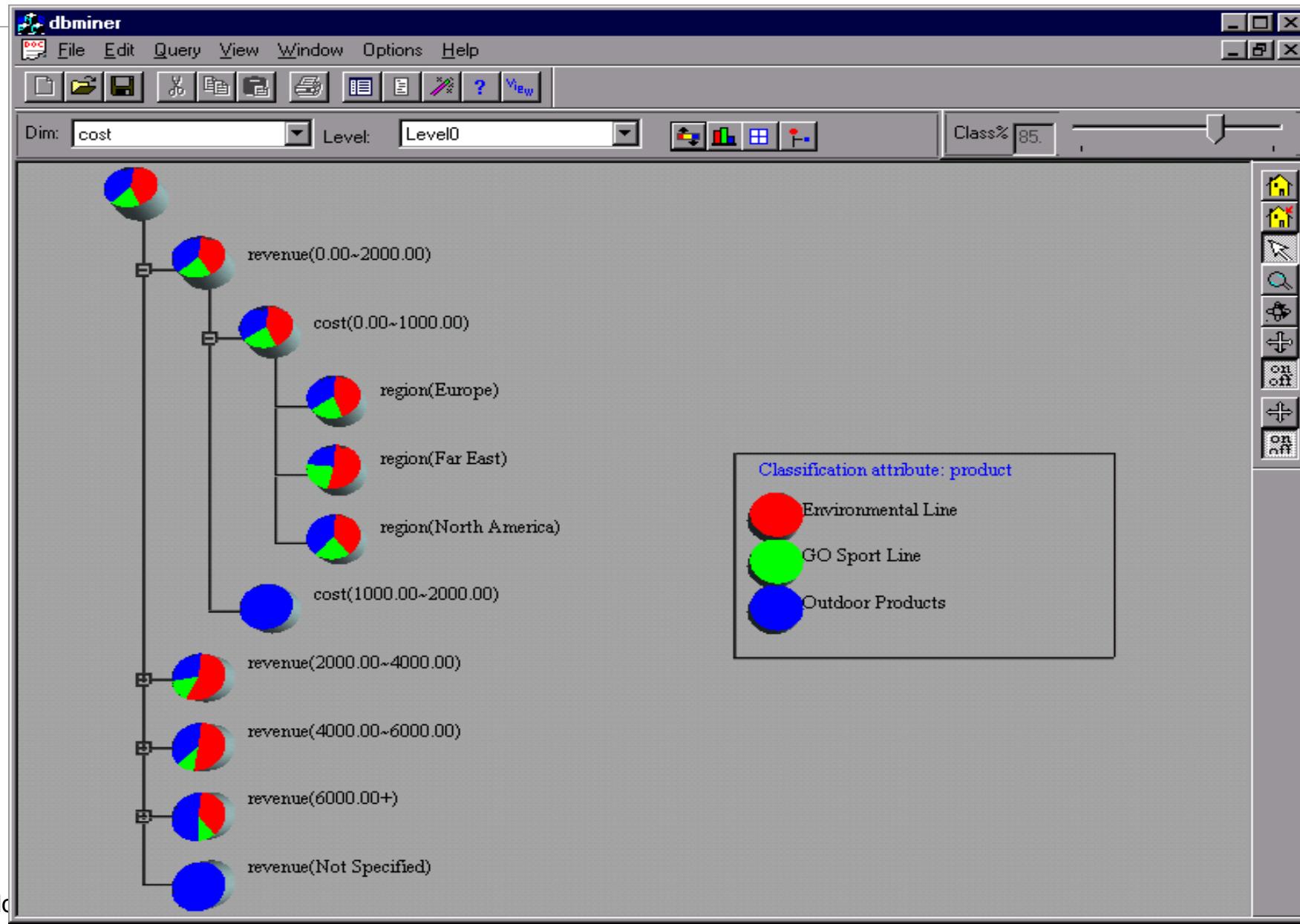
AVC-set on Age		
Age	Buy_Computer	
	yes	no
<=30	2	3
31..40	4	0
>40	3	2

AVC-set on Income		
income	Buy_Computer	
	yes	no
high	2	2
medium	4	2
low	3	1

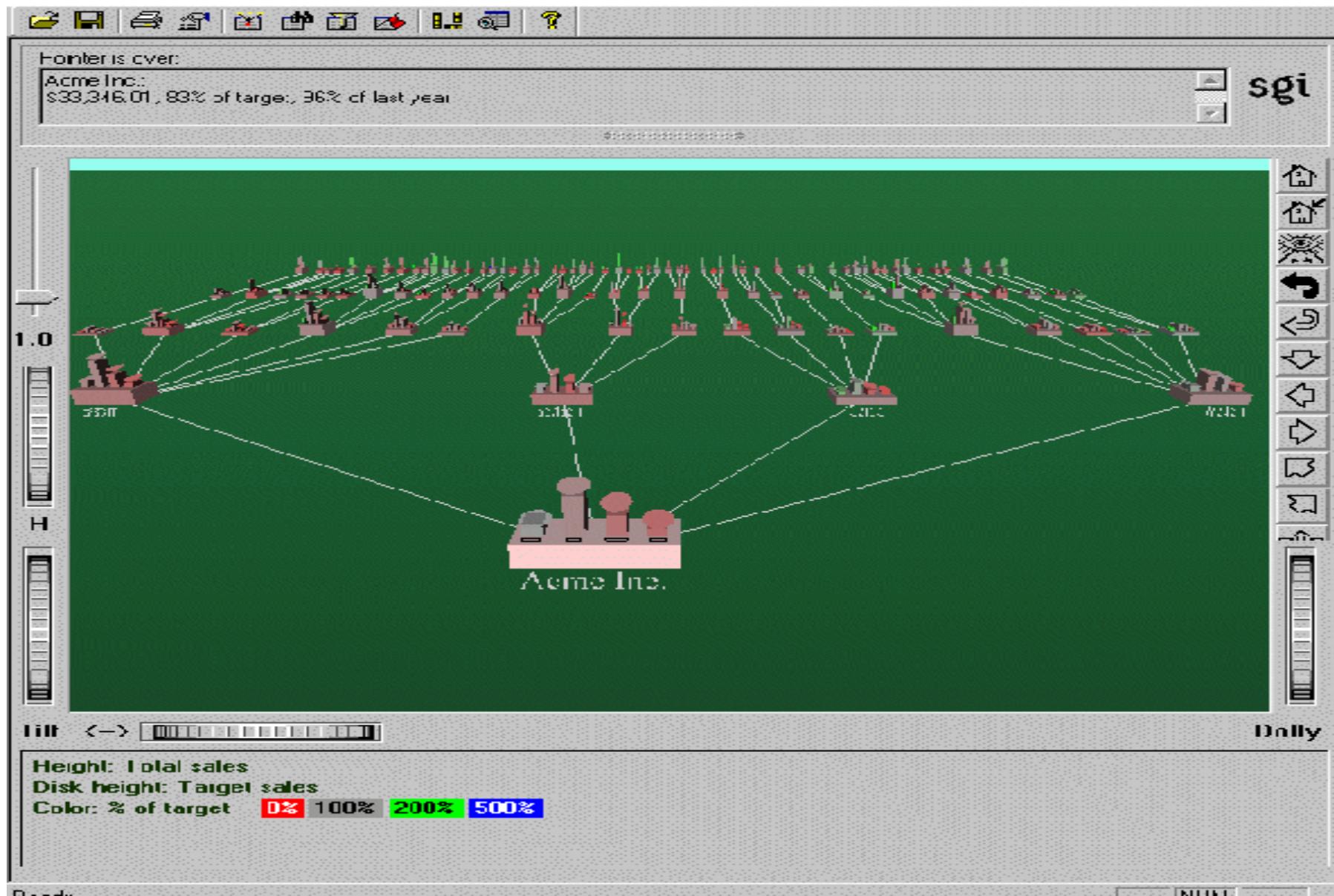
AVC-set on Student		AVC-set on Credit_Rating			
student	Buy_Computer		Credit rating	Buy_Computer	
	yes	no		yes	no
yes	6	1	fair	6	2
no	3	4	excellent	3	3

