# 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)
  - 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 |
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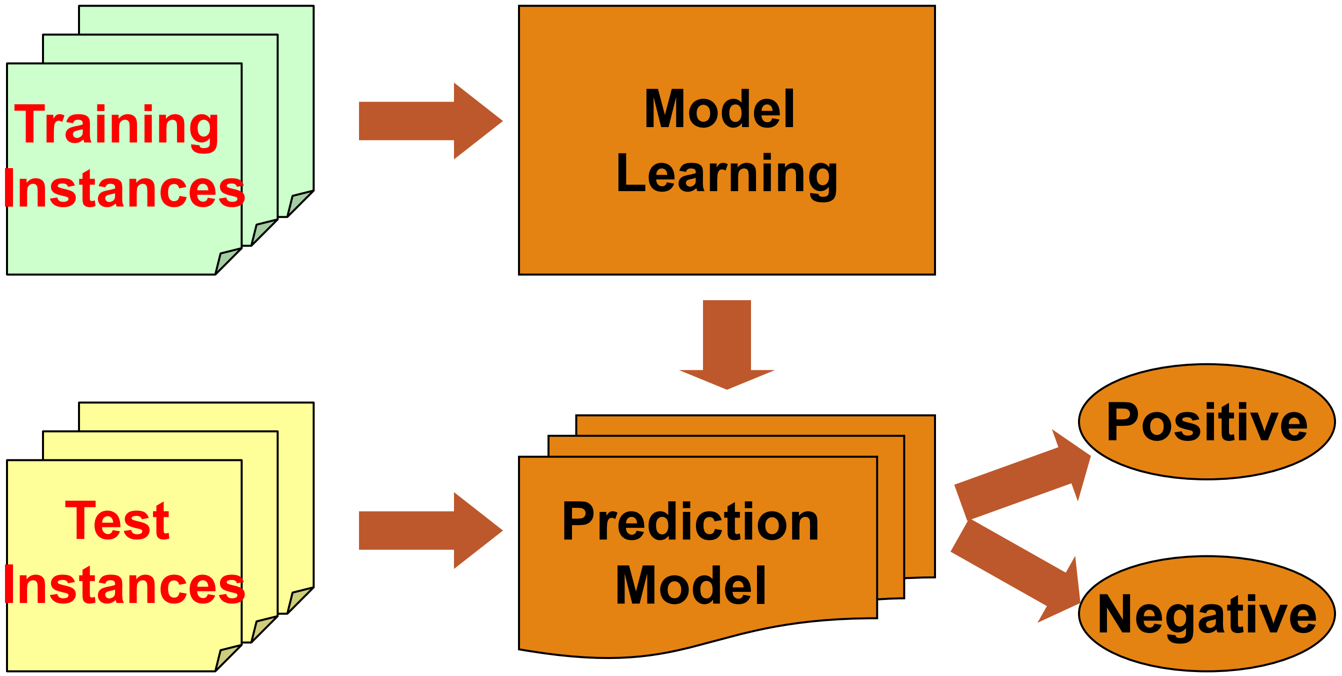
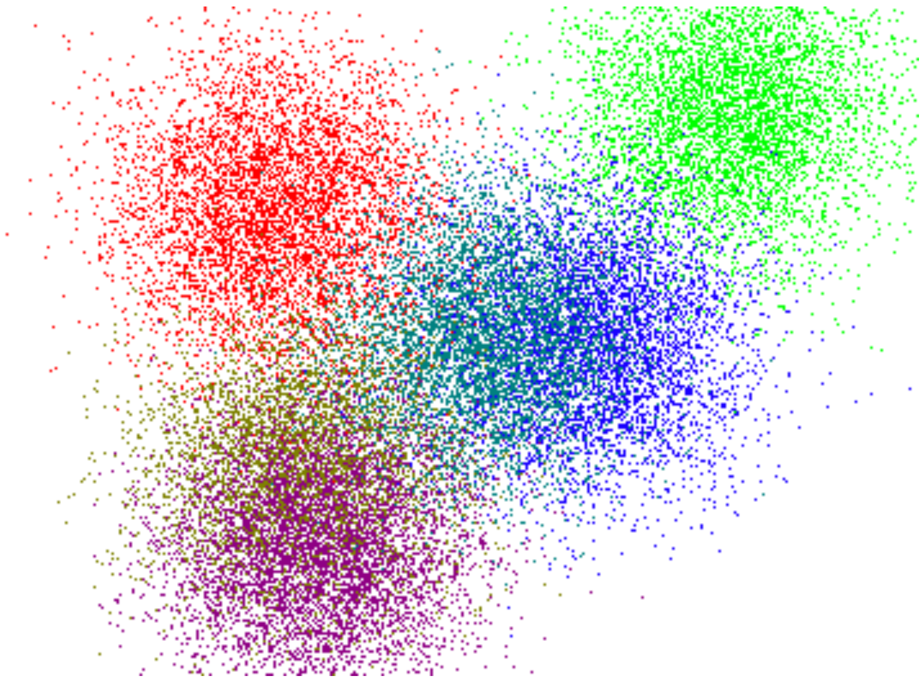


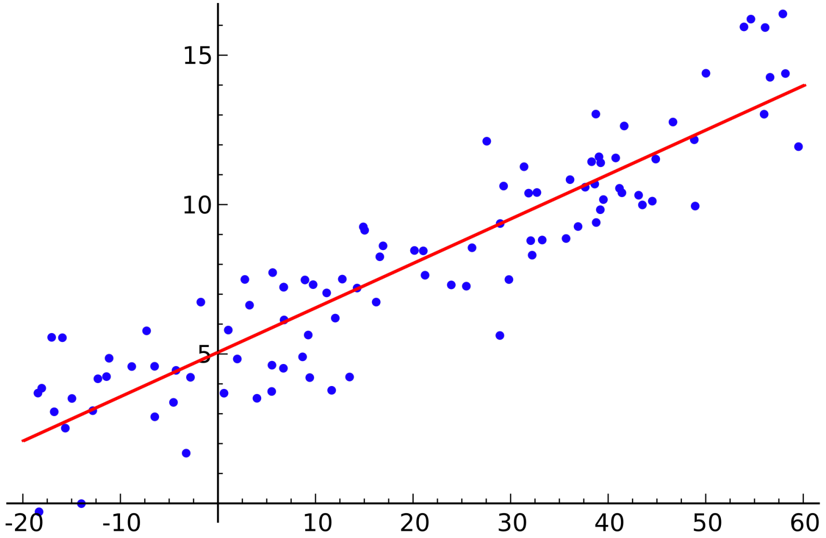
# Supervised vs. Unsupervised Learning (2)

