資料分析與學習基石
(*Fundamental of Data Analytics and Learning*)

-- Basic Classifier

Hung-Yu Kao (高宏宇)
***I**ntelligent **K**nowledge **M**anagement Lab*

Master Program of Artificial Intelligence
Institute of Medical Informatics,
Dept. of Computer Science and Information Engineering
National Cheng Kung University, Tainan, Taiwan

Supervised vs. Unsupervised Learning

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

Classification: Definition

- Given a collection of records (*training set*)
  - Each record contains a set of *attributes*, one of the attributes is the *class*.
- Find a *model* for class attribute as a function of the values of other attributes.

- Goal: previously unseen records should be assigned a class as accurately as possible.
  - A *test set* is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build/train the model and test set used to validate it.

Issues Regarding Classification and Prediction (1): Data Preparation

- Data cleaning
  - Preprocess data in order to reduce noise and handle missing values
- Relevance analysis (feature selection)
  - Remove the irrelevant or redundant attributes
- Data transformation
  - Generalize and/or normalize data

Issues regarding classification and prediction (2): Evaluating Classification Methods

- Predictive accuracy
- Speed and scalability
  - time to construct the model
  - time to use the model
- Robustness
  - handling noise and missing values
- Scalability
  - efficiency in disk-resident databases
- Interpretability
  - understanding and insight provided by the model
- Goodness of rules
  - decision tree size
  - compactness of classification rules

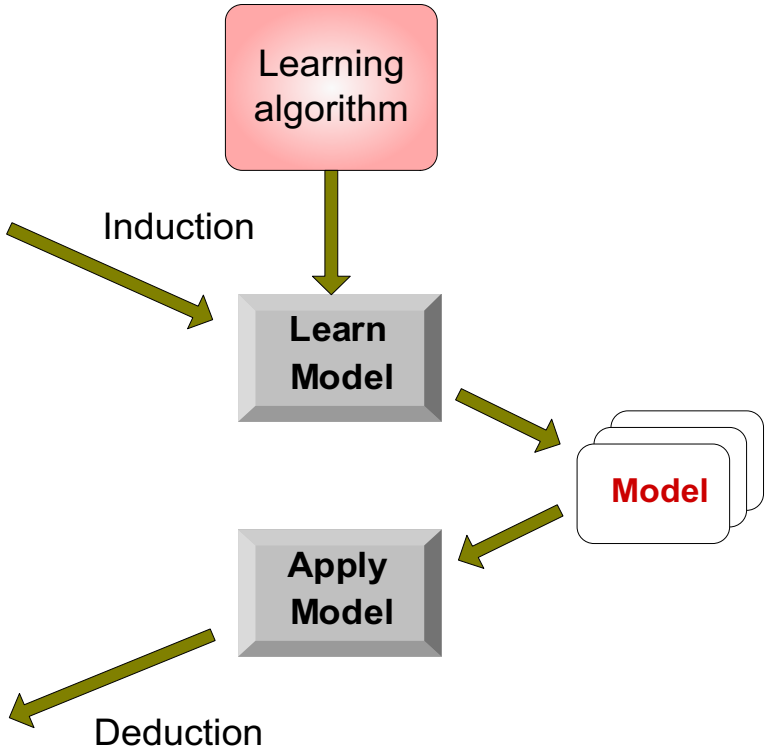
Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

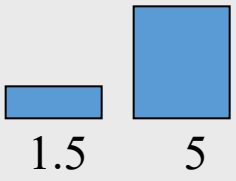
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

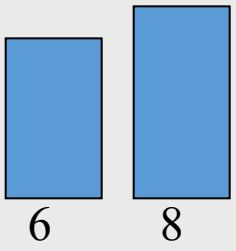
Test Set

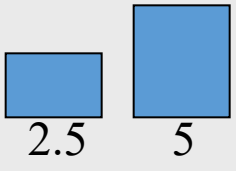


Simple Question 1

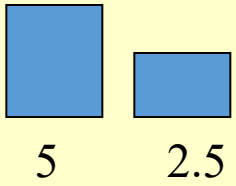
Examples of class A

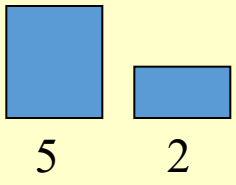


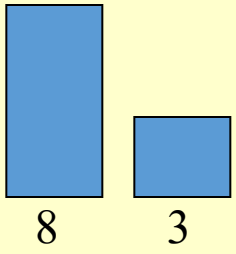


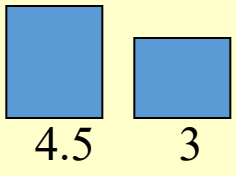


Examples of class B



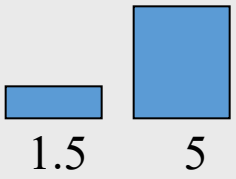


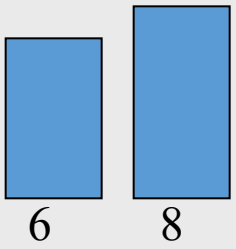


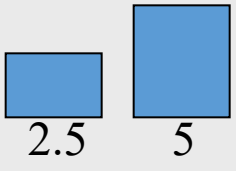


Simple Question 1

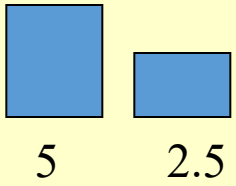
Examples of class A

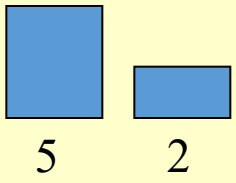


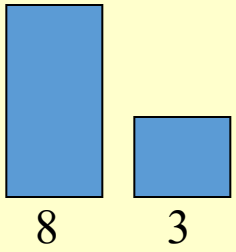


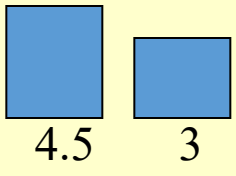


Examples of class B

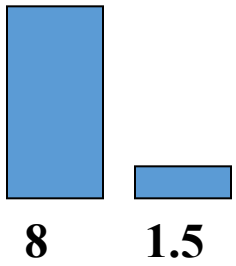




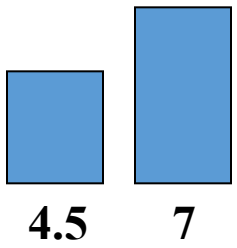




What class is this object?

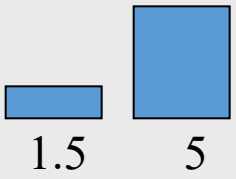


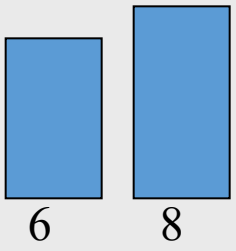
What about this one, A or B?

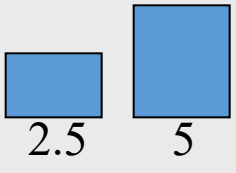


Simple Question 1

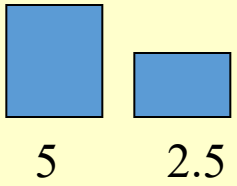
Examples of class A

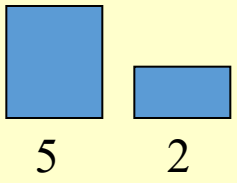


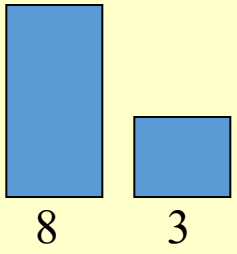


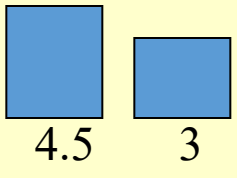


Examples of class B

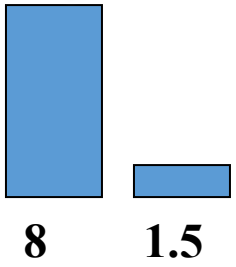








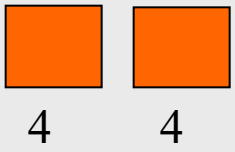
This is a B!

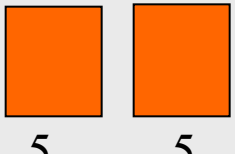


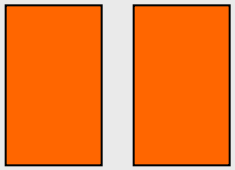
Here is the rule.
If the left bar is smaller than the right bar, it is an A, otherwise it is a B.

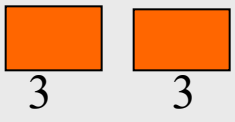
Simple Question 2

Examples of class A

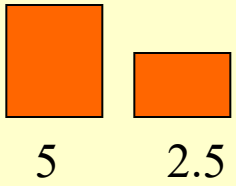


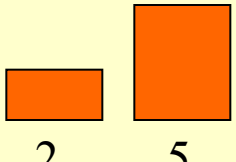


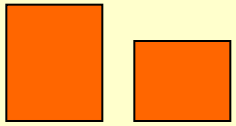


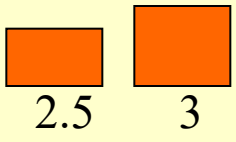


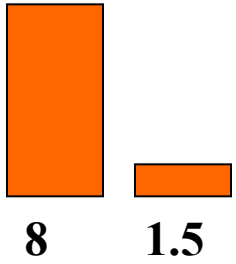
Examples of class B

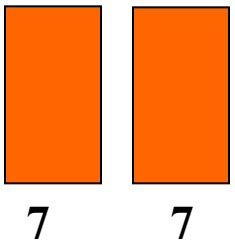






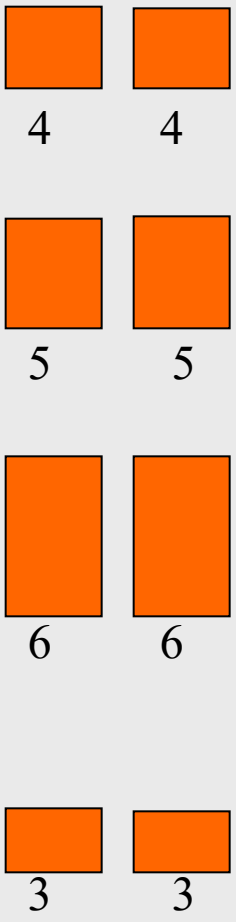




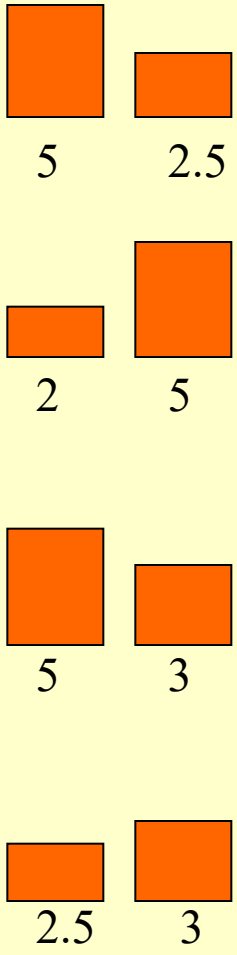


Simple Question 2

Examples of class A

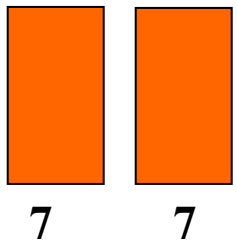


Examples of class B



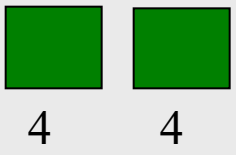
The rule is as follows, if the two bars are equal sizes, it is an A. Otherwise it is a B.

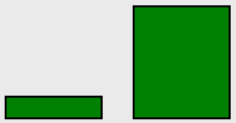
So this one is an A.