Its AVC Sets

Presentation of Classification Results

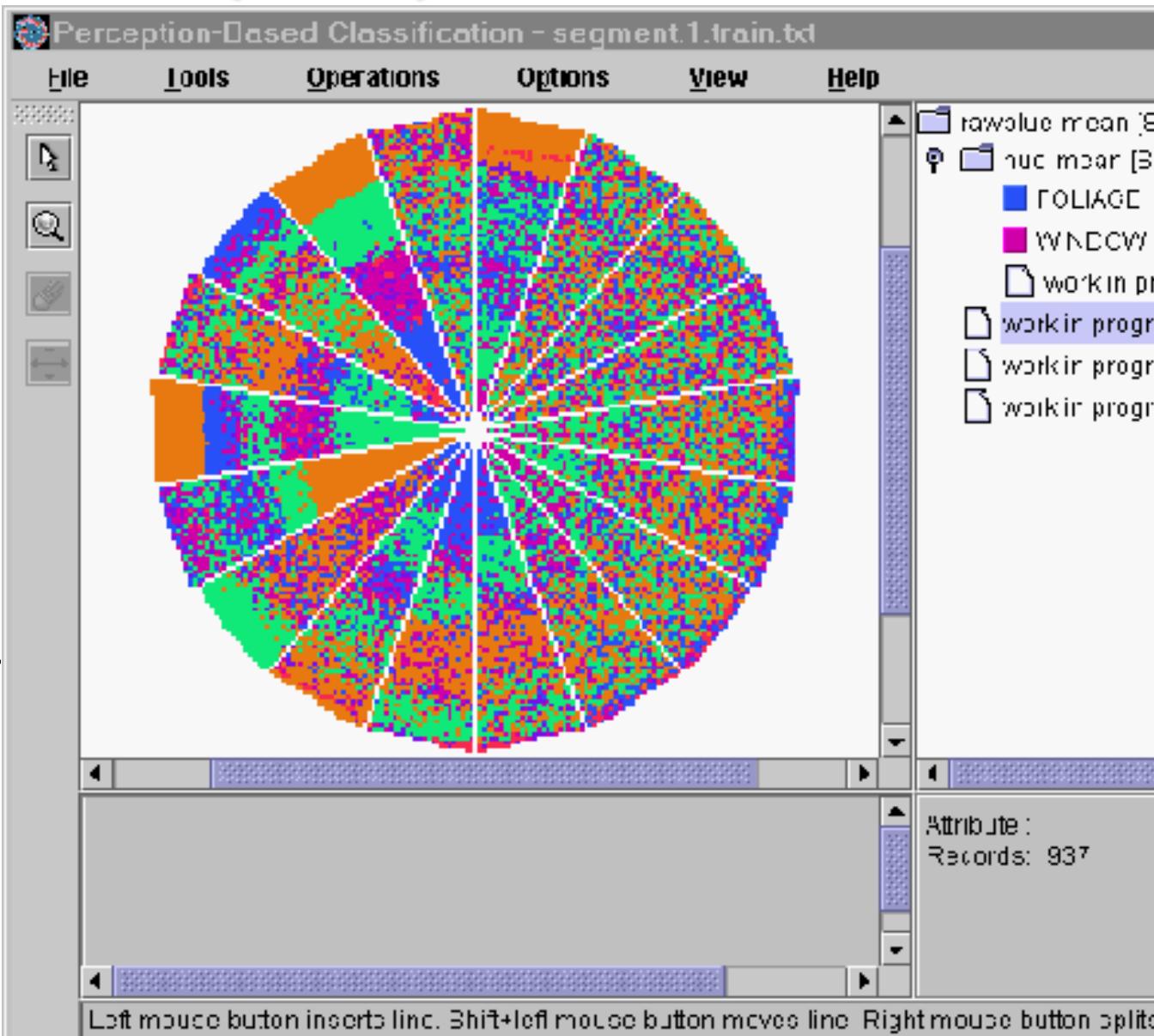


Visualization of a Decision Tree (in SGI/MineSet 3.0)



Interactive Visual Mining by Perception-Based Classification (PBC)

- ❑ Perception-based classifier (PCB): developed at Univ. of Munich (1999)
- ❑ One color represents one class label
- ❑ One pie represents one attribute (or variable)
- ❑ The pie with random spread implies weak classification power
- ❑ The pie with clearly partitioned color strips implies good classification power
- ❑ One can select a good attribute and regenerate new pie charts for classification at the subsequent levels

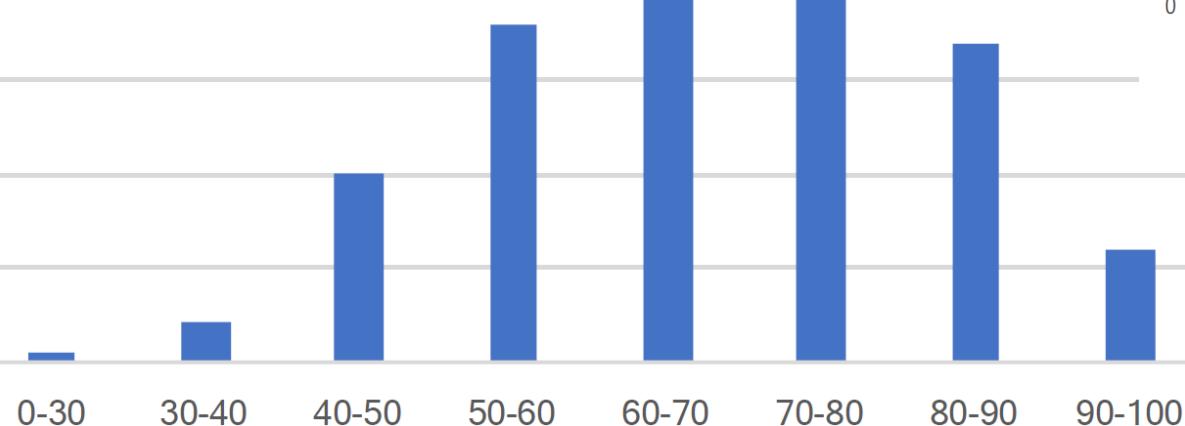


CS412-Fall 2017: Midterm Statistics

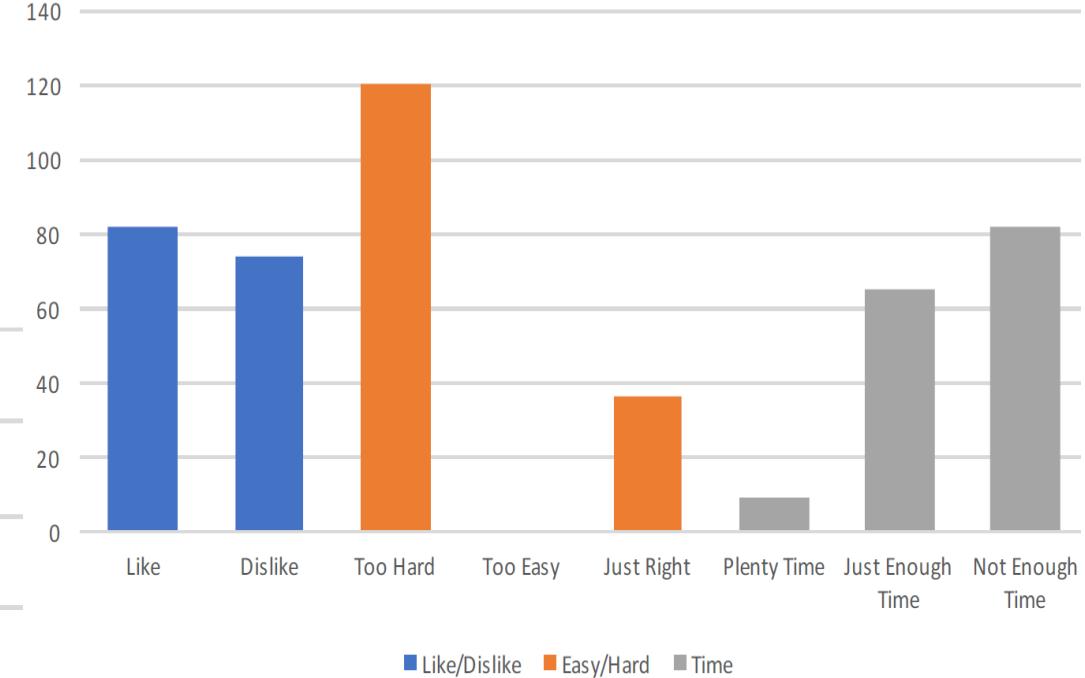
Range	Count
0-30	1
30-40	4
40-50	20
50-60	35
60-70	45
70-80	50
80-90	32
90-100	13

Mean 68.64
Median 69.5
1st quartile 57.75
3rd quartile 79.5

Midterm Scores



Midterm Options



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What Is Bayesian Classification?

- A statistical classifier
 - Perform *probabilistic prediction* (i.e., predict class membership probabilities)
- Foundation—Based on Bayes' Theorem
- Performance
 - A simple Bayesian classifier, *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
- Incremental
 - Each training example can incrementally increase/decrease the probability that a hypothesis is correct—prior knowledge can be combined with observed data
- Theoretical Standard
 - Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

નાયેવી બેસિન્સ ક્લાસિફિકેશન
Classification

Bayes' Theorem: Basics

- Total probability Theorem:

$$p(B) = \sum_i p(B|A_i)p(A_i)$$

- Bayes' Theorem:

$$p(H|X) = \frac{p(X|H)p(H)}{p(X)} \propto p(X|H) P(H)$$

test Data  

posteriori probability likelihood prior probability

What we should choose

What we just see

What we knew previously

- X : a data sample ("evidence")
- H : X belongs to class C

Prediction can be done based on Bayes' Theorem:

Classification is to derive the maximum posteriori

Naïve Bayes Classifier: Making a Naïve Assumption

- Practical difficulty of Naïve Bayes inference: It requires initial knowledge of many probabilities, which may not be available or involving significant computational cost
- A Naïve Special Case
 - Make an additional **assumption** to simplify the model, but achieve comparable performance.

attributes are conditionally independent

(i.e., no dependence relation between attributes)

$$p(X|C_i) = \prod_k p(x_k|C_i) = p(x_1|C_i) \cdot p(x_2|C_i) \cdots p(x_n|C_i)$$

- Only need to count the class distribution w.r.t. features

નેડીવે બેસ ક્લાસિફિકર: નેડીવે અસુમ્પ્શન



Naïve Bayes Classifier: Categorical vs. Continuous Valued Features

- If feature x_k is categorical, $p(x_k = v_k | C_i)$ is the # of tuples in C_i with $x_k = v_k$, divided by $|C_{i,D}|$ (# of tuples of C_i in D)

$$p(X|C_i) = \prod_k p(x_k|C_i) = p(x_1|C_i) \cdot p(x_2|C_i) \cdots p(x_n|C_i)$$

- If feature x_k is continuous-valued, $p(x_k = v_k | C_i)$ is usually computed based on Gaussian distribution with a mean μ and standard deviation σ

$$p(x_k = v_k | C_i) = N(x_k | \mu_{C_i}, \sigma_{C_i}) = \frac{1}{\sqrt{2\pi}\sigma_{C_i}} e^{-\frac{(x-\mu_{C_i})^2}{2\sigma^2}}$$

Naïve Bayes Classifier: Training Dataset

Class:

C1:`buys_computer = 'yes'`

C2:`buys_computer = 'no'`

Data to be classified:

X = (age ≤ 30 , Income = medium,
Student = yes, Credit_rating = Fair)

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
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31...40	medium	no	excellent	yes
31...40	high	yes	fair	yes
> 40	medium	no	excellent	no

Naïve Bayes Classifier: An Example

- $P(C_i)$: $P(\text{buys_computer} = \text{"yes"}) = 9/14 = 0.643$
 $P(\text{buys_computer} = \text{"no"}) = 5/14 = 0.357$
- Compute $P(X|C_i)$ for each class
 $P(\text{age} = \text{"}<=30\text{"} | \text{buys_computer} = \text{"yes"}) = 2/9 = 0.222$
 $P(\text{age} = \text{"}<= 30\text{"} | \text{buys_computer} = \text{"no"}) = 3/5 = 0.6$
 $P(\text{income} = \text{"medium"} | \text{buys_computer} = \text{"yes"}) = 4/9 = 0.444$
 $P(\text{income} = \text{"medium"} | \text{buys_computer} = \text{"no"}) = 2/5 = 0.4$
 $P(\text{student} = \text{"yes"} | \text{buys_computer} = \text{"yes"}) = 6/9 = 0.667$
 $P(\text{student} = \text{"yes"} | \text{buys_computer} = \text{"no"}) = 1/5 = 0.2$
 $P(\text{credit_rating} = \text{"fair"} | \text{buys_computer} = \text{"yes"}) = 6/9 = 0.667$
 $P(\text{credit_rating} = \text{"fair"} | \text{buys_computer} = \text{"no"}) = 2/5 = 0.4$