- Unsupervised learning (clustering)
  - The class labels of training data are unknown
  - 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)
  - 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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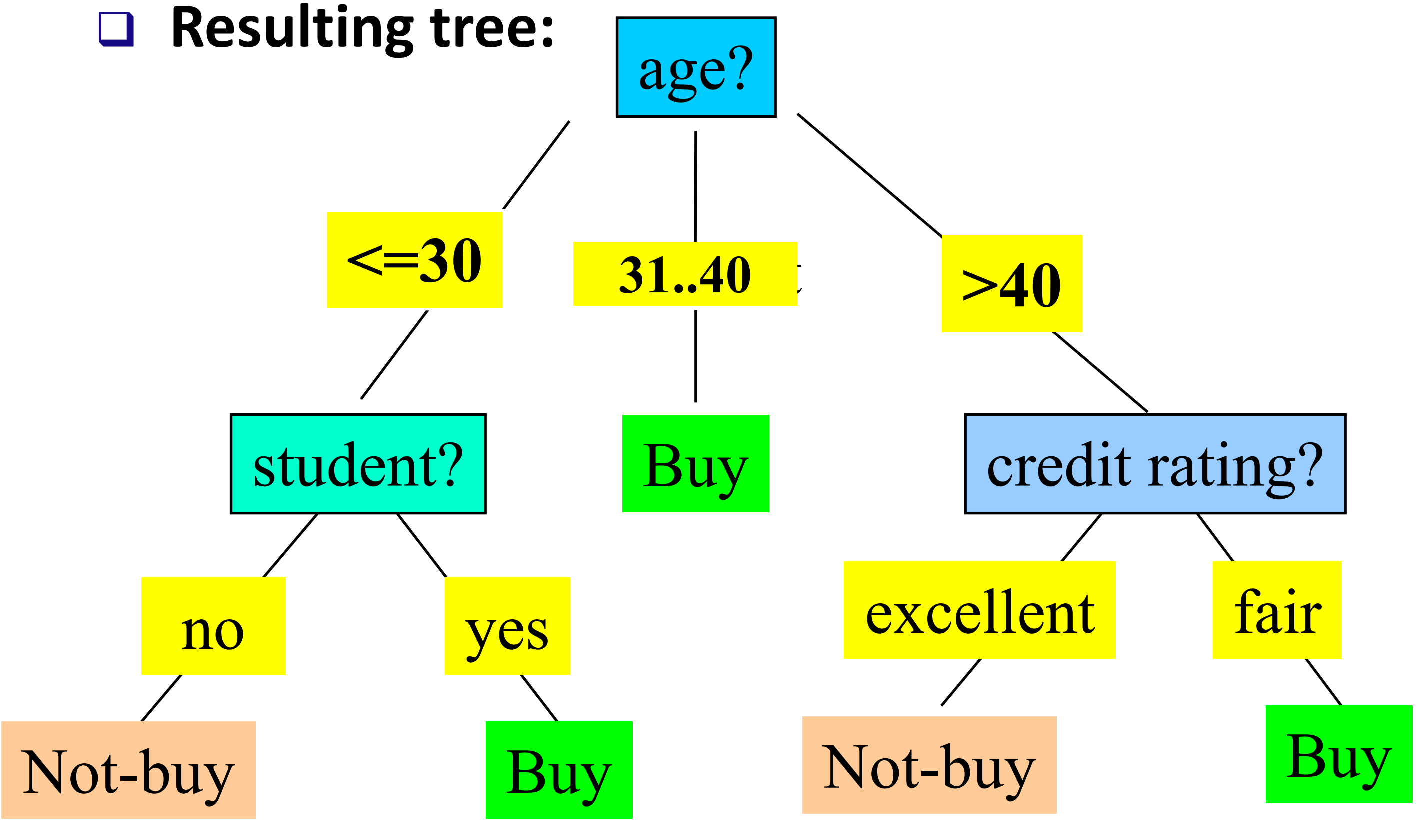
# Decision Tree Induction: An Example

- **Decision tree construction**:
  - A top-down, recursive, divide-and-conquer process
- **Resulting tree:**




Training data set: Who buys computer?

| age | income | student | credit_rating | buys_computer |
|---|---|---|---|---|
| <=30 | high | no | fair | no |
| <=30 | high | no | excellent | no |
| 31…40 | high | no | fair | yes |
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Note: The data set is adapted from "Playing Tennis" example of R. Quinlan

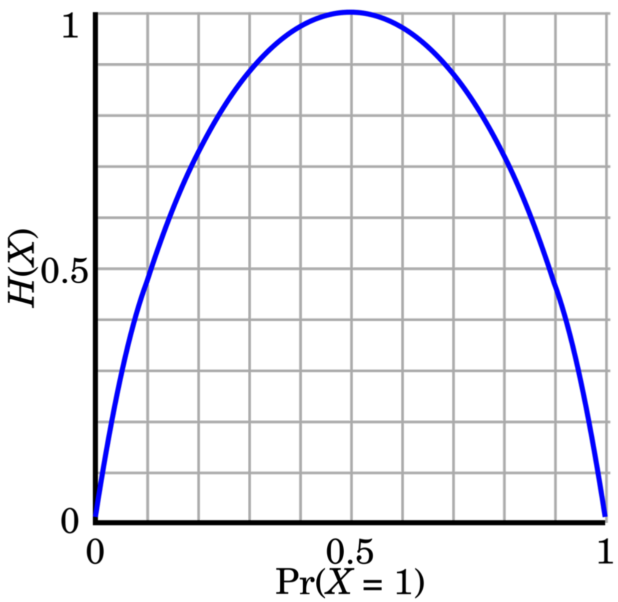
# Decision Tree Induction: Algorithm

- 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

# 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 $\{y_1, y_2, \ldots, y_m\}$

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




**m = 2**

  - Interpretation
    - Higher entropy → higher uncertainty
    - Lower entropy → 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

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

# Example: Attribute Selection with Information Gain

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

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

| 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 |
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| 31…40 | medium | no | excellent | 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

$$Gain(income) = 0.029$$

$$Gain(student) = 0.151$$

$$Gain(credit\_rating) = 0.048$$

# 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, …
  - 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 $A \le P$ 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)

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

  - GainRatio(A) = Gain(A)/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
  - $\text{SplitInfo}_{\text{income}}(\text{D}) = -\frac{4}{14}\log_2\frac{4}{14} - \frac{6}{14}\log_2\frac{6}{14} - \frac{4}{14}\log_2\frac{4}{14} = 1.557$
  - GainRatio(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