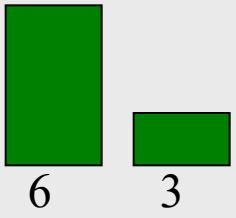


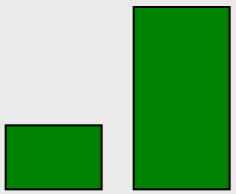
Simple Question 3

Examples of class A

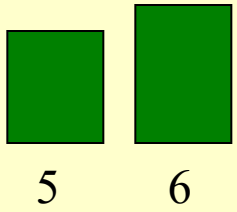


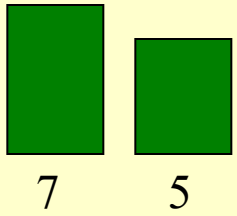


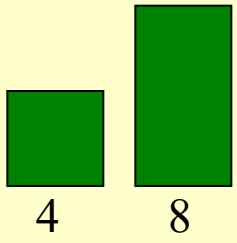


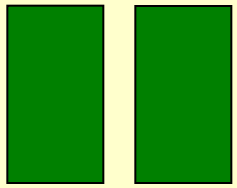


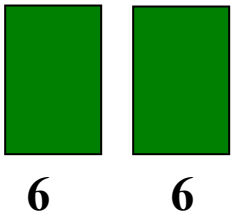
Examples of class B







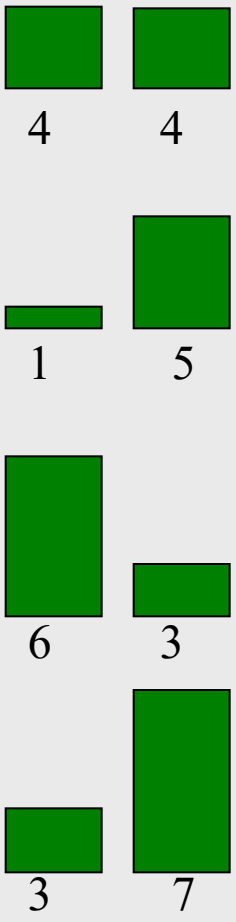




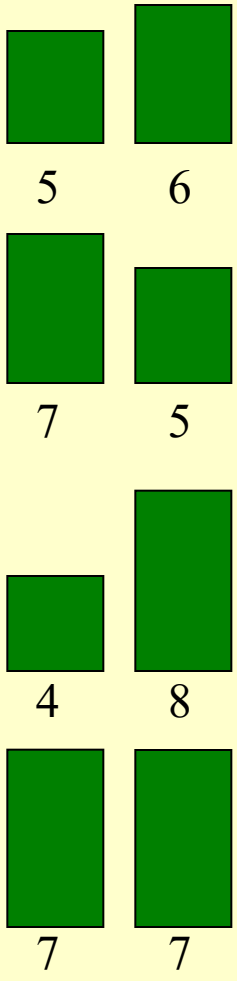
This one is really hard!
What is this, A or B?

Simple Question 3

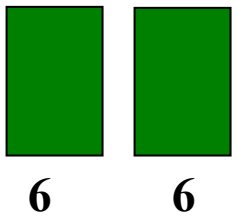
Examples of class A



Examples of class B



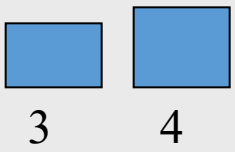
It is a B!

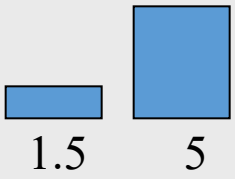


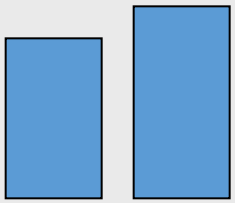
The rule is as follows, if the square of the sum of the two bars is less than or equal to 10, it is an A. Otherwise it is a B.

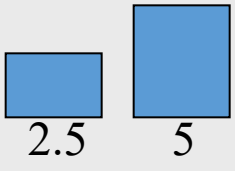
Simple Question 1

Examples of class A

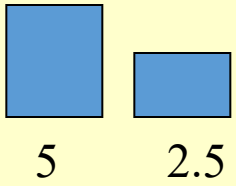


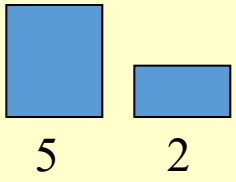


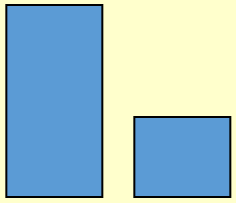


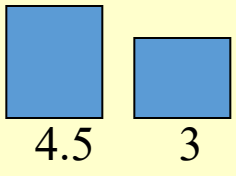


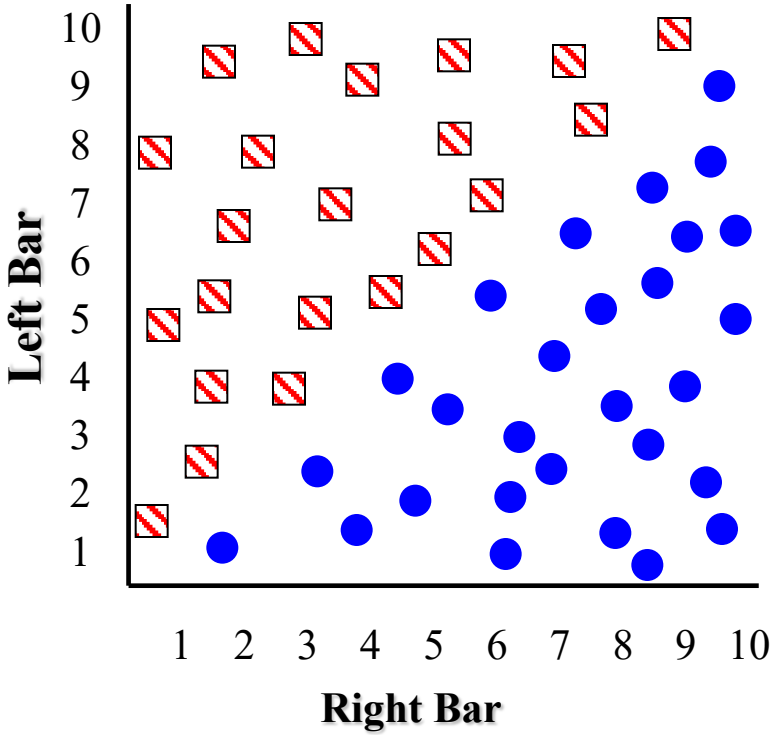
Examples of class B







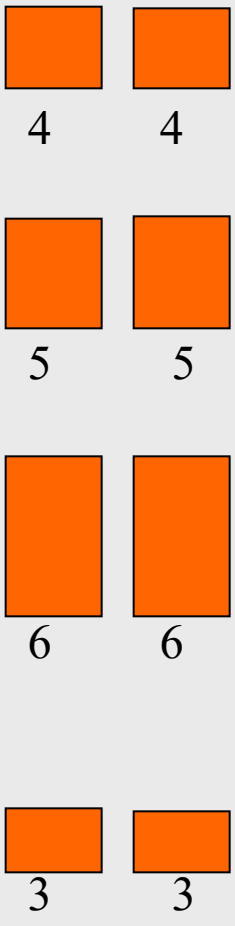




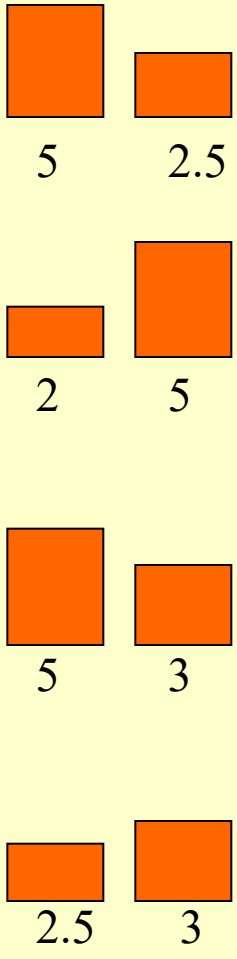
Here is the rule again. If the left bar is smaller than the right bar, it is an A, otherwise it is a B.

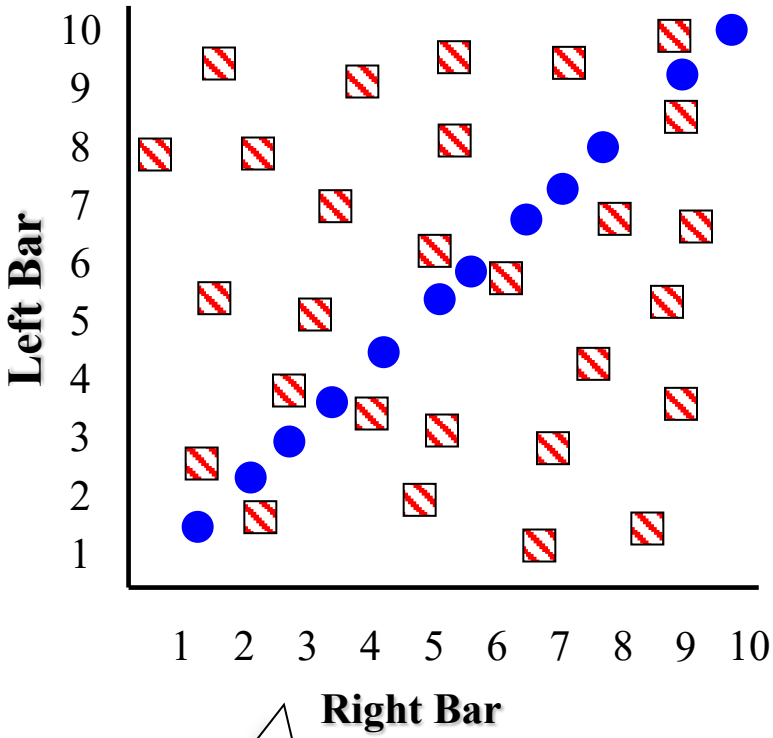
Simple Question 2

Examples of class A



Examples of class B

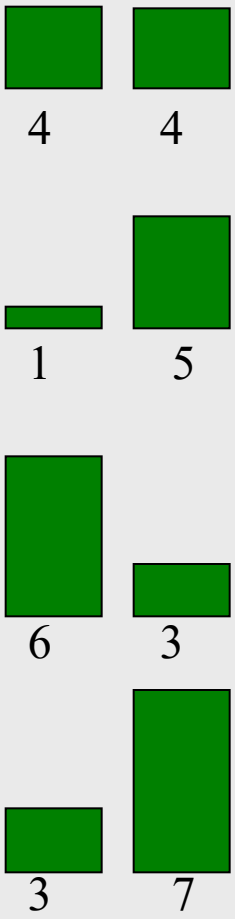




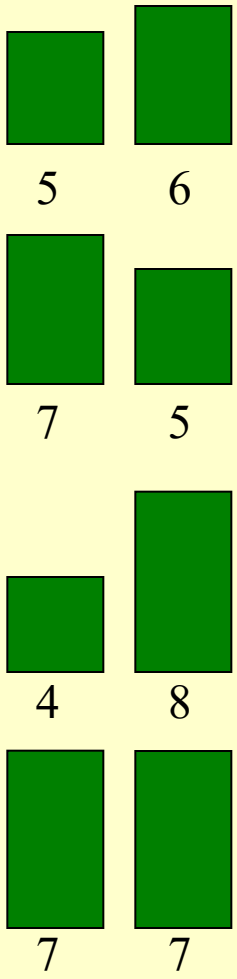
Let me look it up… here it is.. the rule is, if the two bars are equal sizes, it is an A. Otherwise it is a B.