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
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>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

- $X = (\text{age} <= 30, \text{income} = \text{medium}, \text{student} = \text{yes}, \text{credit_rating} = \text{fair})$

$$P(X|C_i) : P(X|\text{buys_computer} = \text{"yes"}) = 0.222 \times 0.444 \times 0.667 \times 0.667 = 0.044$$

$$P(X|\text{buys_computer} = \text{"no"}) = 0.6 \times 0.4 \times 0.2 \times 0.4 = 0.019$$

$$P(X|C_i) * P(C_i) : P(X|\text{buys_computer} = \text{"yes"}) * P(\text{buys_computer} = \text{"yes"}) = 0.028$$

$$P(X|\text{buys_computer} = \text{"no"}) * P(\text{buys_computer} = \text{"no"}) = 0.007$$

0.044 * 0.643

Therefore, X belongs to class ("buys_computer = yes")

Avoiding the Zero-Probability Problem

- Naïve Bayesian prediction requires each conditional probability be **non-zero**
 - Otherwise, the predicted probability will be zero

$$p(X|C_i) = \prod_k p(x_k|C_i) = p(x_1|C_i) \cdot p(x_2|C_i) \cdots p(x_n|C_i)$$

- Example. Suppose a dataset with 1000 tuples:
 - income = low (0), income = medium (990), and income = high (10)
- Use **Laplacian correction** (or Laplacian estimator)
 - *Adding 1 to each case*

$$\text{Prob}(\text{income} = \text{low}) = 1/(1000 + 3)$$

$$\text{Prob}(\text{income} = \text{medium}) = (990 + 1)/(1000 + 3)$$

$$\text{Prob}(\text{income} = \text{high}) = (10 + 1)/(1000 + 3)$$

- The “corrected” probability estimates are close to their “uncorrected” counterparts

Naïve Bayes Classifier: Strength vs. Weakness

- ❑ Strength
 - ❑ Easy to implement
 - ❑ Good results obtained in most of the cases
- ❑ Weakness
 - ❑ Assumption: attributes conditional independence, therefore loss of accuracy
 - ❑ Practically, dependencies exist among variables
 - ❑ E.g., Patients: Profile: age, family history, etc.
Symptoms: fever, cough etc.
Disease: lung cancer, diabetes, etc.
 - ❑ Dependencies among these cannot be modeled by Naïve Bayes Classifier
 - ❑ How to deal with these dependencies?
 - ❑ Use Bayesian Belief Networks (to be covered in the next chapter)

Chapter 8. Classification: Basic Concepts

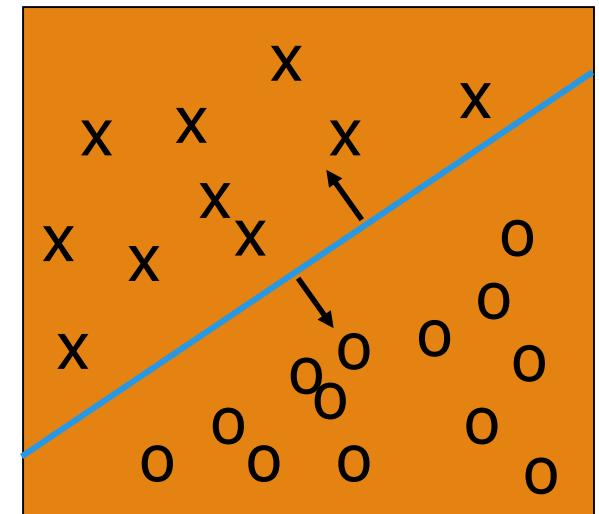
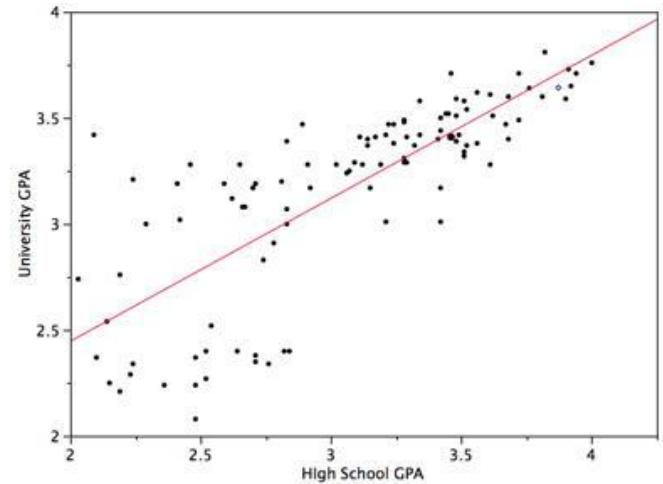
- ❑ Classification: Basic Concepts
- ❑ Decision Tree Induction
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Linear Regression vs. Linear Classifier

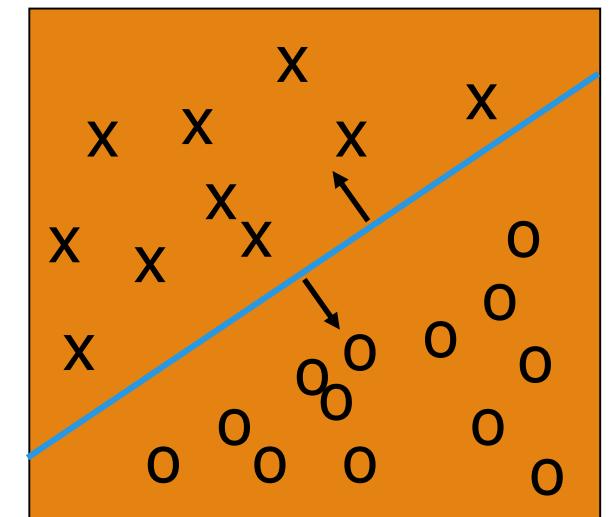
- ❑ Linear regression
 - ❑ Data modeled to fit a straight line
 - ❑ *Linear equation:* $Y = w X + b$
 - ❑ Often uses the least-square method to fit the line
 - ❑ Used to predict continuous values

- ❑ Linear Classifier
 - ❑ Built a classification model using a straight line
 - ❑ Used for (categorical data) binary classification



Linear Classifier: General Ideas

- ❑ Binary Classification
- ❑ $f(x)$ is a linear function based on the example's attribute values
 - ❑ The prediction is based on the value of $f(x)$
 - ❑ Data above the blue line belongs to class 'x' (i.e., $f(x) > 0$)
 - ❑ Data below blue line belongs to class 'o' (i.e., $f(x) < 0$)
- ❑ Classical Linear Classifiers
 - ❑ Linear Discriminant Analysis (LDA) (not covered)
 - ❑ Logistic Regression
 - ❑ Perceptron (later)
 - ❑ SVM (later)