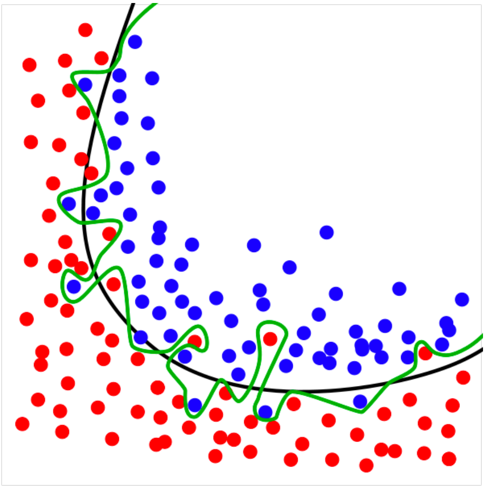
# Comparing Three Attribute Selection Measures

- 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 $\chi^2$ 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 | com |
|---|---|---|---|---|
| <=30 | high | no | fair | no |
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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*

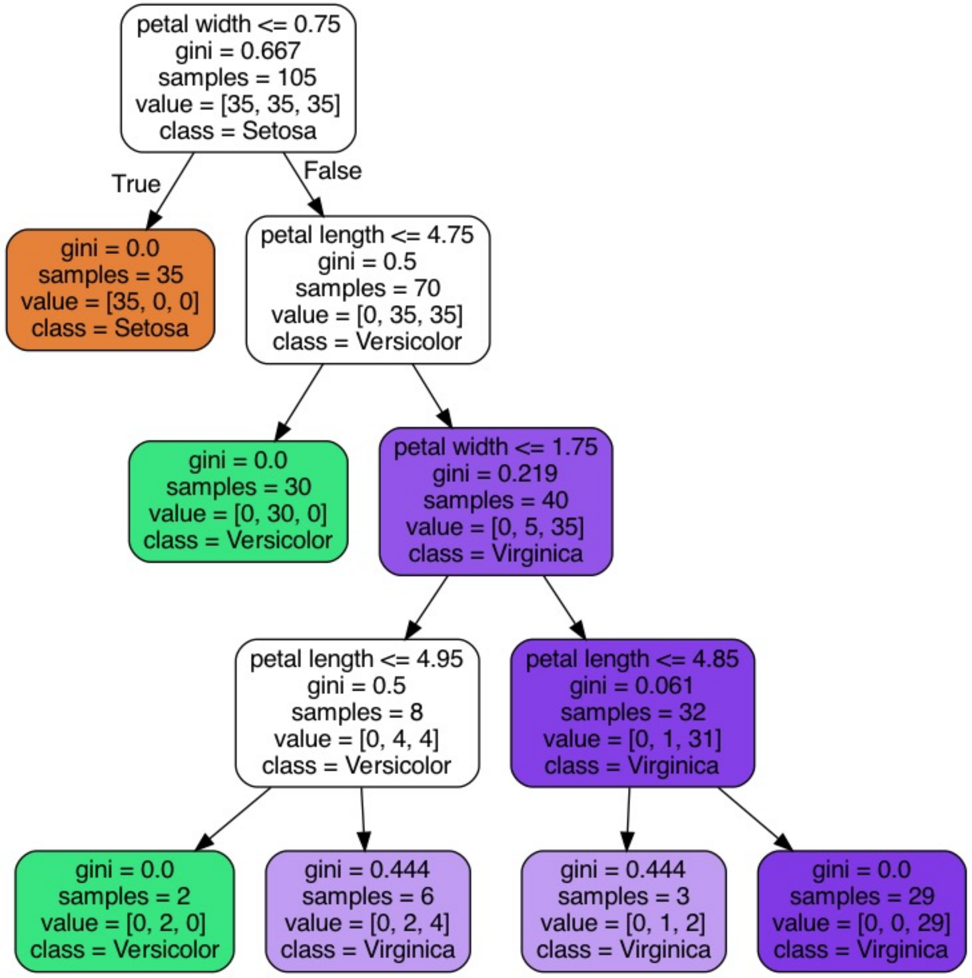
| student | Buy_Computer | |
|---|---|---|
| | yes | no |
| yes | 6 | 1 |
| no | 3 | 4 |

AVC-set on *Credit_Rating*

| Credit rating | Buy_Computer | |
|---|---|---|
| | yes | no |
| fair | 6 | 2 |
| excellent | 3 | 3 |

Its AVC Sets

# Visualization of a Decision Tree



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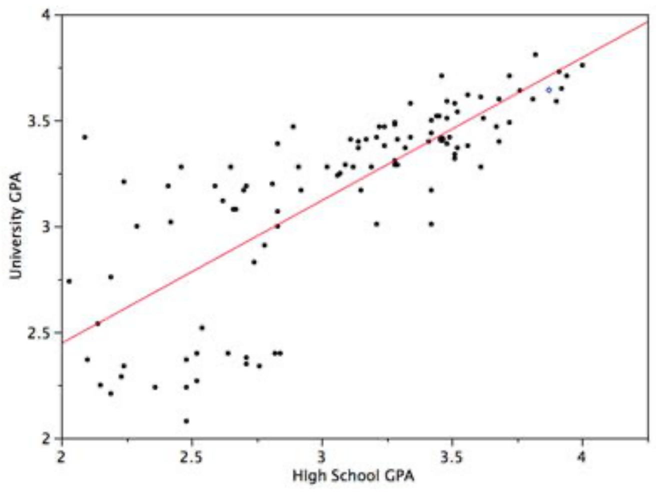
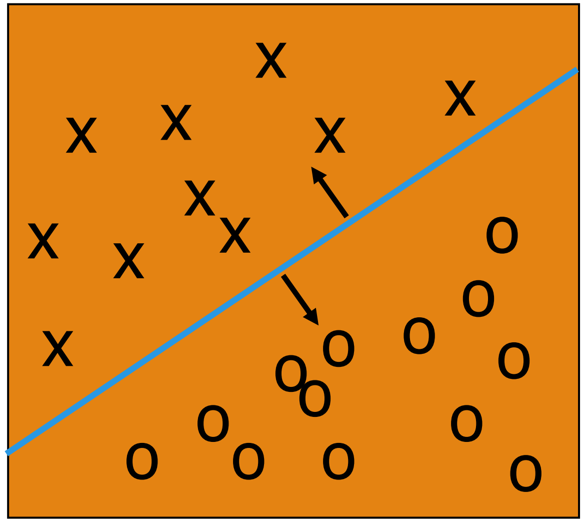
# Linear Regression vs. Linear Classifier

- 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

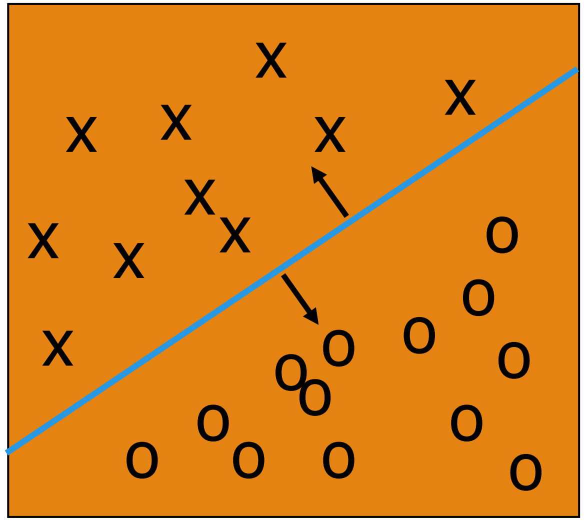



- Linear Classifier
  - Built a classification model using a straight line
  - Used for (categorical data) binary classification