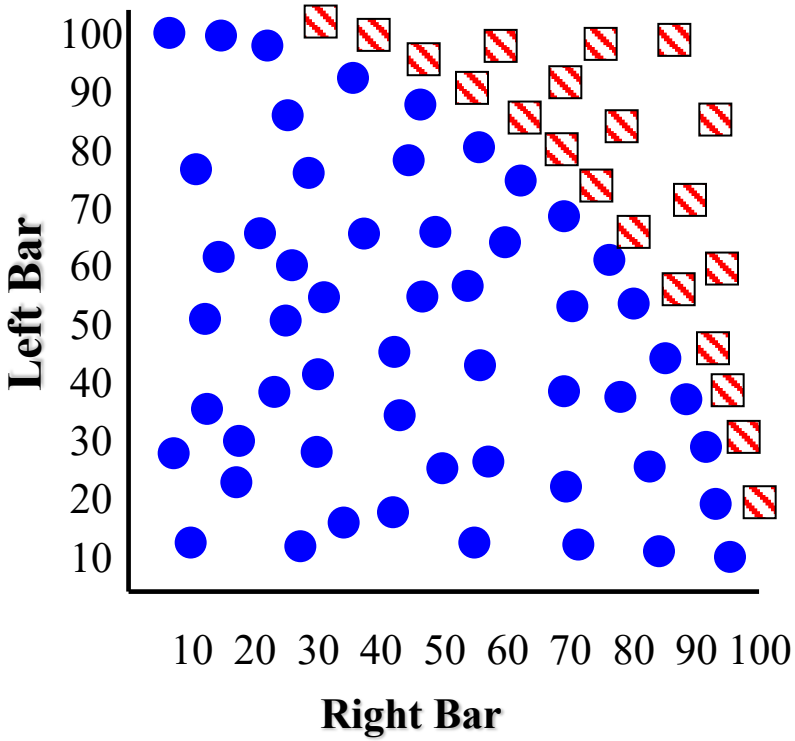
Simple Question 3

Examples of class A



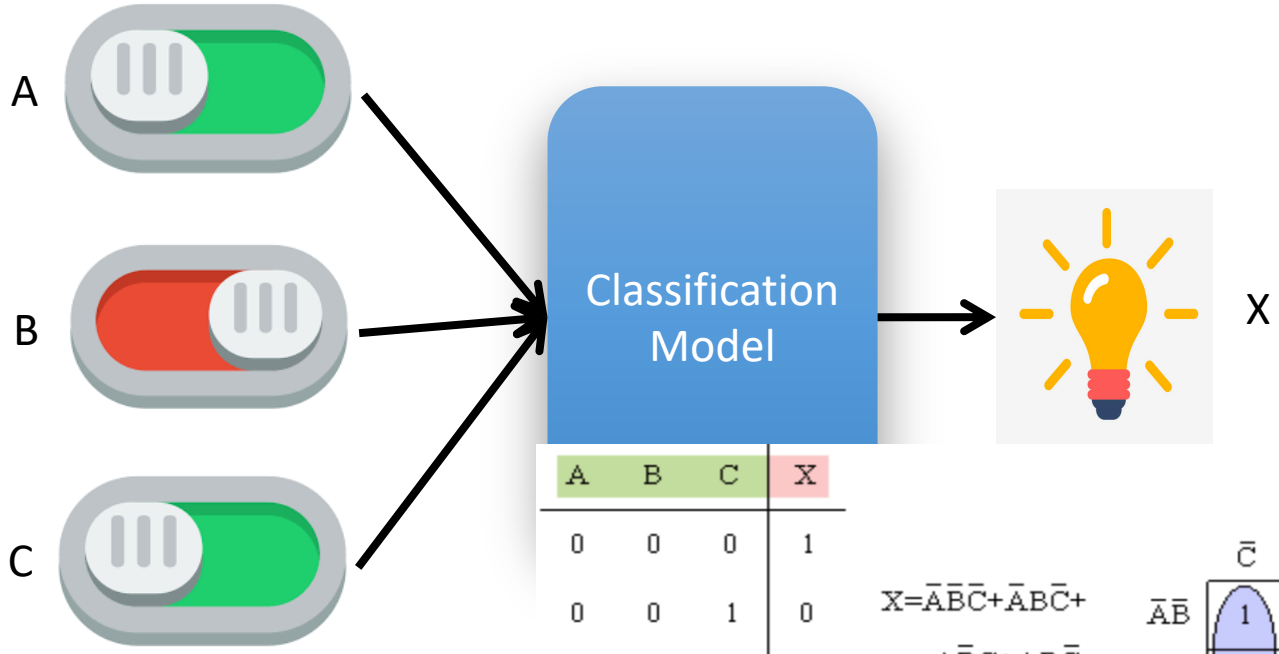
Examples of class B





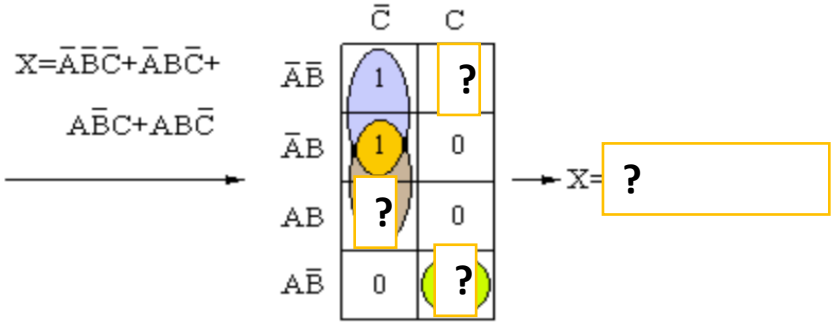
The rule again:
if the square of the sum of the two bars is less than or equal to 10, it is an A. Otherwise it is a B.

Simple Data-Oriented Classification



A	B	C	X
0	0	0	1
0	0	1	0
0	1	0	1
0	1	1	0
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	0

$X=\bar{A}\bar{B}\bar{C}+\bar{A}B\bar{C}+A\bar{B}C+AB\bar{C}$



Karnaugh map (K-map)

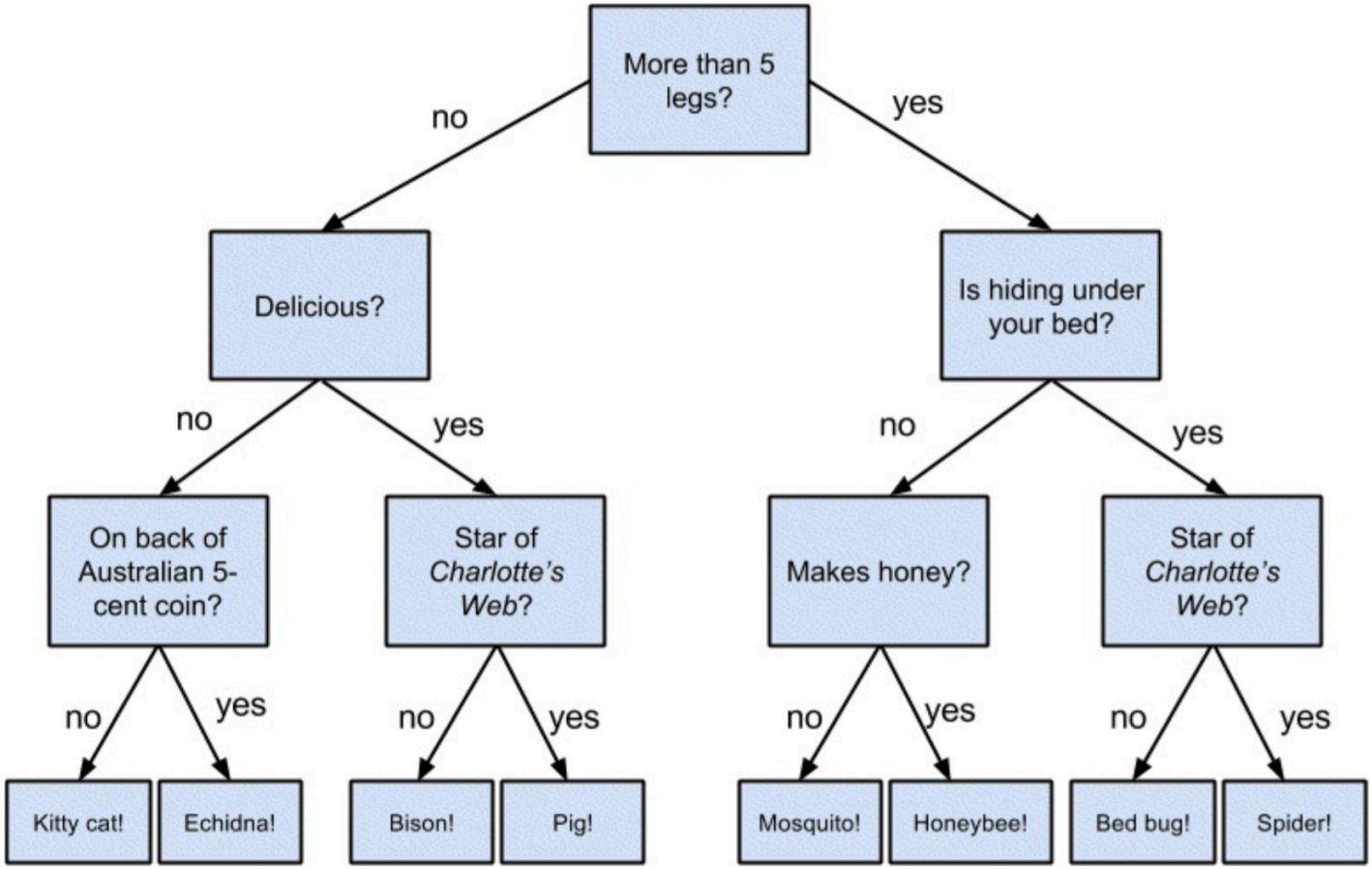
Classification Techniques

- Decision Tree based Methods
- Memory based reasoning (K-NN)
- Naïve Bayes
- Support Vector Machines

- Regression
- Neural Networks
  - DNN
- Ensemble
  - Boosting
  - Random Forest, XGBoost (Regression Tree, Regression Tree Ensemble)
- Semi-supervised Learning

Decision Tree

20 Questions



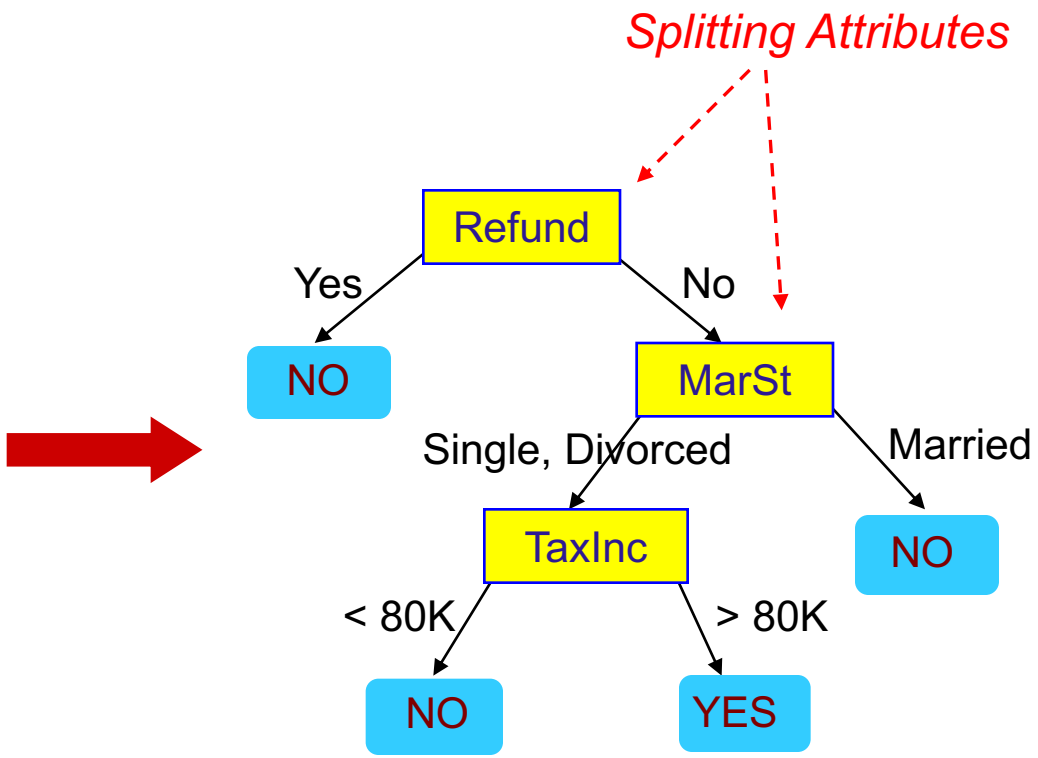
"*Guess the animal*" decision tree

Example of a Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

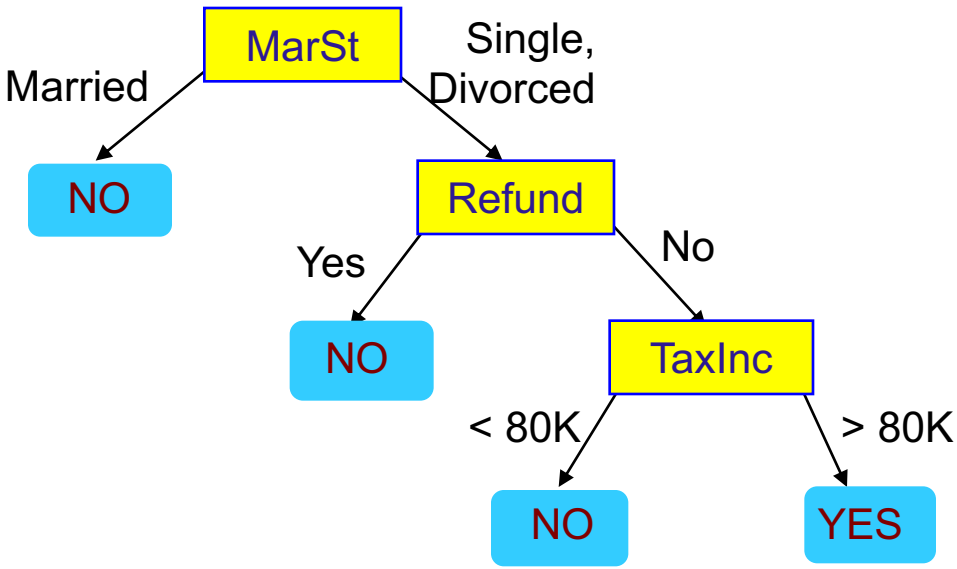
Training Data



Model: Decision Tree

Another Example of Decision Tree

Tid	Refund	Marital Status	Taxable Income	Cheat
	categorical	categorical	continuous	class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



There could be more than one tree that fits the same data!