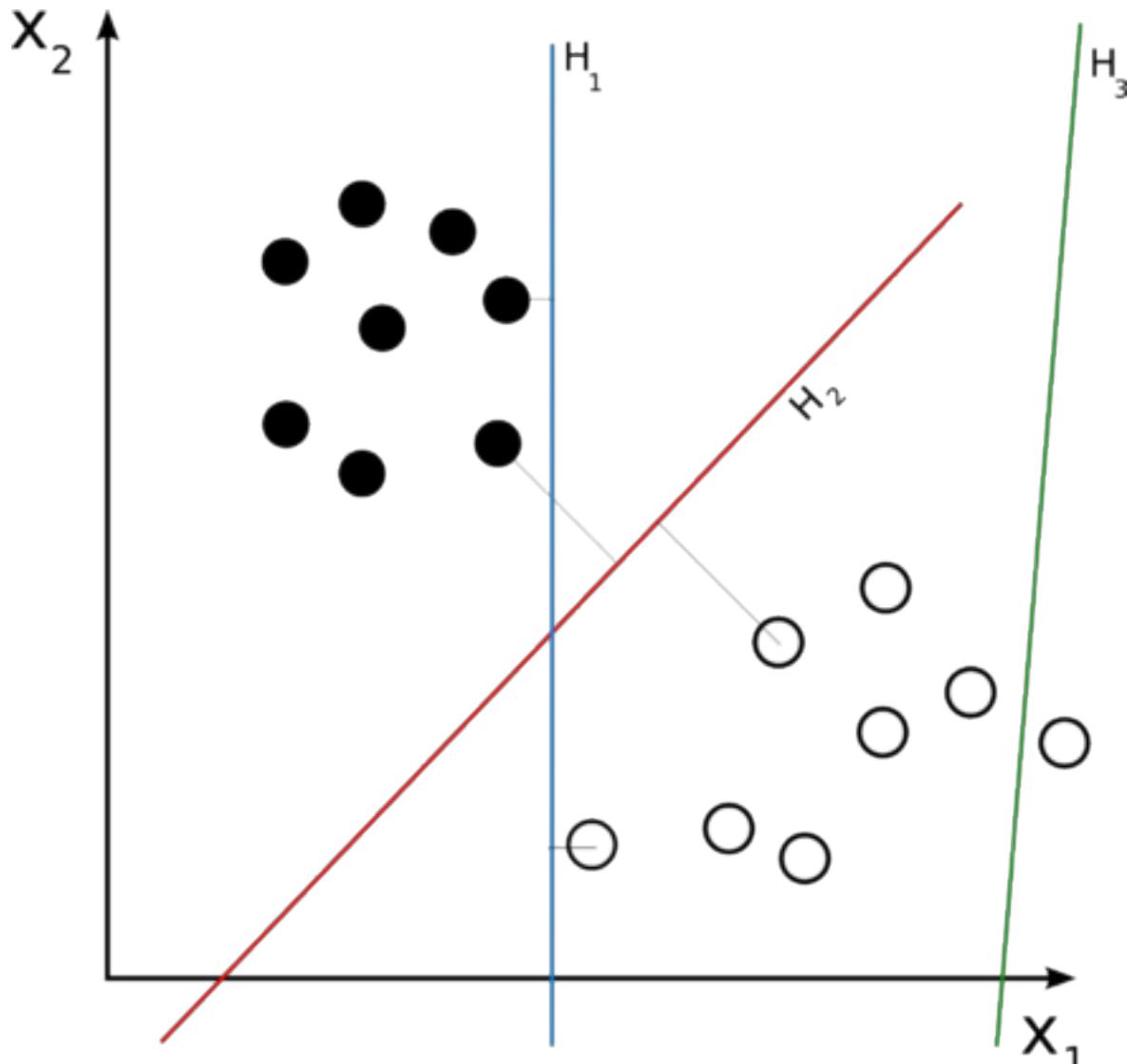


Linear Classifier: An Example

- A toy rule to determine whether a faculty member has tenure
 - Year ≥ 6 or Title = “Professor” \Leftrightarrow Tenure
- How to express the rule as a linear classifier?
- Features
 - $x_1 (x_1 \geq 0)$ is an integer denoting the year
 - x_2 is a Boolean denoting whether the title is “Professor”
- A feasible linear classifier: $f(x) = (x_1 - 5) + 6 \cdot x_2$
 - When x_2 is True, because $x_1 \geq 0$, $f(x)$ is always greater than 0
 - When x_2 is False, because $f(x) > 0 \Leftrightarrow x_1 \geq 6$
- There are many more feasible classifiers
 - $f(x) = (x_1 - 5.5) + 6 \cdot x_2$
 - $f(x) = 2 \cdot (x_1 - 5) + 11 \cdot x_2$
 -

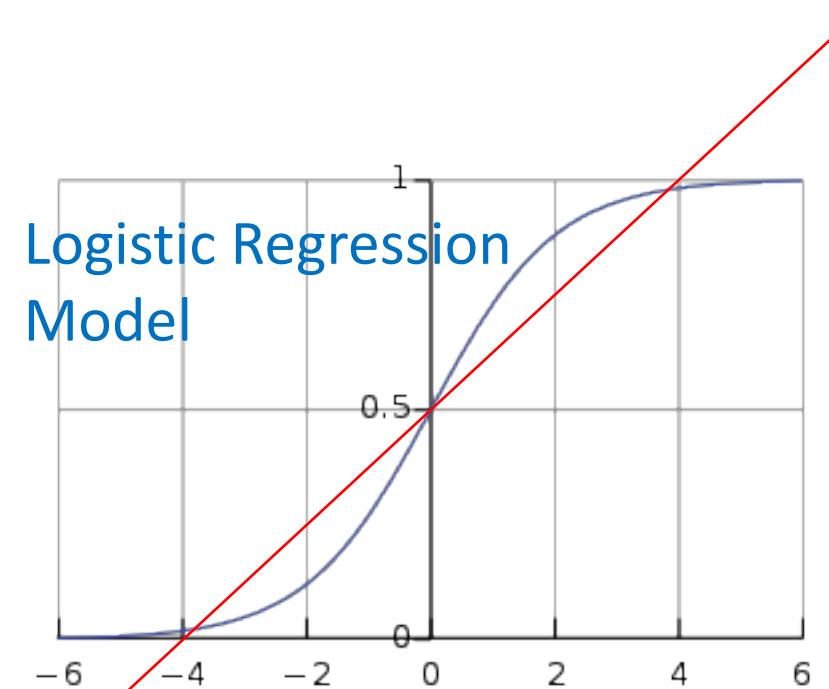
Key Question: Which Line Is Better?

- ❑ There might be many feasible linear functions
 - ❑ Both H_1 and H_2 will work
- ❑ Which one is better?
 - ❑ H_2 looks “better” in the sense that it is also furthest from both groups
 - ❑ We will introduce more in the SVM section



Logistic Regression: General Ideas

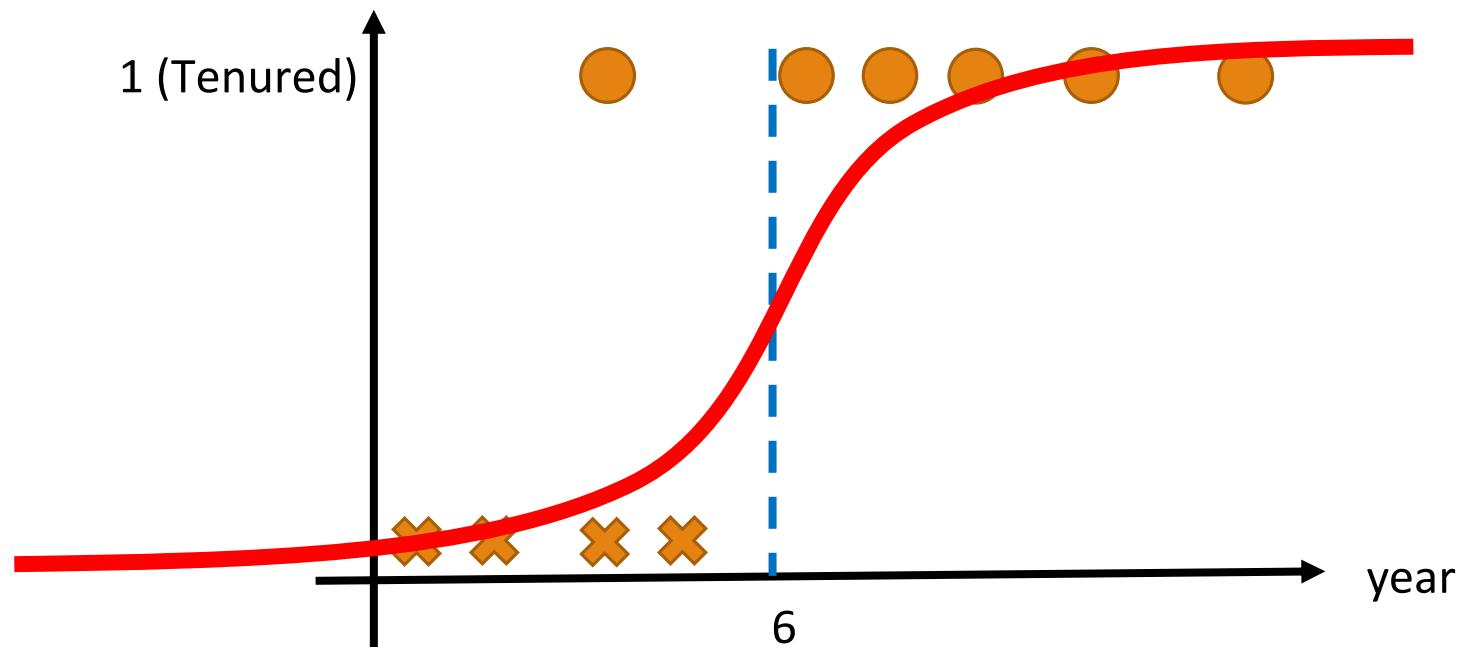
- Key Idea: Turns linear predictions into probabilities
- Sigmoid function:
 - $S(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$
 - Projects $(-\infty, +\infty)$ to $[0, 1]$
- Compare to linear probability model
- More smooth



Linear Probability
Model

Logistic Regression: An Example

- ❑ Suppose we only consider the year as feature



Logistic Regression: Maximum Likelihood

- ❑ The prediction function to learn

- ❑ $p(Y = 1 | X = x; \mathbf{w}) = S(w_0 + \sum_{i=1}^n w_i \cdot x_i)$
 - ❑ $\mathbf{w} = (w_0, w_1, w_2, \dots, w_n)$ are the parameters

- ❑ Maximum Likelihood

- ❑ Log likelihood:

$$l(\mathbf{w}) = \sum_{i=1}^N y_i \log p(Y = 1 | X = x_i; \mathbf{w}) + (1 - y_i) \log(1 - p(Y = 1 | X = x_i; \mathbf{w}))$$

- ❑ There's no close form solution

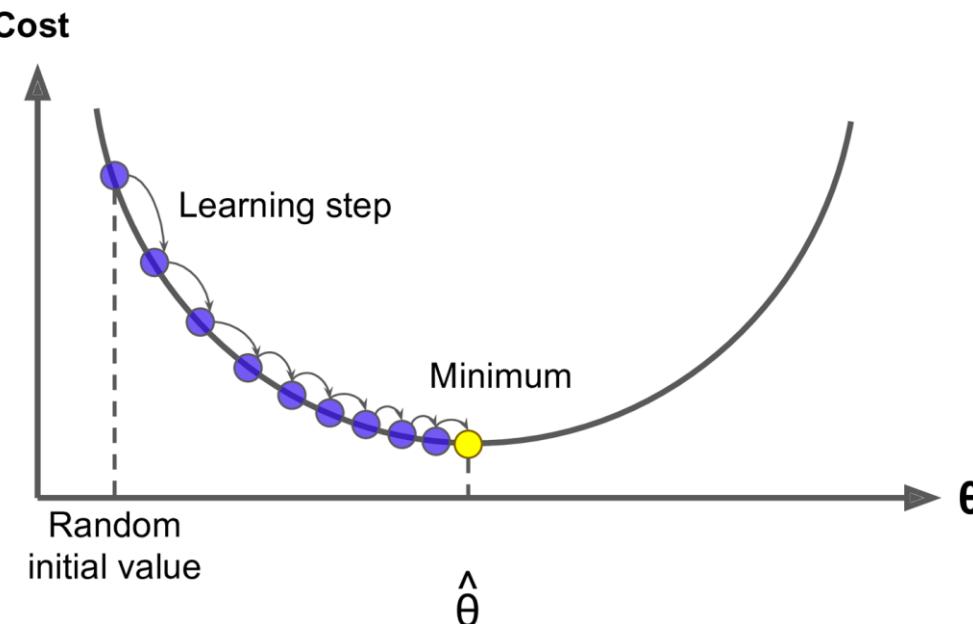
- ❑ Gradient Descent
 - ❑ Update \mathbf{w} based on training data
 - ❑ Chain-rule for the gradient