# 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)

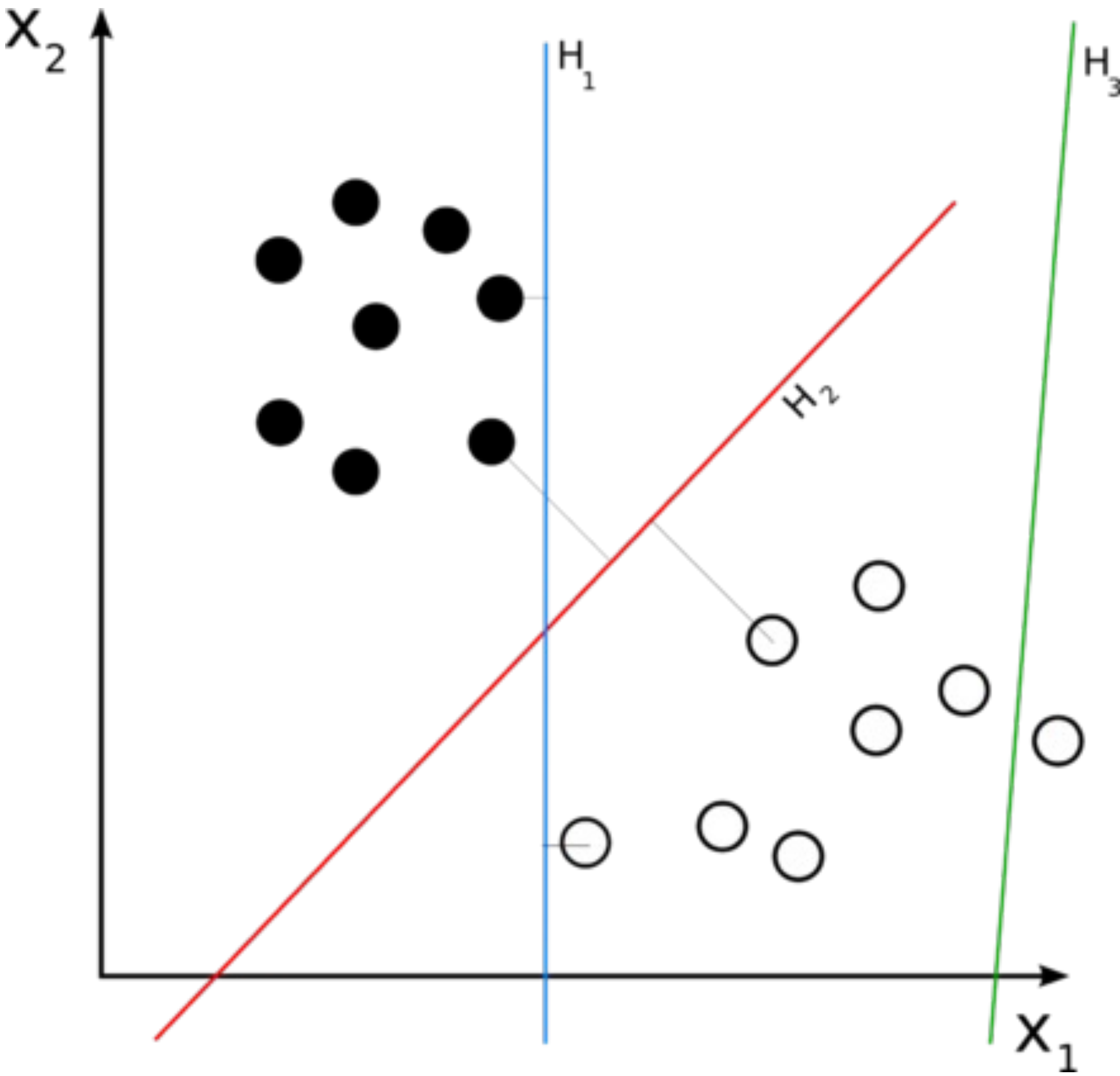


# Linear Classifier: An Example

- A toy rule to determine whether a faculty member has tenure
  - Year >= 6 or Title = "Professor" ⇔ Tenure
- How to express the rule as a linear classifier?
- Features
  - $\mathrm{x}_1 (x_1 \geq 0)$ is an integer denoting the year
  - $\mathrm{x}_2$ 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
  - $f(x) = (x_1 - 5.5) + 6 \cdot x_2$
  - $f(x) = 2 \cdot (x_1 - 5) + 11 \cdot x_2$
  - ……

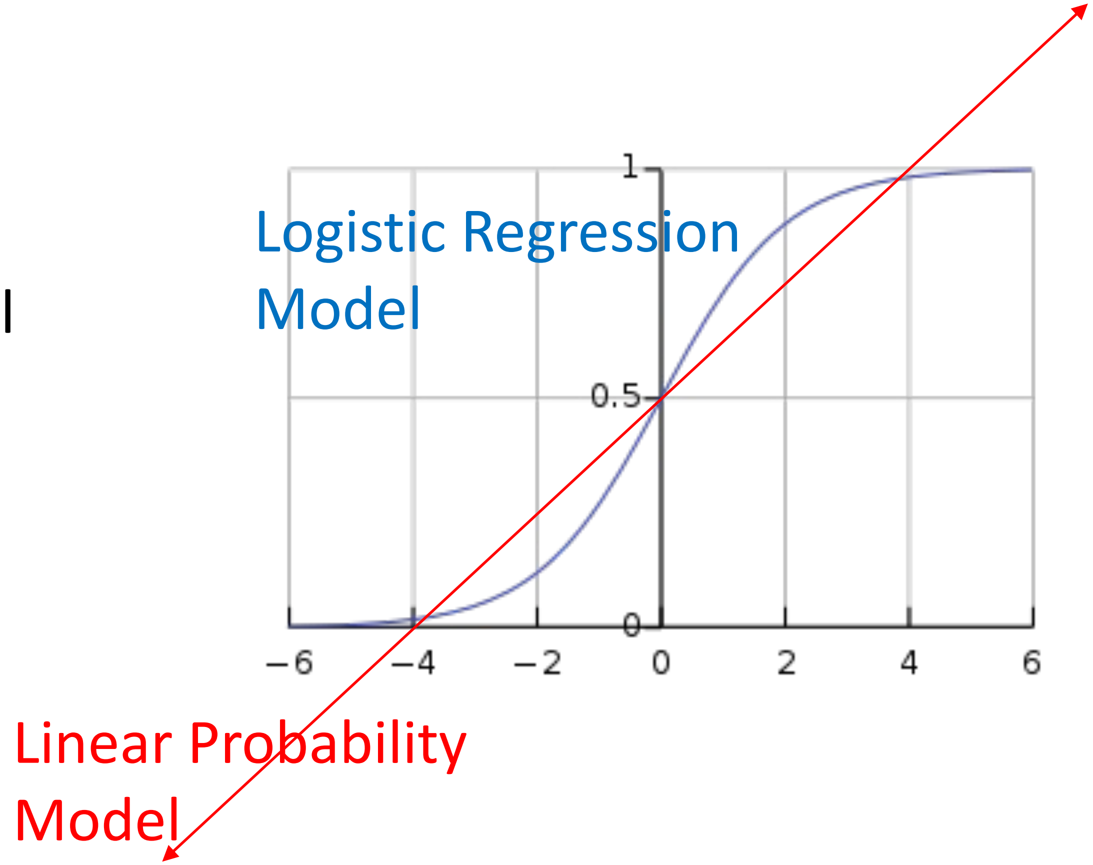
# Key Question: Which Line Is Better?