Test data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

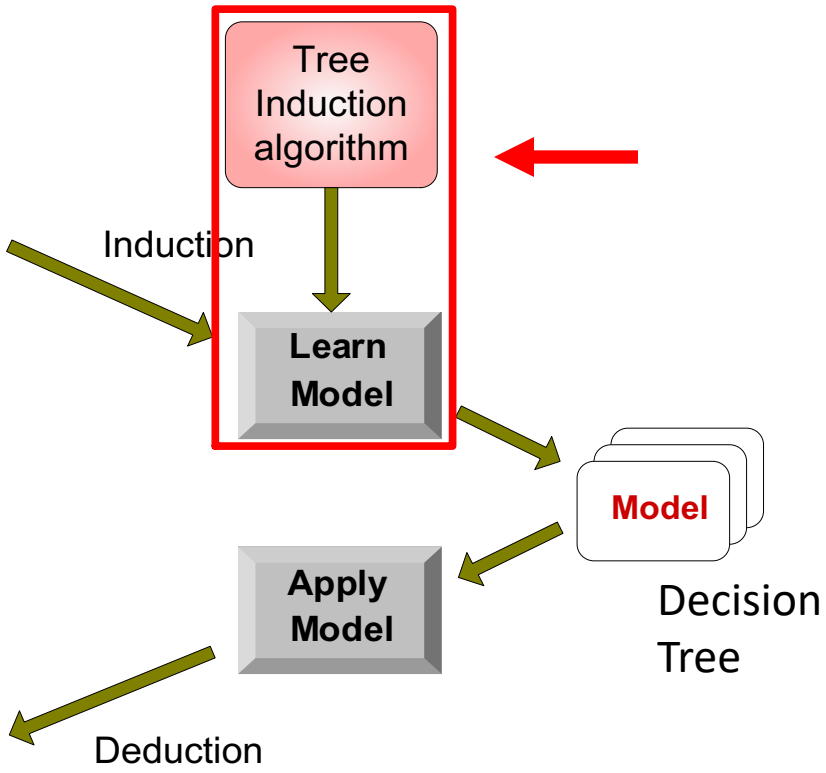
Decision Tree Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set



Decision Tree Induction

- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5, C5.0, See5
  - SLIQ,SPRINT

https://scikit-learn.org/stable/modules/tree.html

Tree Induction

- Greedy strategy
  - Split the records based on an attribute test that optimizes certain criterion.

- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

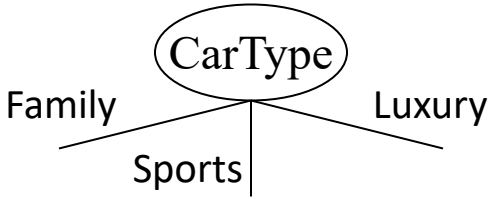
How to Specify Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

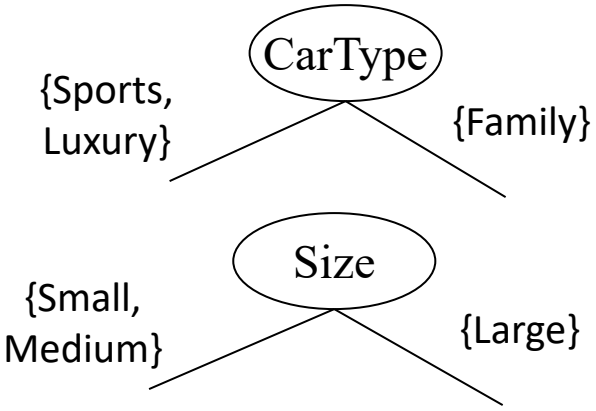
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Based on Nominal Attributes

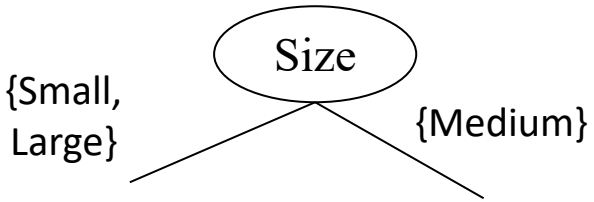
- Multi-way split: Use as many partitions as *distinct values*.

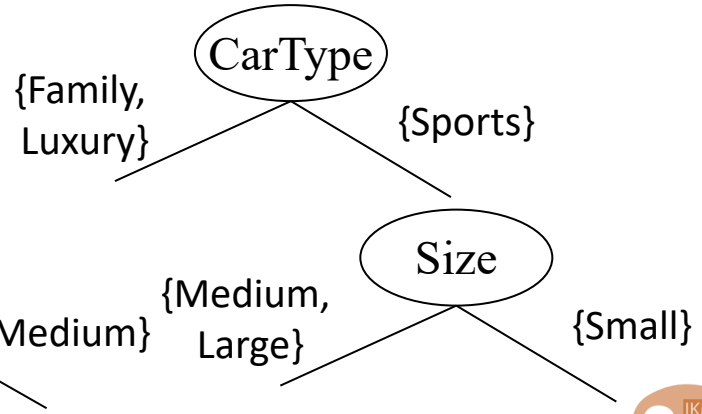


- Binary split: Divides values into two subsets. Need to find optimal partitioning.



OR

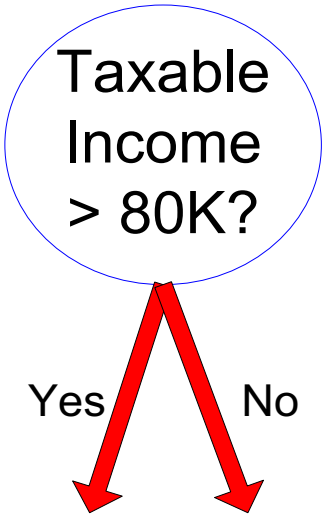




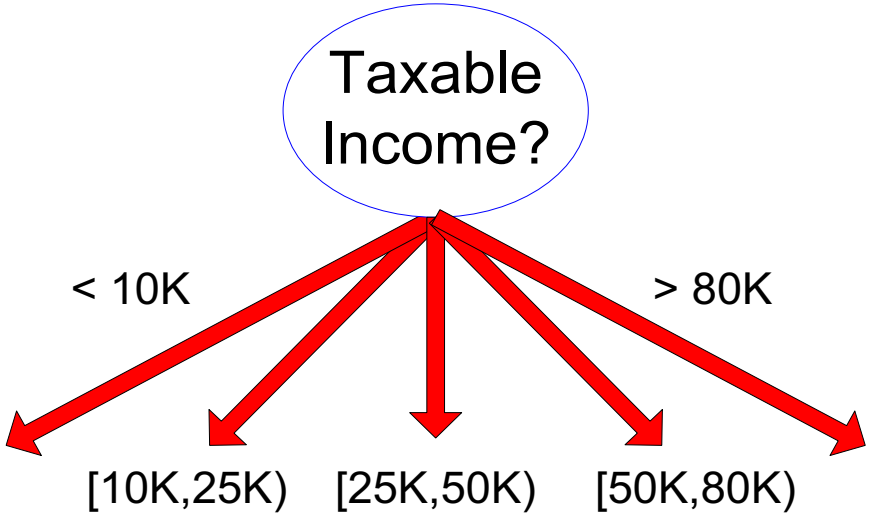
Splitting Based on Continuous Attributes

- Different ways of handling
  - Discretization to form an ordinal categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - Binary Decision: $(A < v)$ or $(A \geq v)$
    - consider all possible splits and finds the best cut
    - can be more compute intensive

Splitting Based on Continuous Attributes



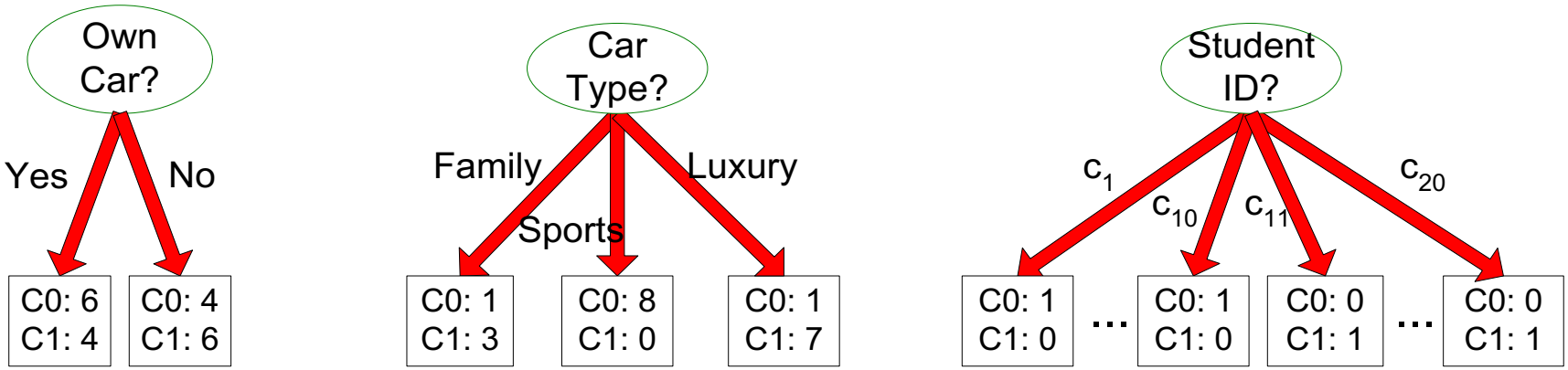
(i) Binary split



(ii) Multi-way split

How to determine the Best Split

Before Splitting: 10 records of class 0, 10 records of class 1



Which test condition is the best?

How to determine the Best Split

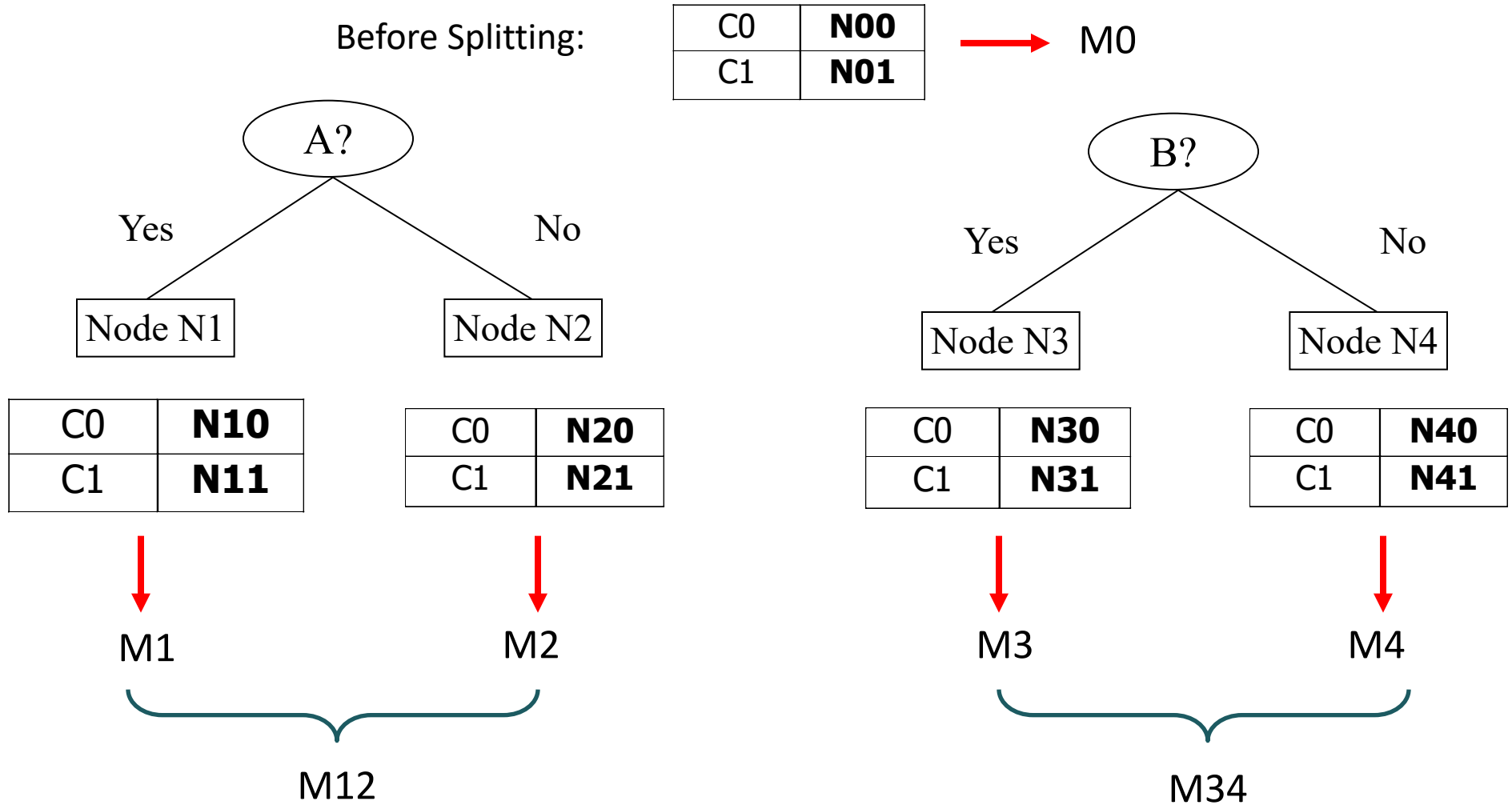
- Greedy approach:
  - Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

C0: 5 C1: 5	C0: 9 C1: 1
Non-homogeneous,	Homogeneous,
High degree of impurity	Low degree of impurity

Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error

How to Find the Best Split



Gain = M0 – M12 vs M0 – M34

Measure of Impurity: GINI

- Gini Index for a given node t :

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

(NOTE: $p(j \mid t)$ is the relative frequency of class j at node t).