Gradient Descent

- Gradient Descent is an iterative optimization algorithm for finding the minimum of a function (e.g., the negative log likelihood)
- For a function $F(x)$ at a point a , $F(x)$ decreases fastest if we go in the direction of the negative gradient of a

$$\mathbf{a}_{n+1} = \mathbf{a}_n - \gamma \nabla F(\mathbf{a}_n)$$

When the gradient is zero, we arrive at the local minimum



Generative vs. Discriminative Classifiers

- X: observed variables (features)
- Y: target variables (class labels)
- A generative classifier models $p(Y, X)$
 - It models how the data was "generated"? "what is the likelihood this or that class generated this instance?" and pick the one with higher probability
- Naïve Bayes
- Bayesian Networks
- A discriminative classifier models $p(Y | X)$
 - It uses the data to create a decision boundary
- Logistic Regression
- Support Vector Machines

Further Comments on Discriminative Classifiers

- Strength
 - Prediction accuracy is generally high
 - As compared to generative models
 - Robust, works when training examples contain errors
 - Fast evaluation of the learned target function
 - Comparing to [\(covered in future\)](#) Bayesian networks (which are normally slow)
- Criticism
 - Long training time
 - Difficult to understand the learned function (weights)
 - Bayesian networks can be used easily for pattern discovery
 - Not easy to incorporate domain knowledge
 - Easy in the form of priors on the data or distributions

Chapter 8. Classification: Basic Concepts

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Model Evaluation and Selection

- Evaluation metrics
 - How can we measure accuracy?
 - Other metrics to consider?
- Use **validation test set** of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy
 - Holdout method
 - Cross-validation
 - Bootstrap
- Comparing classifiers:
 - ROC Curves

Classifier Evaluation Metrics: Confusion Matrix

□ Confusion Matrix:

Actual class\Predicted class	C_1	$\neg C_1$
C_1	True Positives (TP)	False Negatives (FN)
$\neg C_1$	False Positives (FP)	True Negatives (TN)

□ In a confusion matrix w. m classes, $CM_{i,j}$ indicates # of tuples in class i that were labeled by the classifier as class j

□ May have extra rows/columns to provide totals

□ Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	6954	46	7000
buy_computer = no	412	2588	3000
Total	7366	2634	10000

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	$\neg C$	
C	TP	FN	P
$\neg C$	FP	TN	N
	P'	N'	All

- Classifier accuracy, or recognition rate
 - Percentage of test set tuples that are correctly classified
$$\text{Accuracy} = (\text{TP} + \text{TN})/\text{All}$$
- Error rate: $1 - \text{accuracy}$, or
- $$\text{Error rate} = (\text{FP} + \text{FN})/\text{All}$$

- Class imbalance problem
 - One class may be *rare*
 - E.g., fraud, or HIV-positive
 - Significant *majority of the negative class* and minority of the positive class
 - Measures handle the class imbalance problem
 - **Sensitivity** (recall): True positive recognition rate
 - $\text{Sensitivity} = \text{TP}/\text{P}$
 - **Specificity**: True negative recognition rate
 - $\text{Specificity} = \text{TN}/\text{N}$

Classifier Evaluation Metrics: Precision and Recall, and F-measures

- ❑ **Precision:** Exactness: what % of tuples that the classifier labeled as positive are actually positive?

$$P = \text{Precision} = \frac{TP}{TP + FP}$$

- ❑ **Recall:** Completeness: what % of positive tuples did the classifier label as positive?

$$R = \text{Recall} = \frac{TP}{TP + FN}$$

- ❑ Range: $[0, 1]$
- ❑ The “inverse” relationship between precision & recall
- ❑ **F measure (or F-score):** harmonic mean of precision and recall
- ❑ In general, it is the weighted measure of precision & recall

$$F_{\beta} = \frac{1}{\alpha \cdot \frac{1}{P} + (1 - \alpha) \cdot \frac{1}{R}} = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

Assigning β times as much weight to recall as to precision)

- ❑ **F1-measure (balanced F-measure)**

- ❑ That is, when $\beta = 1$,

$$F_1 = \frac{2PR}{P + R}$$

Classifier Evaluation Metrics: Example

- ❑ Use the same confusion matrix, calculate the measure just introduced

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	90	210	300	30.00 (<i>sensitivity</i>)
cancer = no	140	9560	9700	98.56 (<i>specificity</i>)
Total	230	9770	10000	96.50 (<i>accuracy</i>)

- ❑ Sensitivity = $TP/P = 90/300 = 30\%$
- ❑ Specificity = $TN/N = 9560/9700 = 98.56\%$
- ❑ Accuracy = $(TP + TN)/All = (90+9560)/10000 = 96.50\%$
- ❑ Error rate = $(FP + FN)/All = (140 + 210)/10000 = 3.50\%$
- ❑ Precision = $TP/(TP + FP) = 90/(90 + 140) = 90/230 = 39.13\%$
- ❑ Recall = $TP / (TP + FN) = 90/(90 + 210) = 90/300 = 30.00\%$
- ❑ $F1 = 2 P \times R / (P + R) = 2 \times 39.13\% \times 30.00\% / (39.13\% + 30\%) = 33.96\%$

Classifier Evaluation: Holdout & Cross-Validation

- **Holdout method**
 - Given data is randomly partitioned into two independent sets
 - Training set (e.g., 2/3) for model construction
 - Test set (e.g., 1/3) for accuracy estimation
 - Repeated random sub-sampling validation: a variation of holdout
 - Repeat holdout k times, accuracy = avg. of the accuracies obtained
- **Cross-validation (k -fold, where $k = 10$ is most popular)**
 - Randomly partition the data into k *mutually exclusive* subsets, each approximately equal size
 - At i -th iteration, use D_i as test set and others as training set
 - Leave-one-out: k folds where $k = \#$ of tuples, for small sized data
 - *Stratified cross-validation*: folds are stratified so that class distribution, in each fold is approximately the same as that in the initial data

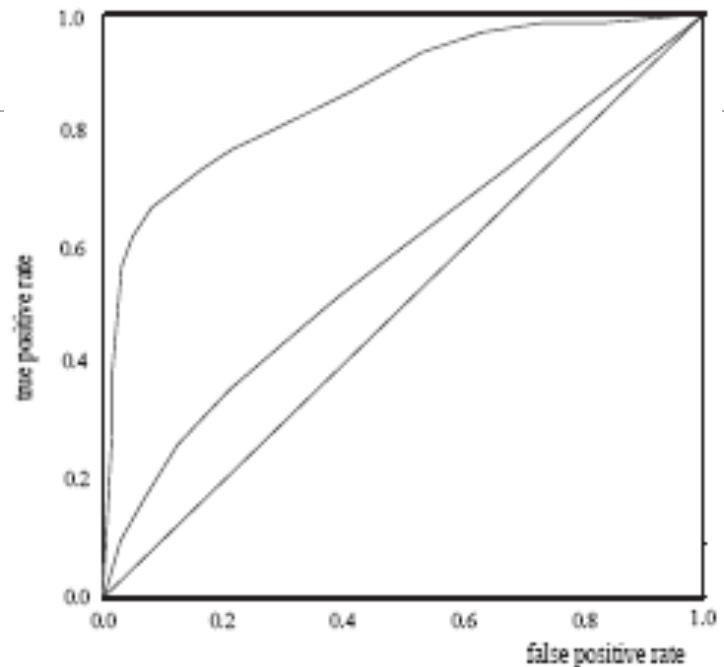
Classifier Evaluation: Bootstrap

- **Bootstrap**
 - Works well with small data sets
 - Samples the given training tuples uniformly *with replacement*
 - Each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several bootstrap methods, and a common one is **.632 bootstrap**
 - A data set with d tuples is sampled d times, with replacement, resulting in a training set of d samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data end up in the bootstrap, and the remaining 36.8% form the test set (since $(1 - 1/d)^d \approx e^{-1} = 0.368$)
 - Repeat the sampling procedure k times, overall accuracy of the model:

$$Acc(M) = \frac{1}{k} \sum_{i=1}^k (0.632 \times Acc(M_i)_{test_set} + 0.368 \times Acc(M_i)_{train_set})$$

Model Selection: ROC Curves

- ❑ ROC (Receiver Operating Characteristics) curves: for visual comparison of classification models
- ❑ Originated from signal detection theory
- ❑ Shows the trade-off between the true positive rate and the false positive rate
- ❑ The area under the ROC curve (**AUC**: Area Under Curve) is a measure of the accuracy of the model
- ❑ Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- ❑ The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model



- ❑ Vertical axis represents the true positive rate
- ❑ Horizontal axis rep. the false positive rate
- ❑ The plot also shows a diagonal line
- ❑ A model with perfect accuracy will have an area of 1.0

Issues Affecting Model Selection

- **Accuracy**
 - classifier accuracy: predicting class label
- **Speed**
 - time to construct the model (training time)
 - time to use the model (classification/prediction time)
- **Robustness:** handling noise and missing values
- **Scalability:** efficiency in disk-resident databases
- **Interpretability**
 - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules

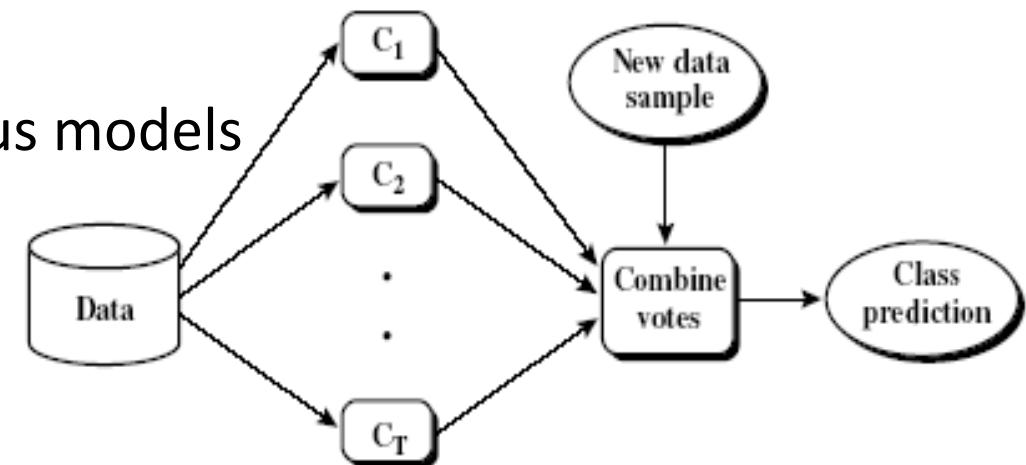
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Ensemble Methods: Increasing the Accuracy