- There might be many feasible linear functions
  - Both H1 and H2 will work
- Which one is better?
  - H2 looks "better" in the sense that it is also furthest from both groups
  - We will introduce more in the SVM section



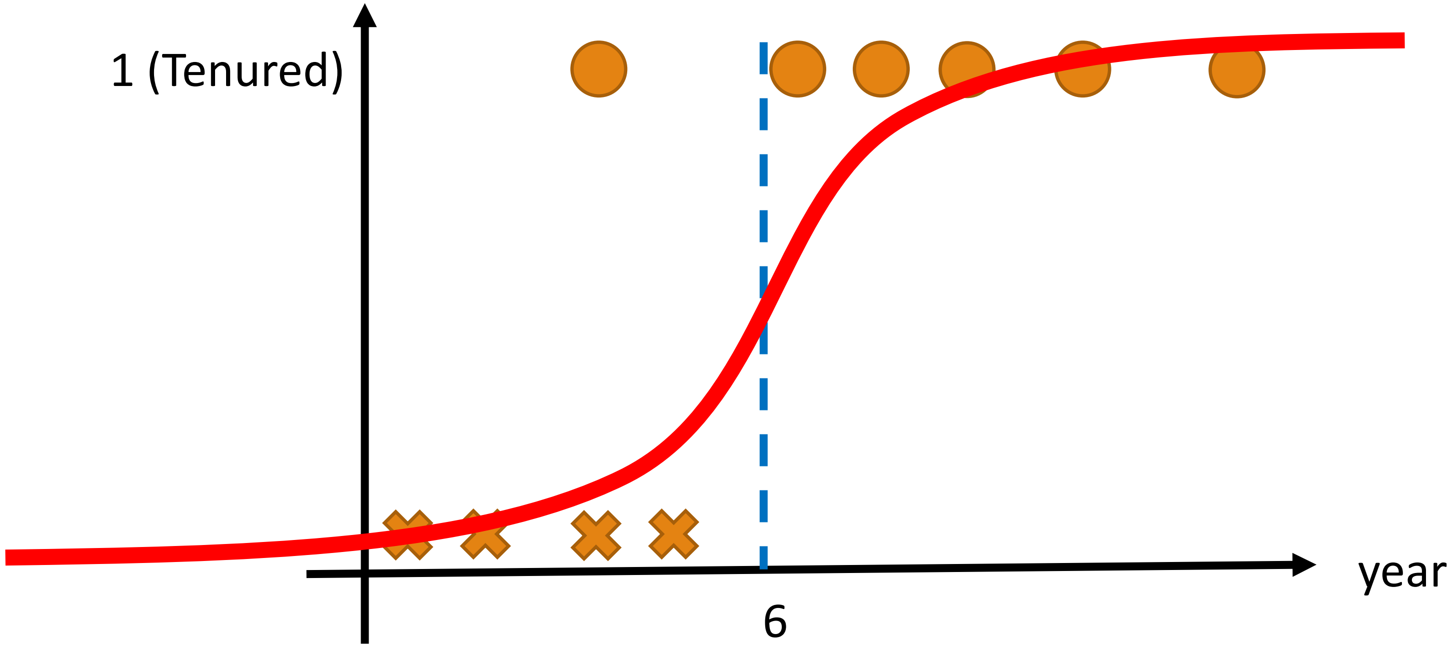
# Logistic Regression: General Ideas

- 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



# Logistic Regression: An Example

- Suppose we only consider the year as feature



# Logistic Regression: Maximum Likelihood

- The prediction function to learn
  - $p(Y=1\,|X=x;\boldsymbol{w}) \;=\; S(w_0+\sum_{i=1}^{n} w_i\cdot x_i)$
  - $\boldsymbol{w}=(w_0,w_1,w_2,\dots,w_n)$ are the parameters
- Maximum Likelihood
  - Log likelihood:

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

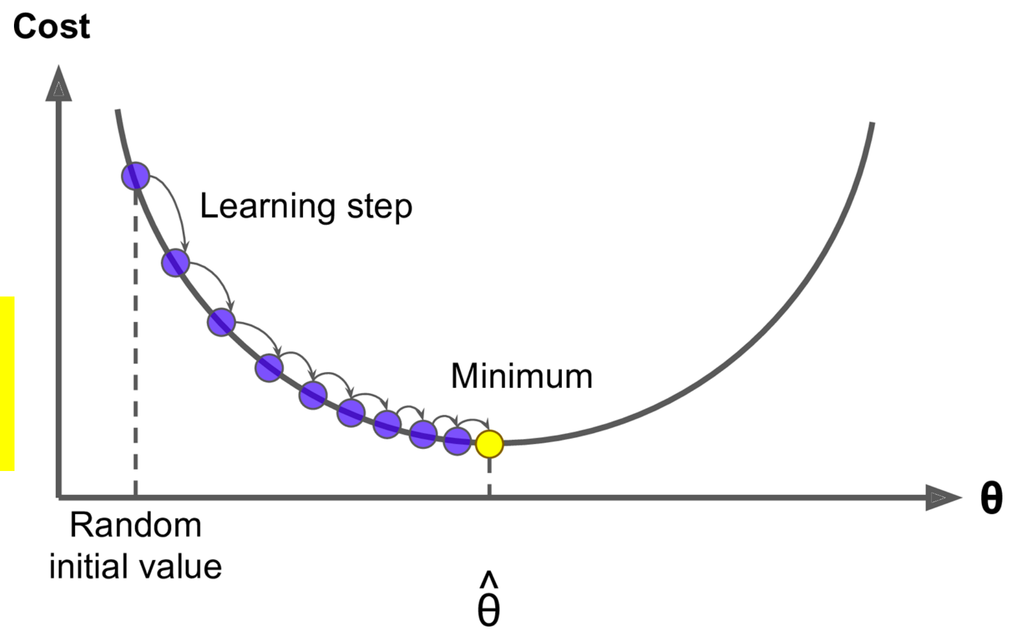
- There's no close form solution
  - Gradient Descent
  - Update w based on training data
    - Chain-rule for the gradient