- Maximum (1 - 1/n_c) when records are equally distributed among all classes, implying least interesting information
- Minimum (0.0) when all records belong to one class, implying most interesting information

C1	**0**
C2	**6**
Gini=0.000	

C1	**1**
C2	**5**
Gini=0.278	

C1	**2**
C2	**4**
Gini=0.444	

C1	**3**
C2	**3**
Gini=0.500	

Examples for computing GINI

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Gini = 1 – P(C1)^2 – P(C2)^2 = 1 – 0 – 1 = 0

C1	**1**
C2	**5**

P(C1) = 1/6 P(C2) = 5/6

Gini = 1 – (1/6)^2 – (5/6)^2 = 0.278

C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

Gini = 1 – (2/6)^2 – (4/6)^2 = 0.444

Splitting Based on GINI

- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

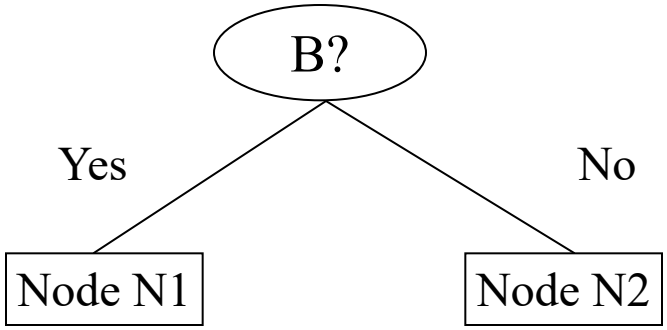
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

where, n_i = number of records at child i,

n = number of records at node p.

Binary Attributes: Computing GINI Index

- Splits into two partitions
- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for.



	Parent
C1	**6**
C2	**6**
Gini = 0.500	

Gini(N1)
$= 1 - (5/7)^2 - (2/7)^2$
$= 0.408$

Gini(N2)
$= 1 - (1/5)^2 - (4/5)^2$
$= 0.32$

	N1	N2
C1	**5**	**1**
C2	**2**	**4**
Gini=0.333		

Gini(Children)
$= 7/12 * 0.408 +$
$5/12 * 0.320 = 0.371$

Categorical Attributes: Computing Gini Index

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

Multi-way split

	CarType		
	Family	Sports	Luxury
C1	1	2	1
C2	4	1	1
Gini	0.393		

Two-way split
(find best partition of values)

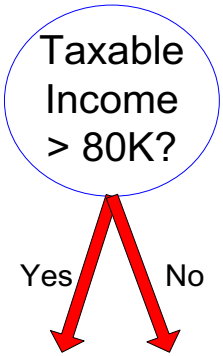
	CarType	
	{Sports, Luxury}	{Family}
C1	3	1
C2	2	4
Gini	0.400	

	CarType	
	{Sports}	{Family, Luxury}
C1	2	2
C2	1	5
Gini	0.419	

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
  - Number of possible splitting values
    = Number of distinct values
- Each splitting value has a count matrix associated with it
  - Class counts in each of the partitions, A < v and A ≥ v
- Simple method to choose best v
  - For each v, scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient! Repetition of work.

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



Continuous Attributes: Computing Gini Index...

- For efficient computation: for each attribute,
  - Sort the attribute on values
  - Linearly scan these values, each time updating the count matrix and computing gini index
  - Choose the split position that has the least gini index

Cheat	No		No		No		Yes		Yes		Yes		No		No		No		No	
Taxable Income																				
Sorted Values →	60		70		75		85		90		95		100		120		125		220	
Split Positions →	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		***0.300***		0.343		0.375		0.400		0.420	

Alternative Splitting Criteria based on INFO

- Entropy at a given node t:

$$Entropy(t) = -\sum_j p(j \mid t) \log p(j \mid t)$$

(NOTE: $p(j \mid t)$ is the relative frequency of class j at node t).

  - Measures homogeneity of a node.
    - Maximum (log n_c) when records are equally distributed among all classes implying least information
    - Minimum (0.0) when all records belong to one class, implying most information
  - Entropy based computations are similar to the GINI index computations

Example of Entropy (cont'd)

Entropy can be measured for a set, e.g.:

S = {a, a, a, a, a, a, a, a, b, b, b, b, b}

$$H(p_1, p_2, ..., p_s) = \sum_{i=1}^{s} (p_i log(1/p_i))$$

(8 a's and 5 b's, 13 total)

$$entropy(S) = -\left[\left(\frac{8}{13}(\log_2 \frac{8}{13})\right) + \left(\frac{5}{13}(\log_2 \frac{5}{13})\right)\right] = 0.96124$$

Remember negative! *for the a's* *for the b's*

Examples for computing Entropy

$$Entropy(t) = -\sum_j p(j \mid t) \log_2 p(j \mid t)$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Entropy = – 0 log 0 – 1 log 1 = – 0 – 0 = 0

C1	**1**
C2	**5**

P(C1) = 1/6 P(C2) = 5/6

Entropy = – (1/6) $\log_2$ (1/6) – (5/6) $\log_2$ (1/6) = 0.65

C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

Entropy = – (2/6) $\log_2$ (2/6) – (4/6) $\log_2$ (4/6) = 0.92

Splitting Based on INFO...

- Information Gain:

$$GAIN_{split} = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_i}{n} Entropy(i) \right)$$

Parent Node, p is split into k partitions;
n_i is number of records in partition i

  - Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
  - Used in ID3 and C4.5
  - Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

Splitting Based on INFO...

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO}$$

$$SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions
n_i is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5
- Designed to overcome the disadvantage of Information Gain

Splitting Criteria based on Classification Error

- Classification error at a node t :

$$Error(t) = 1 - \max_i P(i \mid t)$$

- Measures misclassification error made by a node.
  - Maximum (1 - $1/n_c$) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

Examples for Computing Error

$$Error(t) = 1 - \max_i P(i \mid t)$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Error = 1 – max (0, 1) = 1 – 1 = 0

C1	**1**
C2	**5**

P(C1) = 1/6 P(C2) = 5/6

Error = 1 – max (1/6, 5/6) = 1 – 5/6 = 1/6

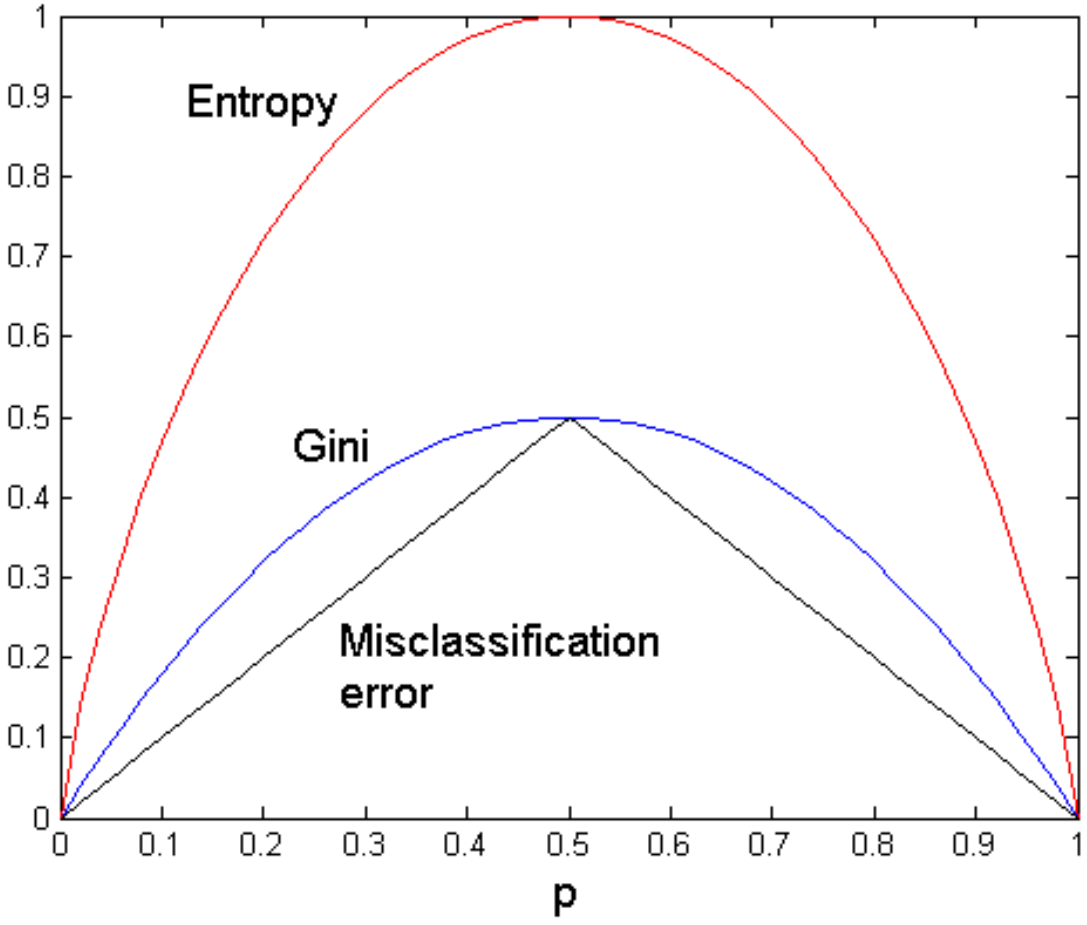
C1	**2**
C2	**4**

P(C1) = 2/6 P(C2) = 4/6

Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Comparison among Splitting Criteria

For a 2-class problem:



Stopping Criteria for Tree Induction

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have similar attribute values
- Early termination (why?)

Decision Tree Based Classification

- Advantages:
  - Inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Accuracy is comparable to other classification techniques for many simple data sets

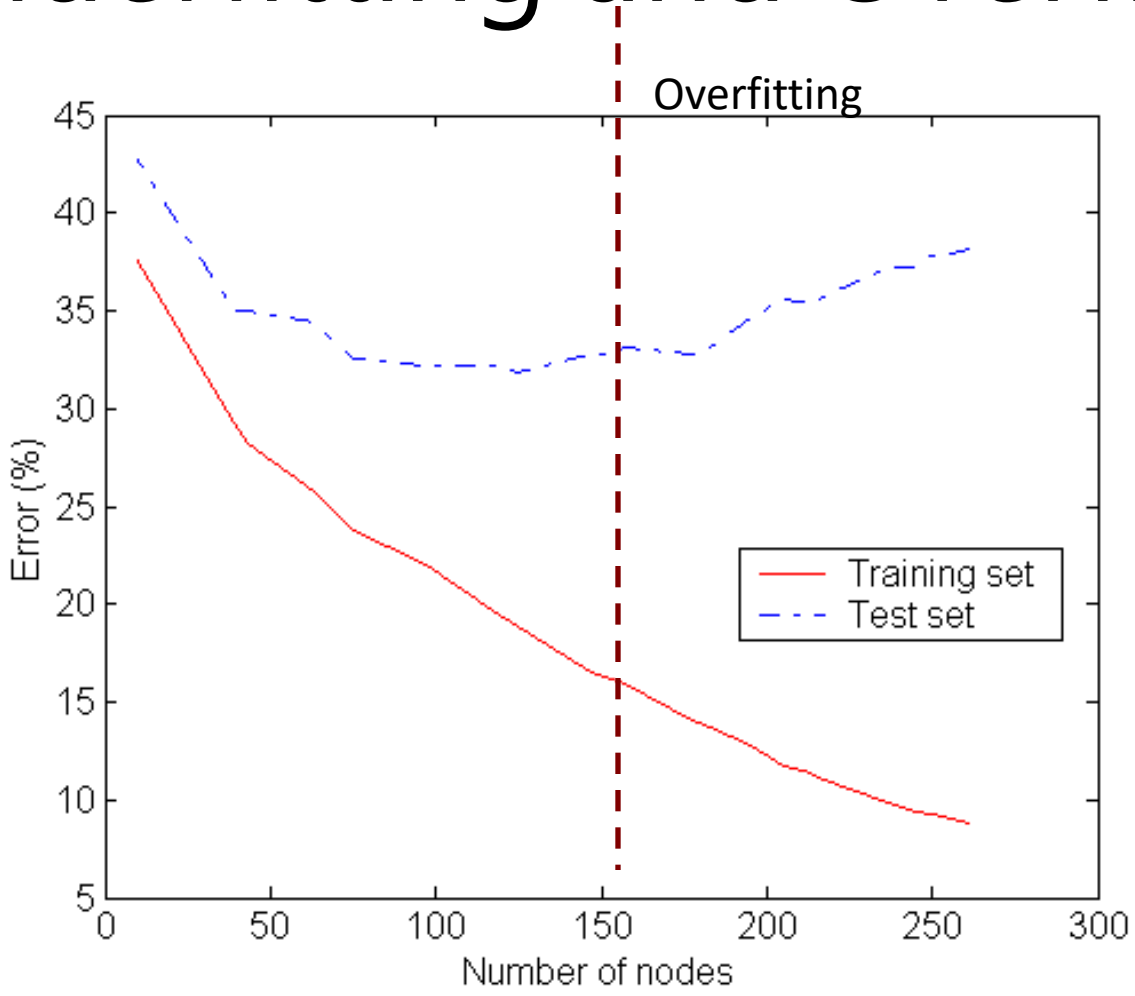
Decision Tree Learning

- Extremely popular method
  - Credit risk assessment
  - Medical diagnosis
  - Market analysis
- Good at dealing with symbolic feature
- Easy to comprehend
  - Compared to logistic regression model and support vector machine