- Ensemble methods
 - Use a combination of models to increase accuracy
 - Combine a series of k learned models, M_1, M_2, \dots, M_k , with the aim of creating an improved model M^*
- Popular ensemble methods
 - Bagging: Trains each model using a subset of the training set, and models learned in parallel
 - Boosting: Trains each new model instance to emphasize the training instances that previous models mis-classified, and models learned in order



Bagging: Bootstrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
 - Given a set D of d tuples, at each iteration i , a training set D_i of d tuples is sampled with replacement from D (i.e., bootstrap)
 - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample X
 - Each classifier M_i returns its class prediction
 - The bagged classifier M^* counts the votes and assigns the class with the most votes to X
- Prediction: It can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple
- Accuracy: Improved accuracy in prediction
 - Often significantly better than a single classifier derived from D
 - For noise data: Not considerably worse, more robust

Random Forest: Basic Concepts

- Random Forest (first proposed by L. Breiman in 2001)
 - A variation of bagging for *decision trees*
 - *Data bagging*
 - Use a subset of training data by sampling with replacement for each tree
 - *Feature bagging*
 - At each node use a random selection of attributes as candidates and split by the best attribute among them
 - Compared to original bagging, increases the diversity among generated trees
 - During classification, each tree votes and the most popular class is returned

Random Forest

- ❑ Two Methods to construct Random Forest:
 - ❑ Forest-RI (*random input selection*): Randomly select, at each node, F attributes as candidates for the split at the node. The CART methodology is used to grow the trees to maximum size
 - ❑ Forest-RC (*random linear combinations*): Creates new attributes (or features) that are a linear combination of the existing attributes (reduces the correlation between individual classifiers)
- ❑ Comparable in accuracy to Adaboost, but more robust to errors and outliers
- ❑ Insensitive to the number of attributes selected for consideration at each split, and faster than typical bagging or boosting

Boosting

- ❑ Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- ❑ How boosting works?
 - ❑ **Weights** are assigned to each training tuple
 - ❑ A series of k classifiers is iteratively learned
 - ❑ After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1} , to **pay more attention to the training tuples that were misclassified** by M_i
 - ❑ The final **M^* combines the votes** of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- ❑ Boosting algorithm can be extended for numeric prediction
- ❑ Comparing with bagging: Boosting tends to have greater accuracy, but it also risks overfitting the model to misclassified data

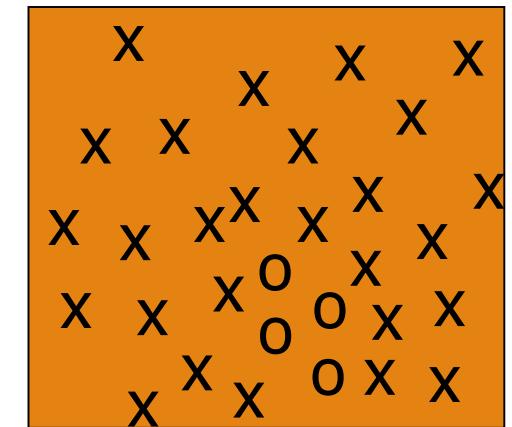
Adaboost (Freund and Schapire, 1997)

- Given a set of d class-labeled tuples, $(\mathbf{X}_1, y_1), \dots, (\mathbf{X}_d, y_d)$
- Initially, all the weights of tuples are set the same ($1/d$)
- Generate k classifiers in k rounds. At round i ,
 - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
 - Each tuple's chance of being selected is based on its weight
 - A classification model M_i is derived from D_i
 - Its error rate is calculated using D_i as a test set
 - If a tuple is misclassified, its weight is increased; otherwise, it is decreased
- Error rate: $\text{err}(\mathbf{X}_j)$ is the misclassification error of tuple \mathbf{X}_j . Classifier M_i error rate is the sum of the weights of the misclassified tuples:
- The weight of classifier M_i 's vote is
$$\log \frac{1 - \text{error}(M_i)}{\text{error}(M_i)}$$

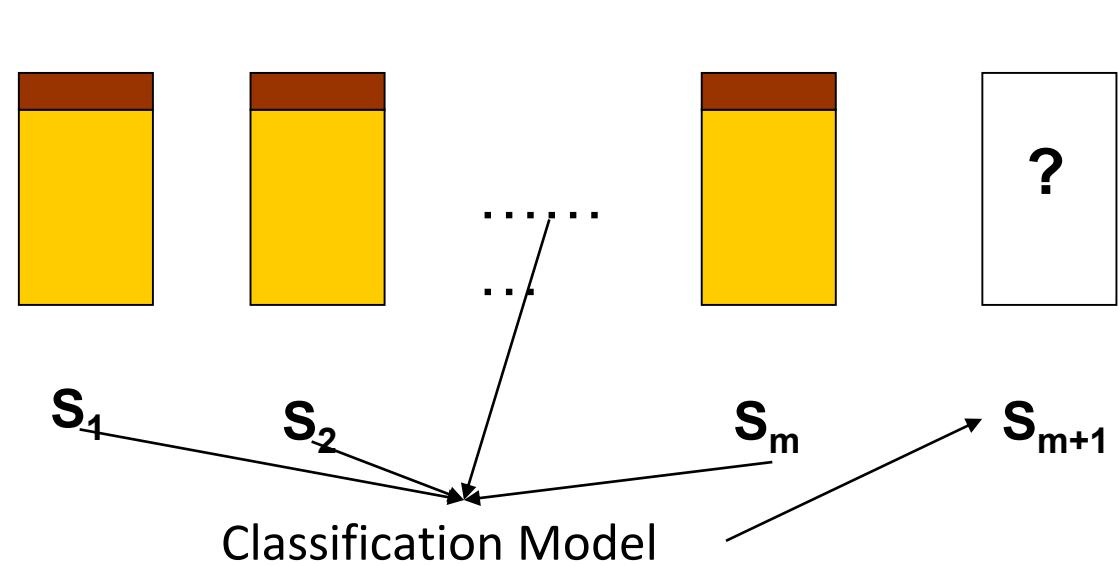
$$\text{error}(M_i) = \sum_j w_j \times \text{err}(\mathbf{X}_j)$$

Classification of Class-Imbalanced Data Sets

- Class-imbalance problem: Rare positive examples but numerous negative ones
 - E.g., medical diagnosis, fraud transaction, accident (oil-spill), and product fault
- Traditional methods assume a balanced distribution of classes and equal error costs: not suitable for class-imbalanced data
- Typical methods on imbalanced data in two-class classification
 - **Oversampling:** Re-sampling of data from positive class
 - **Under-sampling:** Randomly eliminate tuples from negative class
 - **Threshold-moving:** Move the decision threshold, t , so that the rare class tuples are easier to classify, and hence, less chance of costly false negative errors
 - **Ensemble techniques:** Ensemble multiple classifiers introduced above
- Still difficult for class imbalance problem on multiclass tasks



Classifying Data Streams with Skewed Distribution

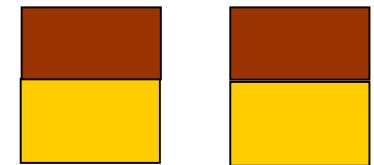


J. Gao, et al., "A General Framework for Mining Concept-Drifting Data Streams with Skewed Distributions", SDM'07

Biased Sampling



Ensemble



$$f^E(x) = \frac{1}{k} \sum_{i=1}^k f^i(x)$$

- Classify data stream with skewed distribution (i.e., rare events)
- **Biased sampling:** Save only the positive examples in the streams
- **Ensemble:** Partition negative examples of S_m into k portions to build k classifiers
- Effectively reduce classification errors on the minority class

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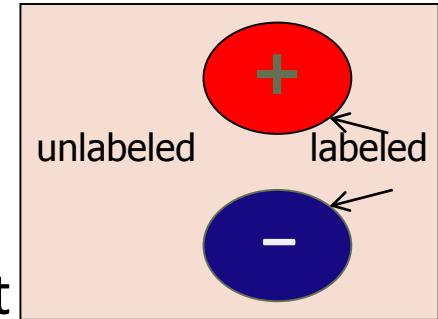


Multiclass Classification

- Classification involving more than two classes (i.e., > 2 Classes)
- Methodology: Reducing the multi-class problem into multiple binary problems
- Method 1. **One-vs.-rest** (or **one-vs.-all**)
 - Given m classes, train m classifiers: one for each class
 - Classifier j: treat tuples in class j as *positive* & **all the rest** as *negative*
 - To classify a tuple X , the set of classifiers vote as an ensemble
- Method 2. **one-vs.-one** (or **all-vs.-all**): Learn a classifier for each pair of classes
 - Given m classes, construct $m(m - 1)/2$ binary classifiers
 - A classifier is trained using tuples of the two classes
 - To classify a tuple X , each classifier votes
 - X is assigned to the class with maximal vote
- Comparison: One-vs.-one tends to perform better than one-vs.-rest
- Many new algorithms have been developed to go beyond binary classifier method

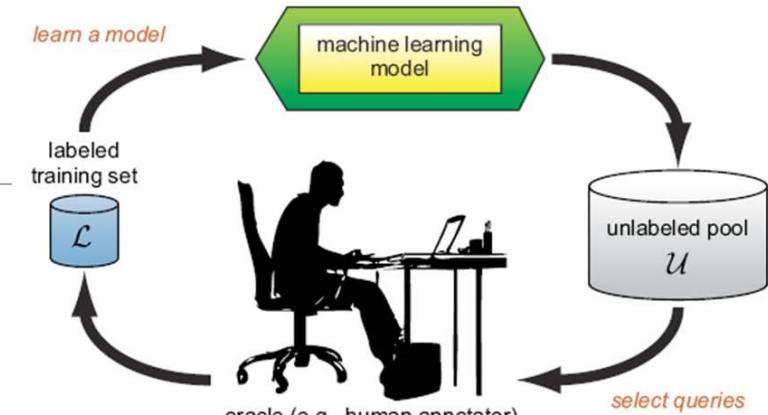
Semi-Supervised Classification

- ❑ Semi-supervised: Uses labeled and unlabeled data to build a classifier
- ❑ Self-training
 - ❑ Build a classifier using the labeled data
 - ❑ Use it to label the unlabeled data, and those with the most confident label prediction are added to the set of labeled data
 - ❑ Repeat the above process
 - ❑ Adv.: easy to understand; Disadv.: may reinforce errors
- ❑ Co-training: Use two or more classifiers to teach each other
 - ❑ Each learner uses a mutually independent set of features of each tuple to train a good classifier, say f_1 and f_2
 - ❑ Then f_1 and f_2 are used to predict the class label for unlabeled data X
 - ❑ Teach each other: The tuple having the most confident prediction from f_1 is added to the set of labeled data for f_2 & vice versa
- ❑ Other methods include joint probability distribution of features and labels