# 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



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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

# Bayes' Theorem: Basics

- Total probability Theorem:

$$p(B) = \sum_{i} p\,(B|A_i)p(A_i)$$

- Bayes' Theorem:

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

posteriori probability — What we should choose

likelihood — What we just see

prior probability — 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: 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 |
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# Naïve Bayes Classifier: An Example

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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 |

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

**$P(X|C_i)$ :** P(X|buys_computer = "yes") = 0.222 x 0.444 x 0.667 x 0.667 = 0.044
P(X|buys_computer = "no") = 0.6 x 0.4 x 0.2 x 0.4 = 0.019

**$P(X|C_i)*P(C_i)$ :** P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028
P(X|buys_computer = "no") * P(buys_computer = "no") = 0.007

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

# 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)

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

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

# Avoiding the Zero-Probability Problem

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

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

- 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*

    Prob(income = low) = 1/(1000 + 3)

    Prob(income = medium) = (990 + 1)/(1000 + 3)

    Prob(income = 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
- Bayes Classification Methods
- Linear Classifier
- Model Evaluation and Selection
- Techniques to Improve Classification Accuracy: Ensemble Methods
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- Summary

# 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 | ¬C | |
|---|---|---|---|
| C | **TP** | **FN** | **P** |
| ¬C | **FP** | **TN** | **N** |
| | **P’** | **N’** | **All** |

- **Classifier accuracy,** or recognition rate
  - Percentage of test set tuples that are correctly classified

  **Accuracy = (TP + TN)/All**
- **Error rate:** *1 – accuracy*, or

  **Error rate = (FP + FN)/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
      - **Sensitivity = TP/P**
    - **Specificity**: True negative recognition rate
      - **Specificity = TN/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 β = 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 (*sensitivity*) |
| cancer = no | **140** | **9560** | 9700 | 98.56 (*specificity*) |
| Total | 230 | 9770 | 10000 | 96.50 (*accuracy*) |

- 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 × R /(P + R) = 2 × 39.13% × 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

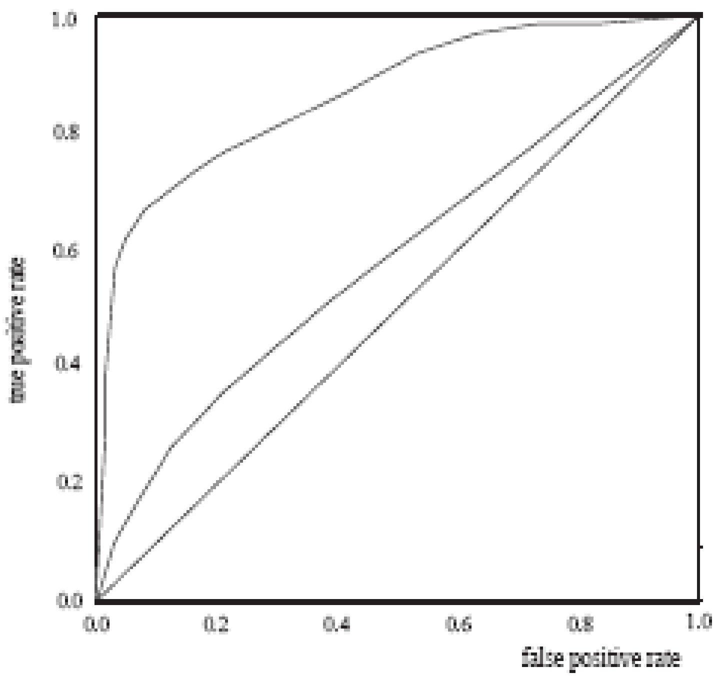
# Classifier Evaluation: Bootstrap

- **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

# Chapter 8. Classification: Basic Concepts

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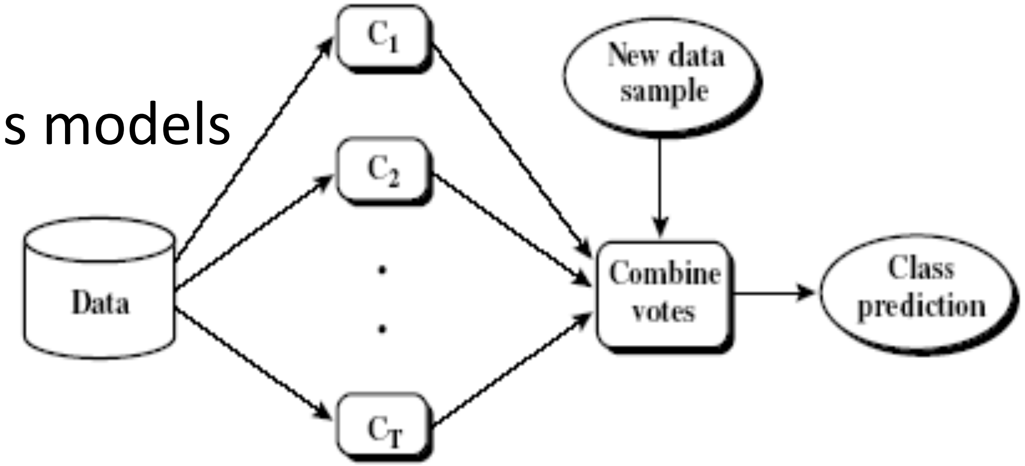
# Ensemble Methods: Increasing the Accuracy

- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of *k* learned models, $M_1$, $M_2$, …, $M_k$, 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)

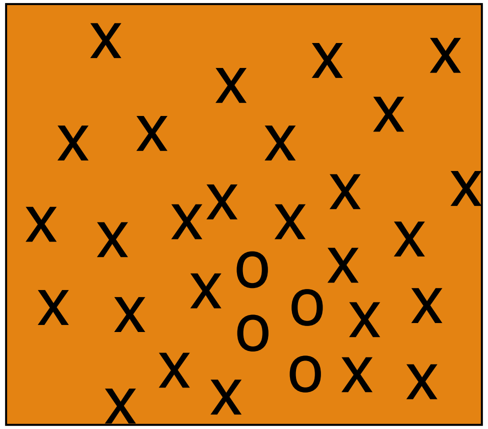
- Given a set of *d* class-labeled tuples, $(\mathbf{X_1}, y_1), \ldots, (\mathbf{X_d}, y_d)$
- Initially, all the weights of tuples are set the same (1/d)
- Generate *k* classifiers in *k* rounds. At round i,
  - Tuples from D are sampled (with replacement) to form a training set $D_i$ of the same size
  - 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: $err(\mathbf{X_j})$ is the misclassification error of tuple $\mathbf{X_j}$. Classifier $M_i$ error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_{j}^{d} w_j \times err(\mathbf{X_j})$$