Practical Issues of Classification

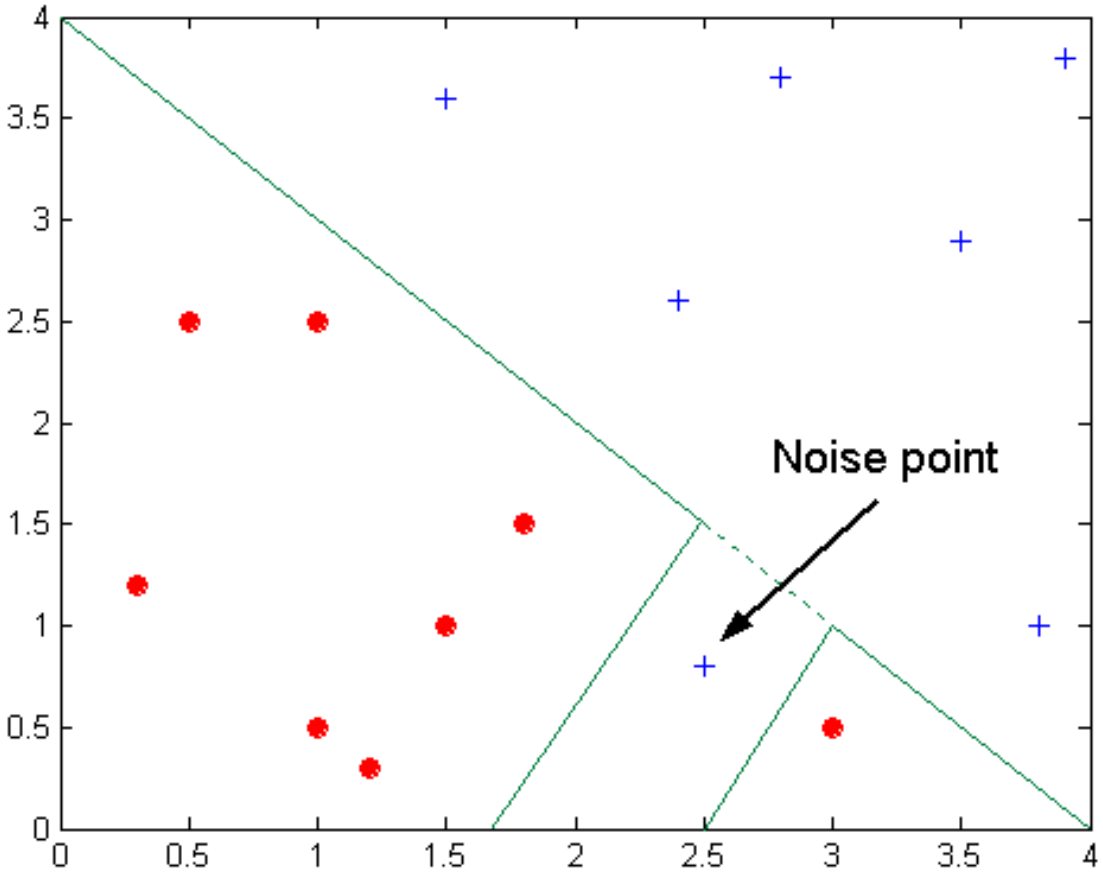
- Underfitting and Overfitting
- Missing Values
- Costs of Classification

Underfitting and Overfitting



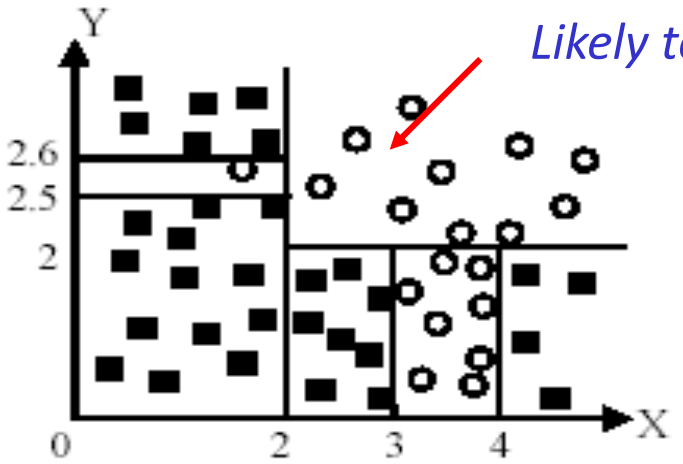
Underfitting: when model is too simple, both training and test errors are large

Overfitting due to Noise



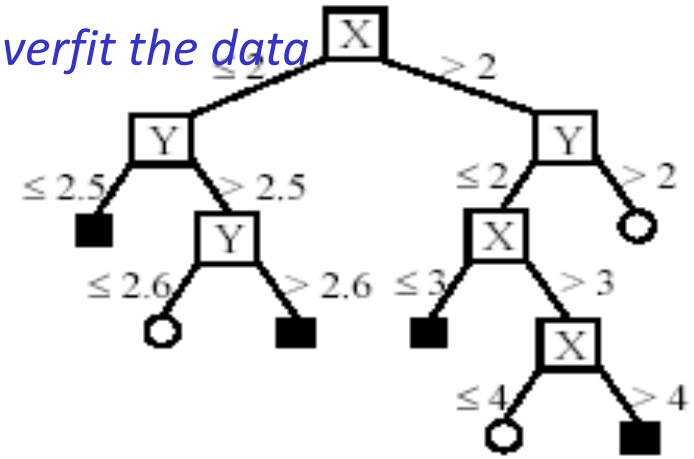
Decision boundary is distorted by noise point

An overfitting example

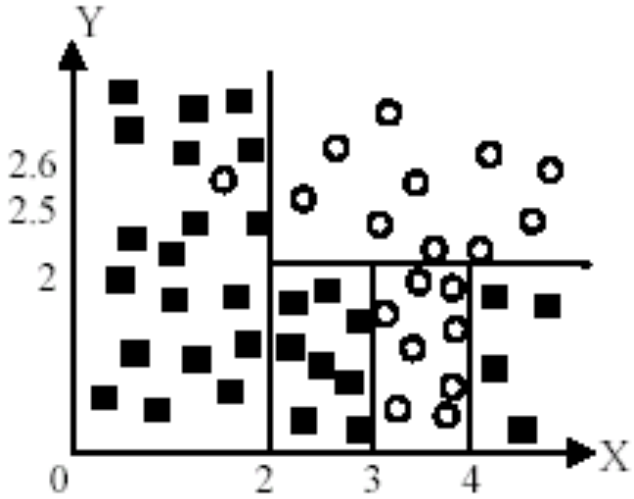


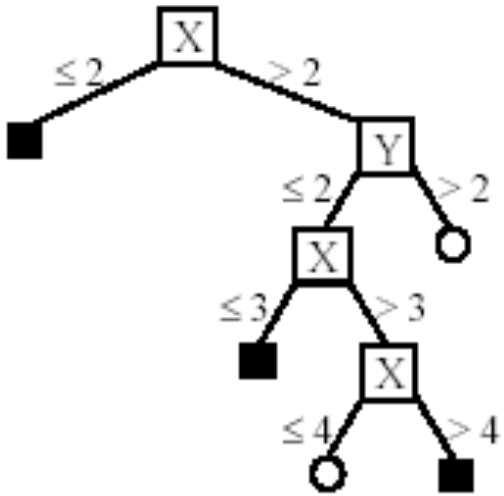
Likely to overfit the data

(A) A partition of the data space



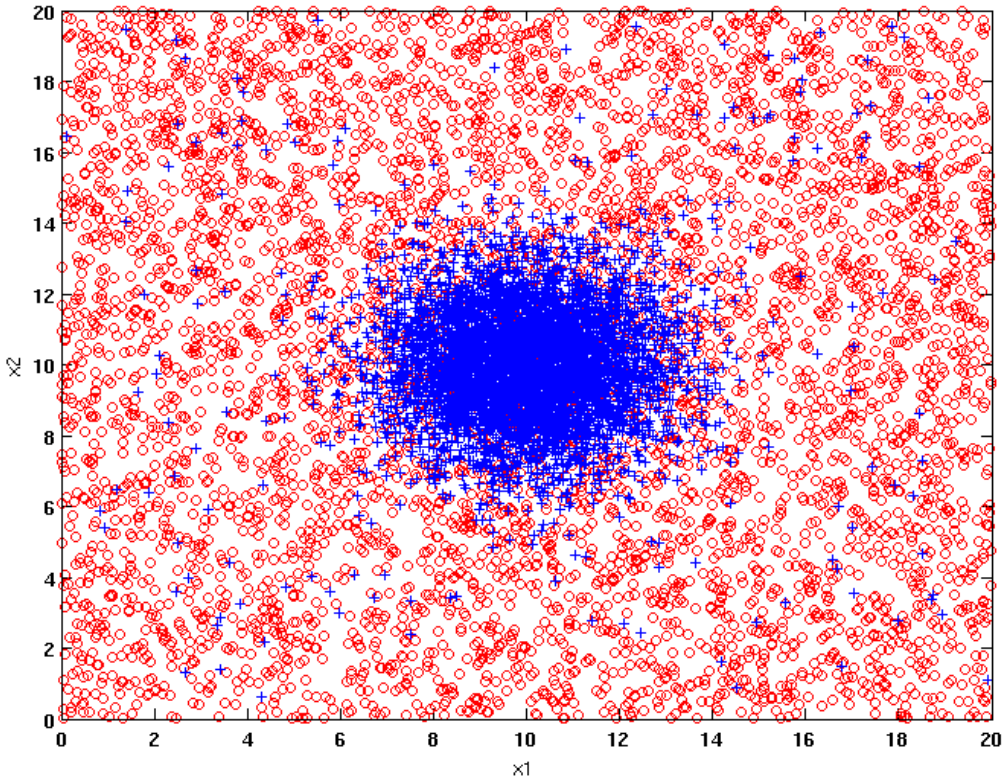
(B). The decision tree





Example Data Set

可乘位了fit外面藍色點兒overfitting
什麼時候該停？經驗、嘗試



Two class problem:

+ : 5200 instances

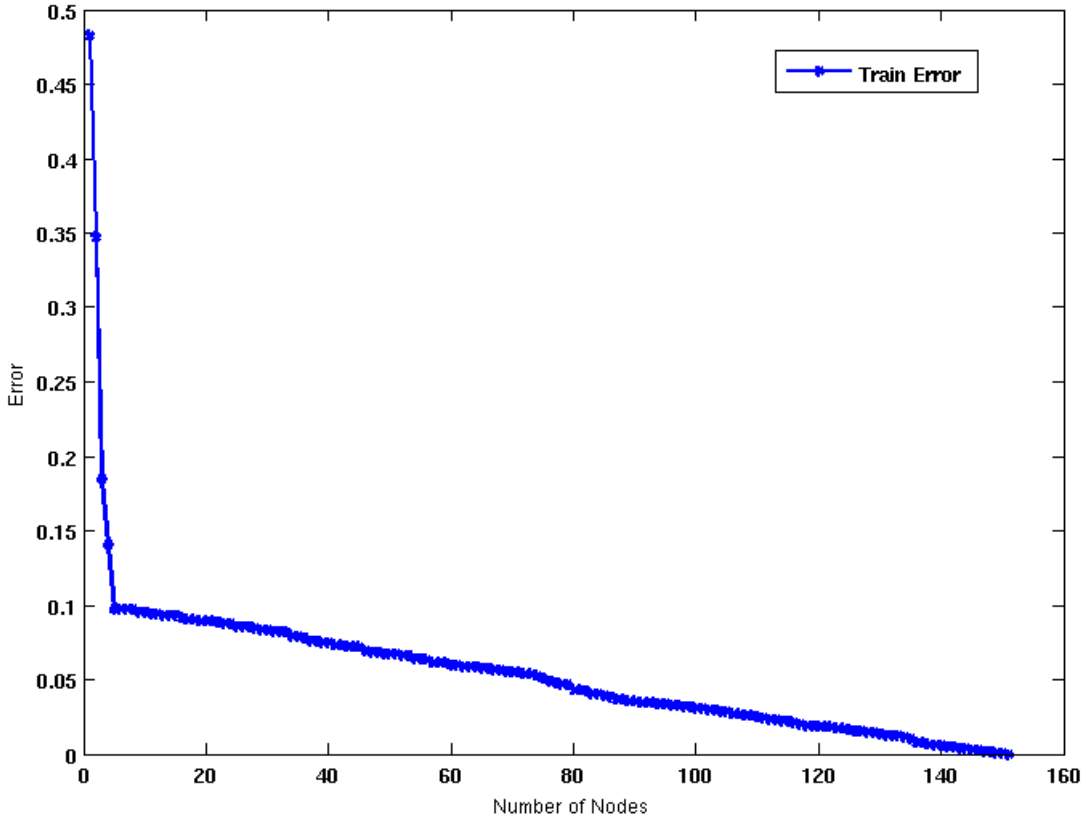
- **5000 instances generated from a Gaussian centered at (10,10)**
- **200 noisy instances added**

o : 5200 instances

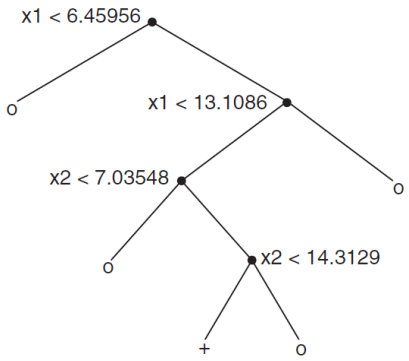
- **Generated from a uniform distribution**