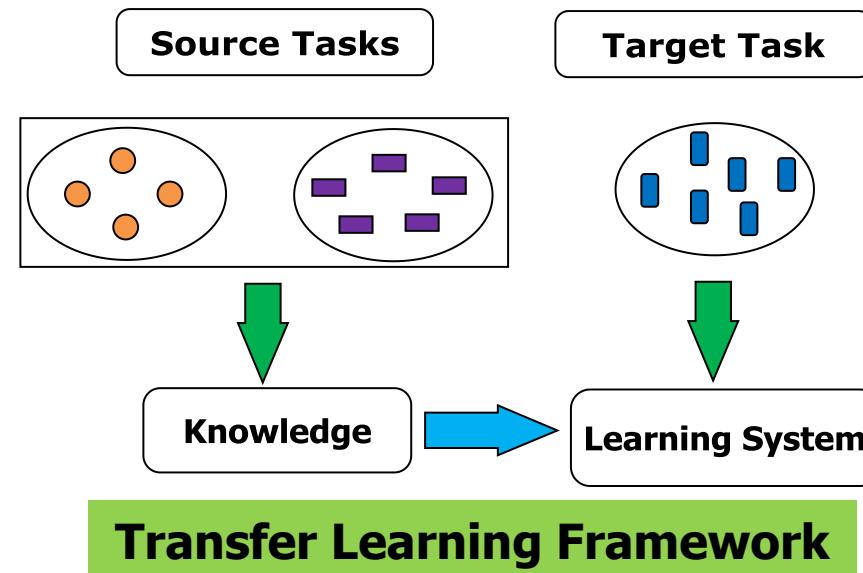
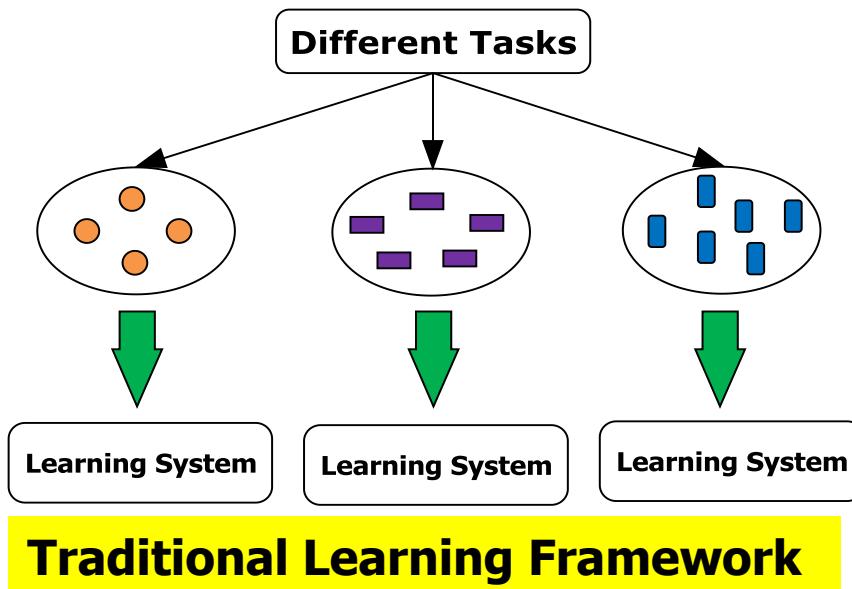
Active Learning

- A special case of semi-supervised learning
 - Unlabeled data: Abundant
 - Class labels are expensive to obtain
- Active learner: Interactively query teachers (oracle) for labels
- Pool-based approach: Uses a pool of unlabeled data
 - L: a small subset of D is labeled, U: a pool of unlabeled data in D
 - Use a query function to carefully select one or more tuples from U and request labels from an oracle (a human annotator)
 - The newly labeled samples are added to L, and learn a model
 - Goal: **Achieve high accuracy using as few labeled data as possible**
- Evaluated using *learning curves*: Accuracy as a function of the number of instances queried (# of tuples to be queried should be small)
- A lot of algorithms have been developed for active learning



Transfer Learning: Conceptual Framework

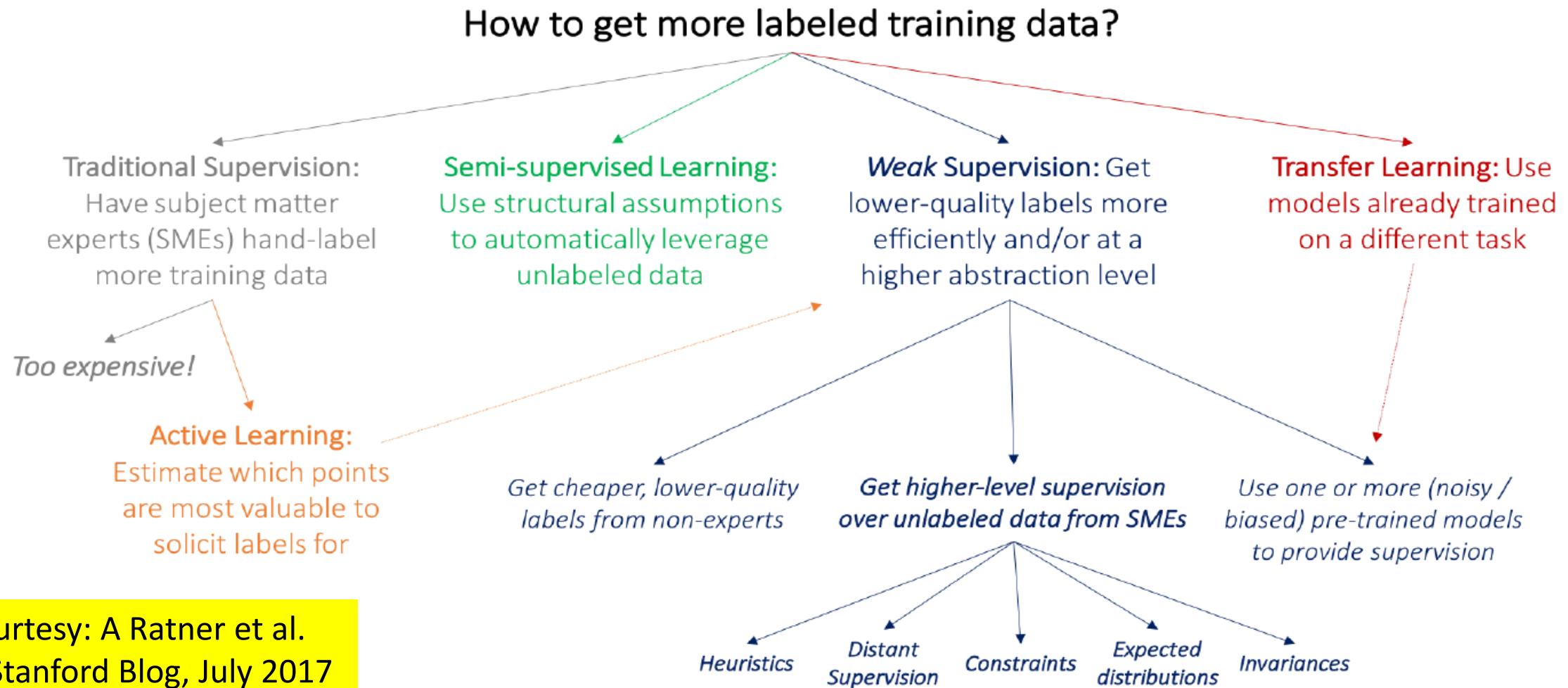
- Transfer learning: Extract knowledge from one or more source tasks (e.g., recognizing cars) and apply the knowledge to a target task (e.g., recognizing trucks)
- Traditional learning: Build a new classifier for each new task
- Transfer learning: Build new classifier by applying existing knowledge learned from source tasks
- Many algorithms are developed, applied to text classification, spam filtering, etc.



Weak Supervision: A New Programming Paradigm for Machine Learning

- ❑ Overcome the training data bottleneck
 - ❑ Leverage higher-level and/or noisier input from experts
- ❑ Exploring weak label distributions provided more cheaply and efficiently by
 - ❑ Higher-level, less precise supervision (e.g., heuristic rules, expected label distributions)
 - ❑ Cheaper, lower-quality supervision (e.g. crowdsourcing)
 - ❑ Existing resources (e.g. knowledge bases, pre-trained models)
- ❑ These weak label distributions could take many forms
 - ❑ Weak Labels from crowd workers, output of heuristic rules, or the result of distant supervision (from KBs), or the output of other classifiers, etc.
 - ❑ Constraints and invariances (e.g., from physics, logic, or other experts)
 - ❑ Probability distributions (e.g., from weak or biased classifiers or user-provided label or feature expectations or measurements)

Relationships Among Different Kinds of Supervisions



Many areas of machine learning are motivated by the bottleneck of labeled training data, but are divided at a high-level by what information they leverage instead.