- The weight of classifier $M_i$'s vote is $\log \frac{1 - error(M_i)}{error(M_i)}$

# 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

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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

# References (1)


- C. Apte and S. Weiss. **Data mining with decision trees and decision rules**. Future Generation Computer Systems, 13, 1997
- P. K. Chan and S. J. Stolfo. **Learning arbiter and combiner trees from partitioned data for scaling machine learning**. KDD'95
- A. J. Dobson. **An Introduction to Generalized Linear Models**. Chapman & Hall, 1990.
- R. O. Duda, P. E. Hart, and D. G. Stork. **Pattern Classification**, 2ed. John Wiley, 2001
- U. M. Fayyad. **Branching on attribute values in decision tree generation**. AAAI'94.
- Y. Freund and R. E. Schapire. **A decision-theoretic generalization of on-line learning and an application to boosting**. J. Computer and System Sciences, 1997.
- J. Gehrke, R. Ramakrishnan, and V. Ganti. **Rainforest: A framework for fast decision tree construction of large datasets**. VLDB'98.
- J. Gehrke, V. Gant, R. Ramakrishnan, and W.-Y. Loh, **BOAT -- Optimistic Decision Tree Construction**. SIGMOD'99.
- T. Hastie, R. Tibshirani, and J. Friedman. **The Elements of Statistical Learning: Data Mining, Inference, and Prediction.** Springer-Verlag, 2001.

# References (2)


- T.-S. Lim, W.-Y. Loh, and Y.-S. Shih. **A comparison of prediction accuracy, complexity, and training time of thirty-three old and new classification algorithms.** Machine Learning, 2000
- J. Magidson. **The Chaid approach to segmentation modeling: Chi-squared automatic interaction detection**. In R. P. Bagozzi, editor, Advanced Methods of Marketing Research, Blackwell Business, 1994
- M. Mehta, R. Agrawal, and J. Rissanen. **SLIQ : A fast scalable classifier for data mining**. EDBT'96
- T. M. Mitchell. **Machine Learning**. McGraw Hill, 1997
- S. K. Murthy, **Automatic Construction of Decision Trees from Data: A Multi-Disciplinary Survey**, Data Mining and Knowledge Discovery 2(4): 345-389, 1998
- J. R. Quinlan. **Induction of decision trees**. *Machine Learning*, 1:81-106, 1986.
- J. R. Quinlan. **C4.5: Programs for Machine Learning**. Morgan Kaufmann, 1993.
- J. R. Quinlan. **Bagging, boosting, and c4.5**. AAAI'96.

# References (3)


- R. Rastogi and K. Shim. **Public: A decision tree classifier that integrates building and pruning**. VLDB'98
- J. Shafer, R. Agrawal, and M. Mehta. **SPRINT : A scalable parallel classifier for data mining**. VLDB'96
- J. W. Shavlik and T. G. Dietterich. **Readings in Machine Learning**. Morgan Kaufmann, 1990
- P. Tan, M. Steinbach, and V. Kumar. **Introduction to Data Mining**. Addison Wesley, 2005
- S. M. Weiss and C. A. Kulikowski. **Computer Systems that Learn: Classification and Prediction Methods from Statistics, Neural Nets, Machine Learning, and Expert Systems**. Morgan Kaufman, 1991
- S. M. Weiss and N. Indurkhya. **Predictive Data Mining**. Morgan Kaufmann, 1997
- I. H. Witten and E. Frank. **Data Mining: Practical Machine Learning Tools and Techniques**, 2ed. Morgan Kaufmann, 2005

# 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 **X** be a data sample ("*evidence*"): class label is unknown
  - Let H be a *hypothesis* that X belongs to class C
  - Classification is to determine P(H|**X**), (i.e., *posteriori probability):* the probability that the hypothesis holds given the observed data sample **X**
  - P(H) (*prior probability*): the initial probability
    - E.g., **X** will buy computer, regardless of age, income, …
  - P(**X**): probability that sample data is observed
  - P(**X**|H) (likelihood): the probability of observing the sample **X**, given that the hypothesis holds
    - E.g., Given that **X** will buy computer, the prob. that 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 **X** = $(x_1, x_2, \ldots, x_n)$
- Suppose there are *m* classes $C_1, C_2, \ldots, C_m$.
- Classification is to derive the maximum posteriori, i.e., the maximal $P(C_i|\mathbf{X})$
- This can be derived from Bayes' theorem

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

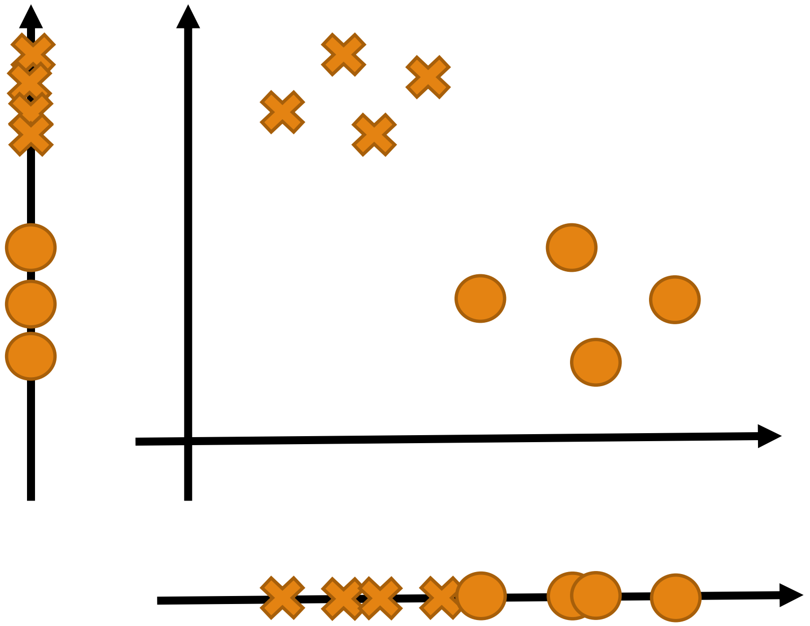
- Since P(X) is constant for all classes, only