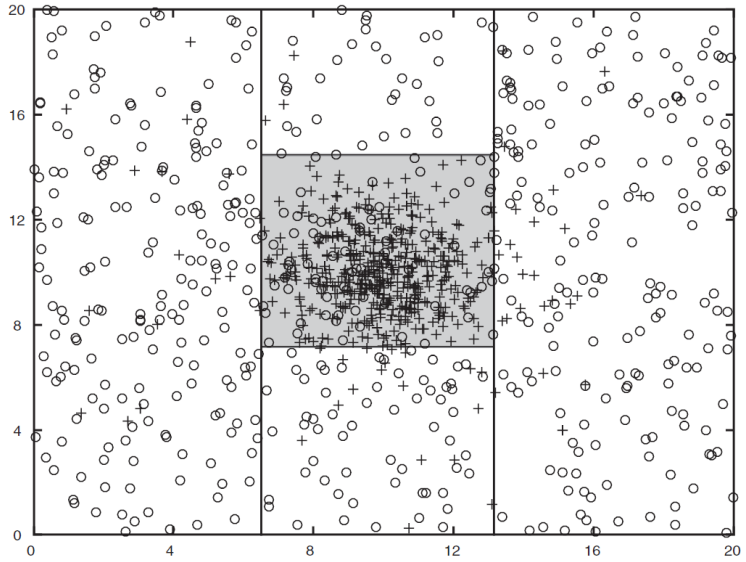
10 % of the data used for training and 90% of the data used for testing

Increasing number of nodes in Decision Trees

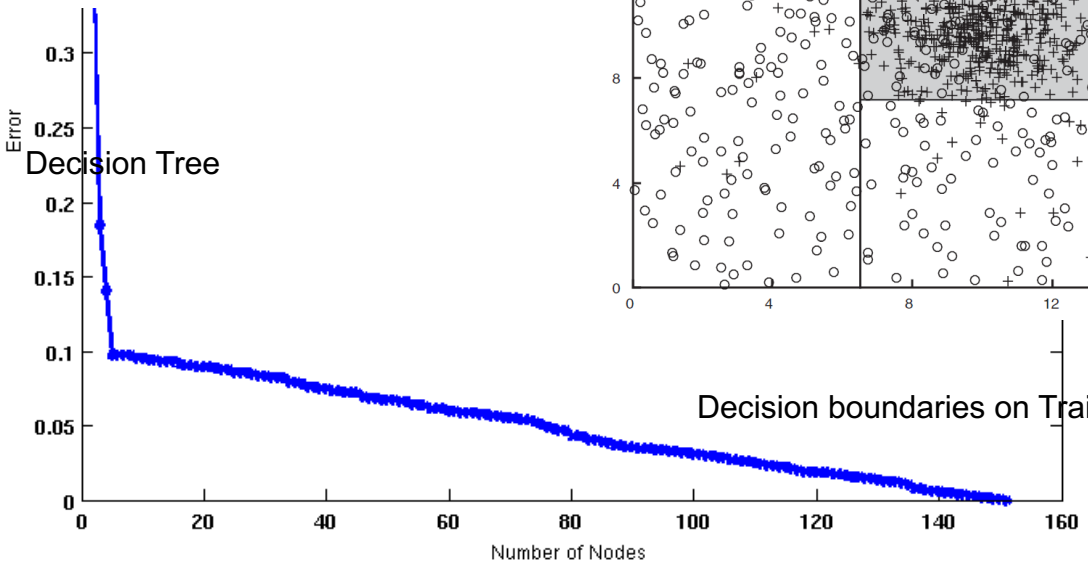


Decision Tree with 4 nodes

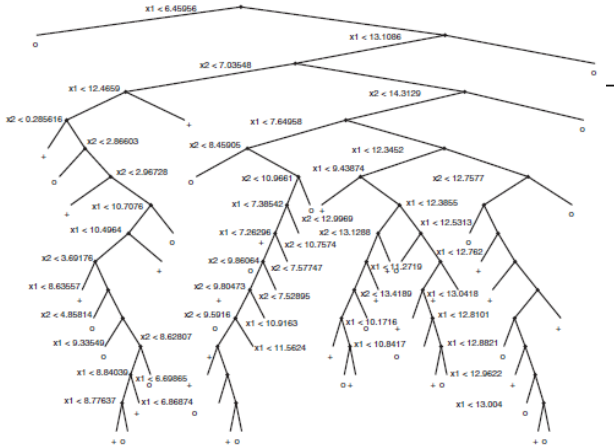


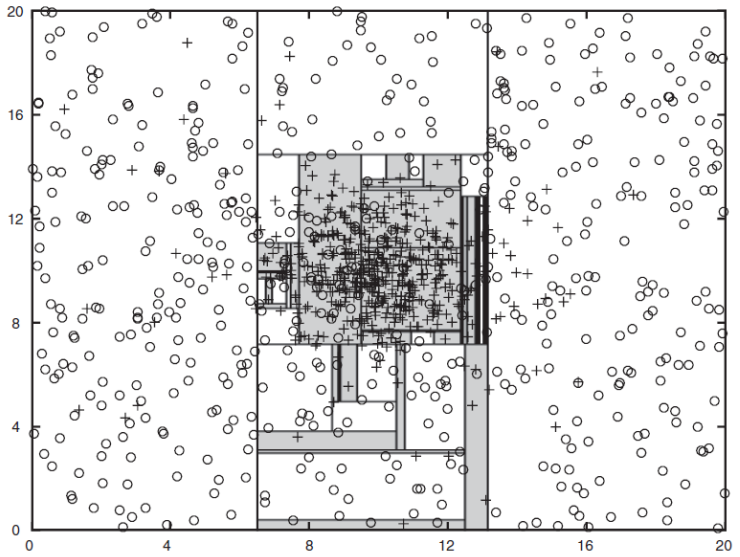


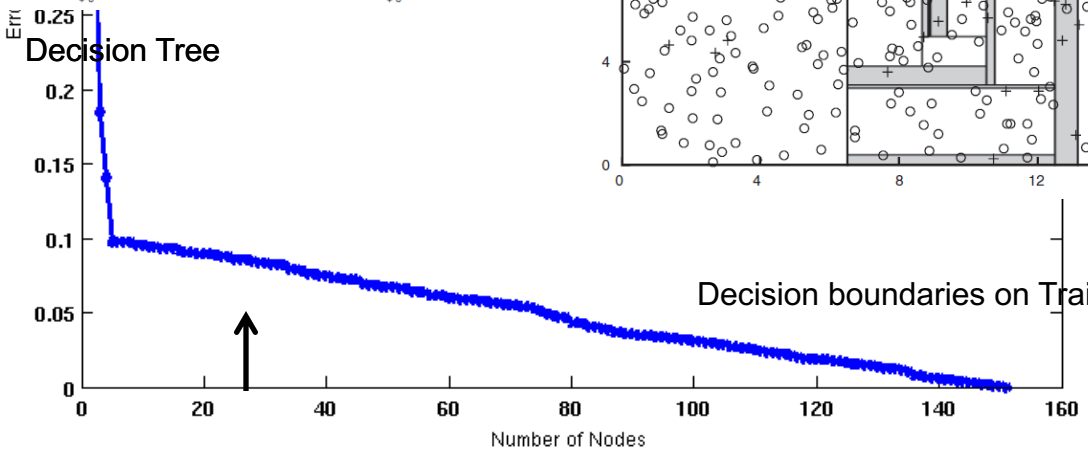
Decision boundaries on Training data



Decision Tree with 50 nodes



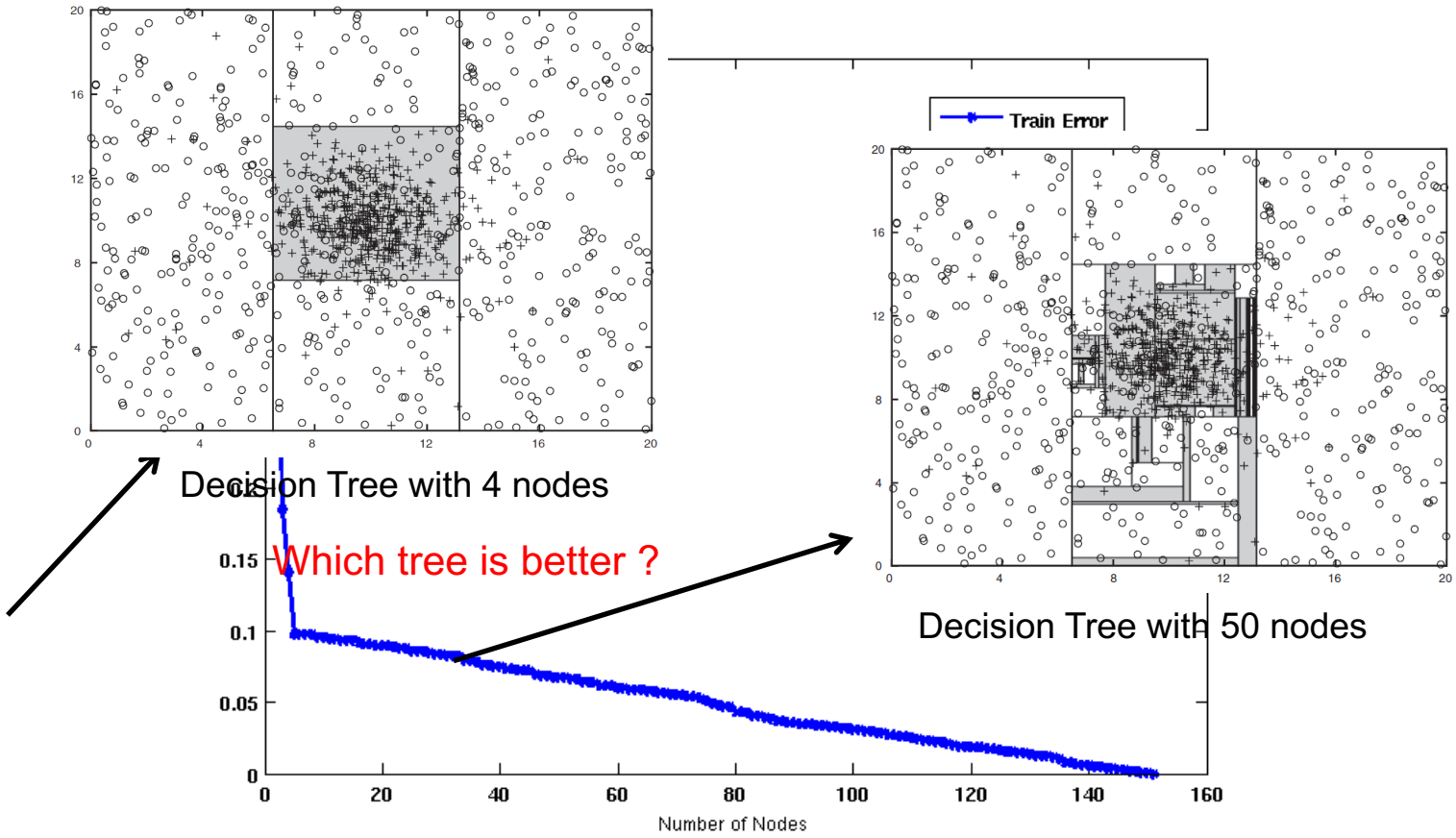




Decision Tree

Decision boundaries on Training data

Which tree is better?