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Summary

- Classification: Model construction from a set of training data
- Effective and scalable methods
 - Decision tree induction, Bayes classification methods, linear classifier, ...
 - No single method has been found to be superior over all others for all data sets
- Evaluation metrics: Accuracy, sensitivity, specificity, precision, recall, F measure
- Model evaluation: Holdout, cross-validation, bootstrapping, ROC curves (AUC)
- Improve Classification Accuracy: Bagging, boosting
- Additional concepts on classification: Multiclass classification, semi-supervised classification, active learning, transfer learning, weak supervision

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Bayes' Theorem: Basics

- Total probability Theorem:

$$P(B) = \sum_{i=1}^M P(B|A_i)P(A_i)$$

- Bayes' Theorem:

$$P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$$

- Let \mathbf{X} be a data sample (“evidence”): class label is unknown
- Let H be a *hypothesis* that \mathbf{X} belongs to class C
- Classification is to determine $P(H|\mathbf{X})$, (i.e., *posteriori probability*): the probability that the hypothesis holds given the observed data sample \mathbf{X}
- $P(H)$ (*prior probability*): the initial probability
 - E.g., \mathbf{X} will buy computer, regardless of age, income, ...
- $P(\mathbf{X})$: probability that sample data is observed
- $P(\mathbf{X}|H)$ (likelihood): the probability of observing the sample \mathbf{X} , given that the hypothesis holds
 - E.g., Given that \mathbf{X} will buy computer, the prob. that \mathbf{X} is 31..40, medium income

Classification Is to Derive the Maximum Posteriori

- Let D be a training set of tuples and their associated class labels, and each tuple is represented by an n -D attribute vector $\mathbf{X} = (x_1, x_2, \dots, x_n)$
- Suppose there are m classes C_1, C_2, \dots, C_m .
- Classification is to derive the maximum posteriori, i.e., the maximal $P(C_i | \mathbf{X})$
- This can be derived from Bayes' theorem

$$P(C_i | \mathbf{X}) = \frac{P(\mathbf{X} | C_i)P(C_i)}{P(\mathbf{X})}$$

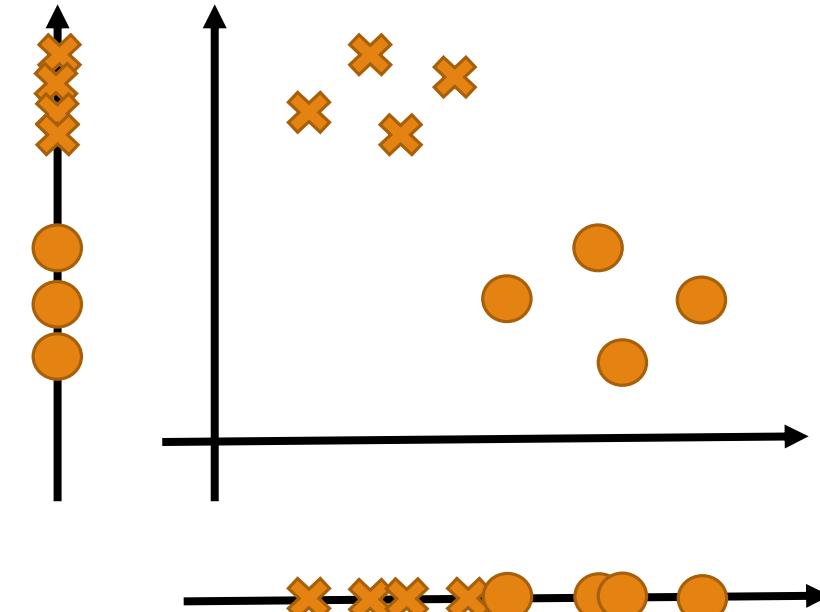
- Since $P(X)$ is constant for all classes, only

$$P(C_i | \mathbf{X}) \propto P(\mathbf{X} | C_i)P(C_i)$$

needs to be maximized

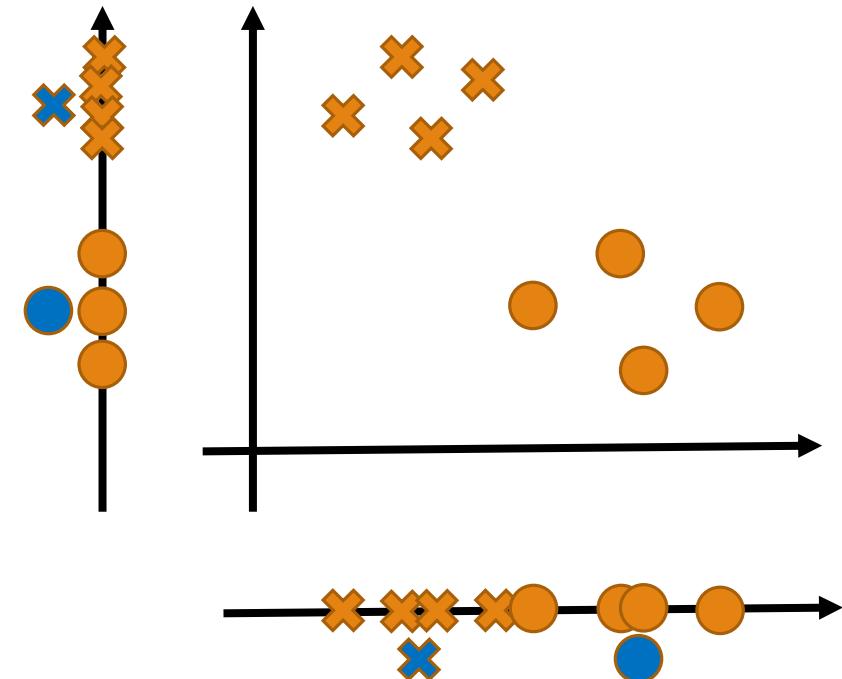
Linear Discriminant Analysis (LDA)

- Linear Discriminant Analysis (LDA) works when the attributes are all continuous
 - For the categorical attributes, discriminant correspondence analysis is the equivalent technique
- Basic Ideas: Project all samples on a line such that different classes are well separated
- Example: Suppose we have 2 classes and 2-dimensional samples x_1, \dots, x_n
 - n_1 samples come from class 1
 - n_2 samples come from class 2
- Let the line direction be given by unit vector ν
- There are two candidates of projections
 - Vertical: $\nu = (0,1)$
 - Horizontal: $\nu = (1,0)$
- Which one looks better?
- How to mathematically measure it?



Fisher's LDA (Linear Discriminant Analysis)

- $v^T x_i$ is the distance of projection of x_i from the origin
- Let μ_1 and μ_2 be the means of class 1 and class 2 in the original space
 - $\mu_1 = \frac{1}{n_1} \sum_{i \in \text{class 1}} x_i$
 - $\mu_2 = \frac{1}{n_2} \sum_{i \in \text{class 2}} x_i$
- The distance between the means of the projected points
 - $|v^T \mu_1 - v^T \mu_2|$
 - Good? No. Horizontal one may have larger distance



Fisher's LDA (con't)

- ❑ Normalization needed
- ❑ Scatter: Sample variance multiplied by n

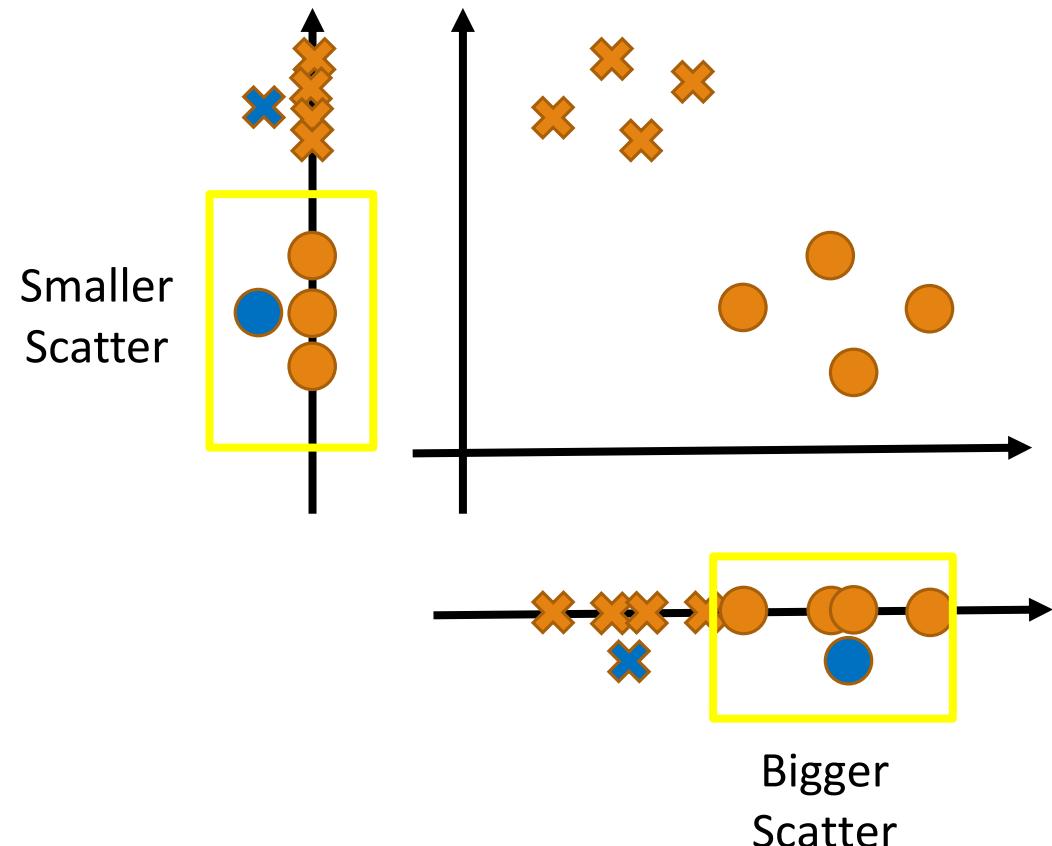
- ❑ $s_1 = \sum_{i \in \text{class 1}} (\mathbf{v}^T \mathbf{x}_i - \mathbf{v}^T \boldsymbol{\mu}_1)^2$

- ❑ $s_2 = \sum_{i \in \text{class 2}} (\mathbf{v}^T \mathbf{x}_i - \mathbf{v}^T \boldsymbol{\mu}_2)^2$

- ❑ Fisher's LDA

- ❑ Maximize $J(\mathbf{v}) = \frac{(\mathbf{v}^T \boldsymbol{\mu}_1 - \mathbf{v}^T \boldsymbol{\mu}_2)^2}{s_1 + s_2}$

- ❑ Closed-form optimal solution



Fisher's LDA: Summary

- Advantages
 - Useful for dimension reduction
 - Easy to extend to multi-classes

- Fisher's LDA will fail
 - When $\mu_1 = \mu_2, J(\nu)$ is always 0.
 - When classes have large overlap when projected to any line