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

needs to be maximized

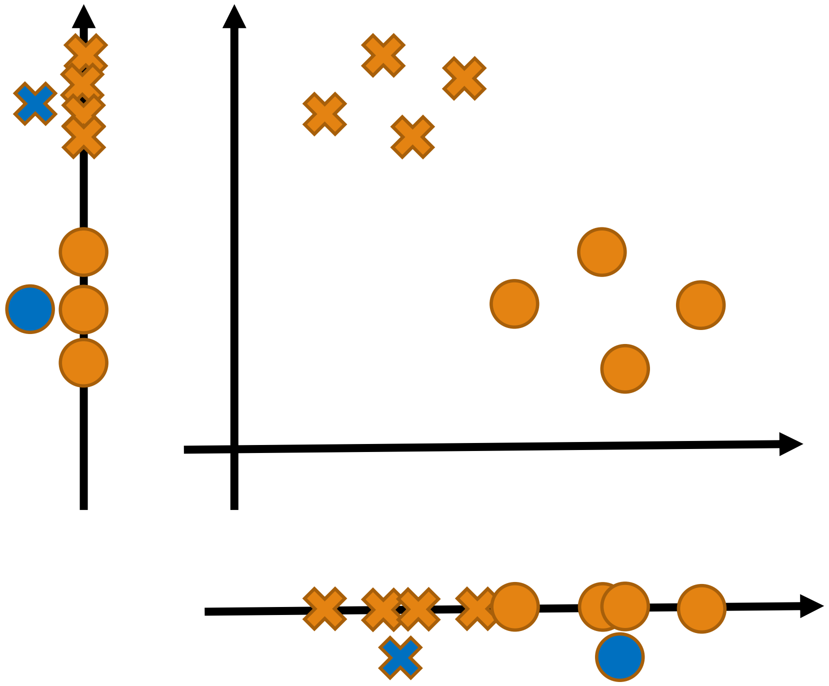
# Linear Discriminant Analysis (LDA)

- 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 $\boldsymbol{v}$
- There are two candidates of projections
  - Vertical: $\boldsymbol{v} = (0,1)$
  - Horizontal: $\boldsymbol{v} = (1,0)$
- Which one looks better?
- How to mathematically measure it?



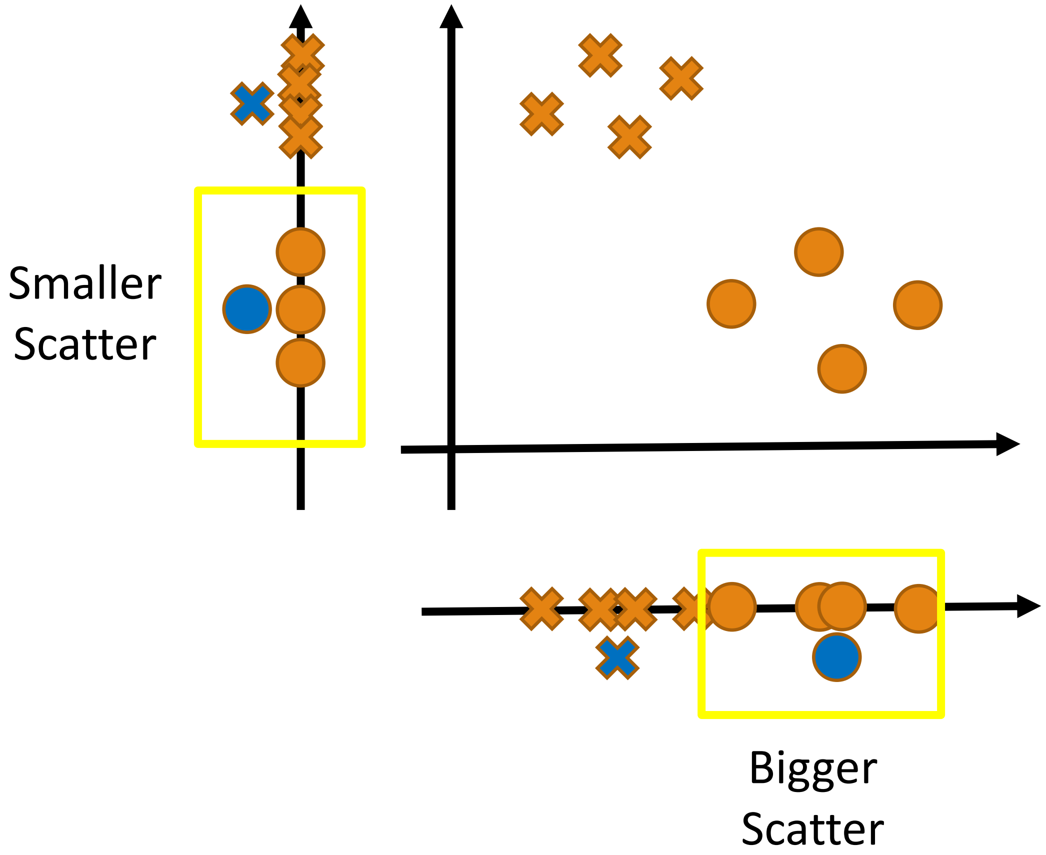
# Fisher's LDA (Linear Discriminant Analysis)

- $\boldsymbol{v}^T\boldsymbol{x}_i$ is the distance of projection of $\boldsymbol{x}_i$ from the origin
- Let $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ be the means of class 1 and class 2 in the original space
  - $\boldsymbol{\mu}_1 = \frac{1}{n_1}\sum_{i \in \text{class } 1} \boldsymbol{x}_i$
  - $\boldsymbol{\mu}_2 = \frac{1}{n_2}\sum_{i \in \text{class } 2} \boldsymbol{x}_i$
- The distance between the means of the projected points
  - $|\boldsymbol{v}^T\boldsymbol{\mu}_1 - \boldsymbol{v}^T\boldsymbol{\mu}_2|$
  - Good? No. Horizontal one may have larger distance



# Fisher's LDA (con't)

- Normalization needed
- Scatter: Sample variance multiplied by $n$
  - $s_1 = \sum_{i\in \text{class } 1}\left(\boldsymbol{v}^T\boldsymbol{x}_i - \boldsymbol{v}^T\boldsymbol{\mu}_1\right)^2$
  - $s_2 = \sum_{i\in \text{class } 2}\left(\boldsymbol{v}^T\boldsymbol{x}_i - \boldsymbol{v}^T\boldsymbol{\mu}_2\right)^2$
- Fisher's LDA
  - Maximize $J(\boldsymbol{v}) = \frac{\left(\boldsymbol{v}^T\boldsymbol{\mu}_1 - \boldsymbol{v}^T\boldsymbol{\mu}_2\right)^2}{s_1+s_2}$
  - 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 $\boldsymbol{\mu_1} = \boldsymbol{\mu_2}$, $J(\boldsymbol{v})$ is always 0.
  - When classes have large overlap when projected to any line