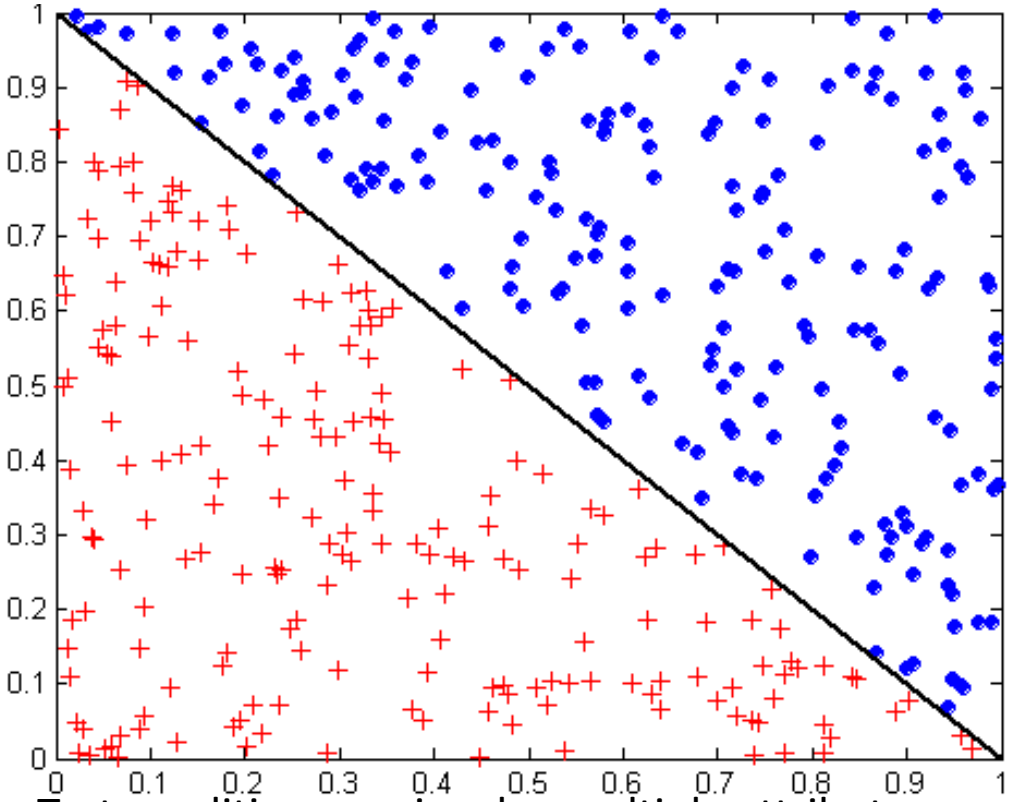
How to Address Overfitting

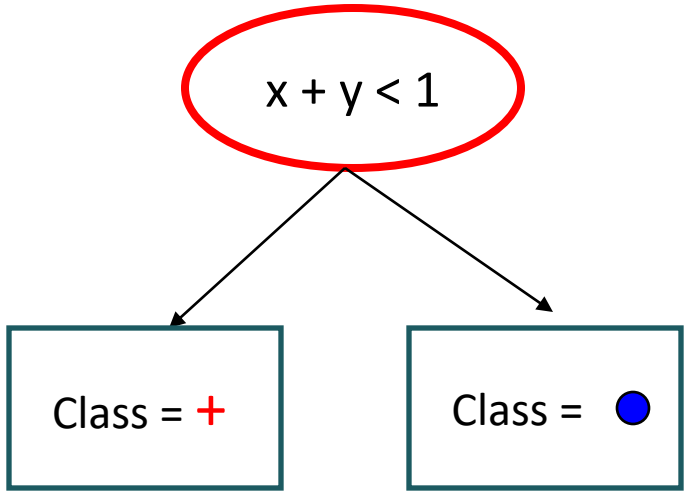
- Pre-Pruning (Early Stopping Rule)
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of instances is less than some user-specified threshold
    - Stop if class distribution of instances are independent of the available features (e.g., using χ^2 test)
    - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

How to Address Overfitting…

- Post-pruning
  - Grow decision tree to its entirety
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node.
  - Class label of leaf node is determined from majority class of instances in the sub-tree
  - Can use MDL for post-pruning

Oblique Decision Trees

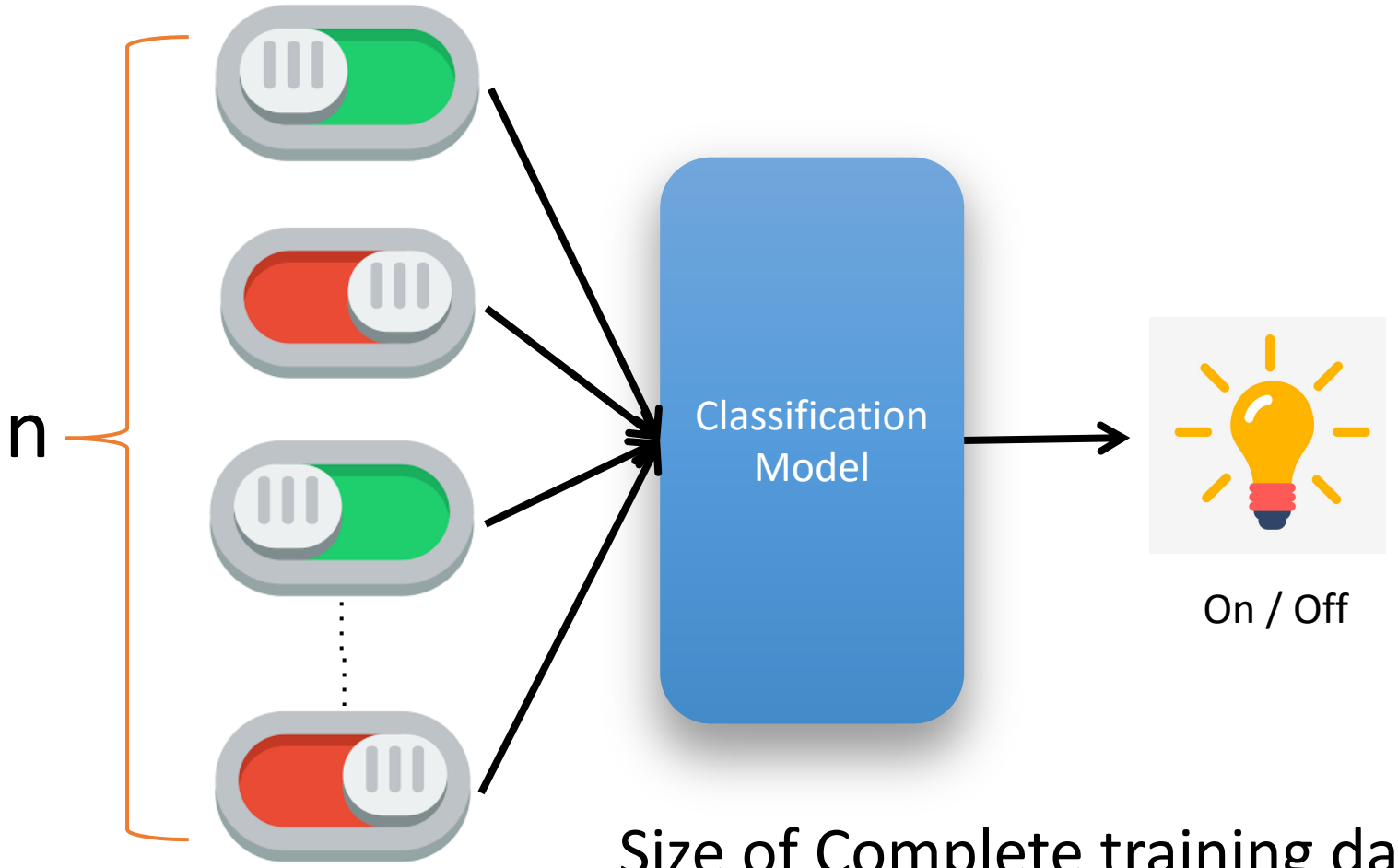




F1	F2	C
+	+	1
-	+	0
+	-	0
-	-	1

- Test condition may involve multiple attributes
- More expressive representation
- Finding optimal test condition is computationally expensive

Curse of Dimensionality



Size of Complete training data=2^n

Complex Decision Tree

- Regression Tree, Random Forest

`sklearn.ensemble`: Ensemble Methods

The `sklearn.ensemble` module includes ensemble-based methods for classification, regression and anomaly detection.

User guide: See the Ensemble methods section for further details.

`ensemble.AdaBoostClassifier` ([…])	An AdaBoost classifier.
`ensemble.AdaBoostRegressor` ([base_estimator, …])	An AdaBoost regressor.
`ensemble.BaggingClassifier` ([base_estimator, …])	A Bagging classifier.
`ensemble.BaggingRegressor` ([base_estimator, …])	A Bagging regressor.
`ensemble.ExtraTreesClassifier` ([…])	An extra-trees classifier.
`ensemble.ExtraTreesRegressor` ([n_estimators, …])	An extra-trees regressor.
`ensemble.GradientBoostingClassifier` ([loss, …])	Gradient Boosting for classification.
`ensemble.GradientBoostingRegressor` ([loss, …])	Gradient Boosting for regression.
`ensemble.IsolationForest` ([n_estimators, …])	Isolation Forest Algorithm
`ensemble.RandomForestClassifier` ([…])	A random forest classifier.
`ensemble.RandomForestRegressor` ([…])	A random forest regressor.
`ensemble.RandomTreesEmbedding` ([…])	An ensemble of totally random trees.
`ensemble.VotingClassifier` (estimators[, …])	Soft Voting/Majority Rule classifier for unfitted estimators.

新的資料來，就跟舊的資料比較，歸到最接近的class

最一開始觀察資料時使用KNN，ex:一開始把K設一，發現只有50%->可能有一堆雜訊、取的屬性有問題

很好做檢測的工具

Instance-Based Classifiers

Set of Stored Cases

Atr1	……	AtrN	Class
			A
			B
			B
			C
			A
			C
			B

- Store the training records
- Use training records to predict the class label of unseen cases

Unseen Case

Atr1	……	AtrN

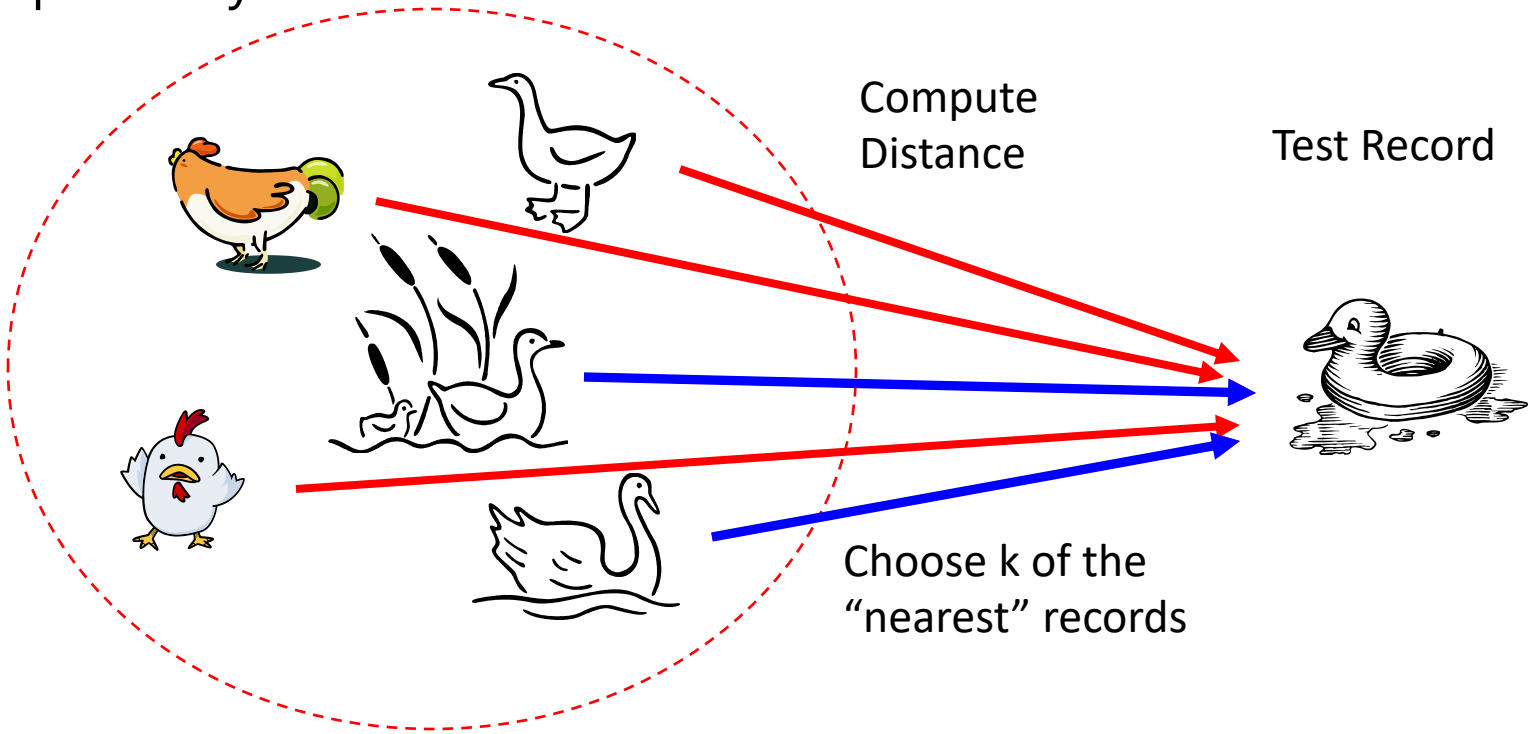
可以看三個最近的，看他們的類別是什麼，再投票

- Nearest neighbor: Uses k “closest” points (nearest neighbors) for performing classification

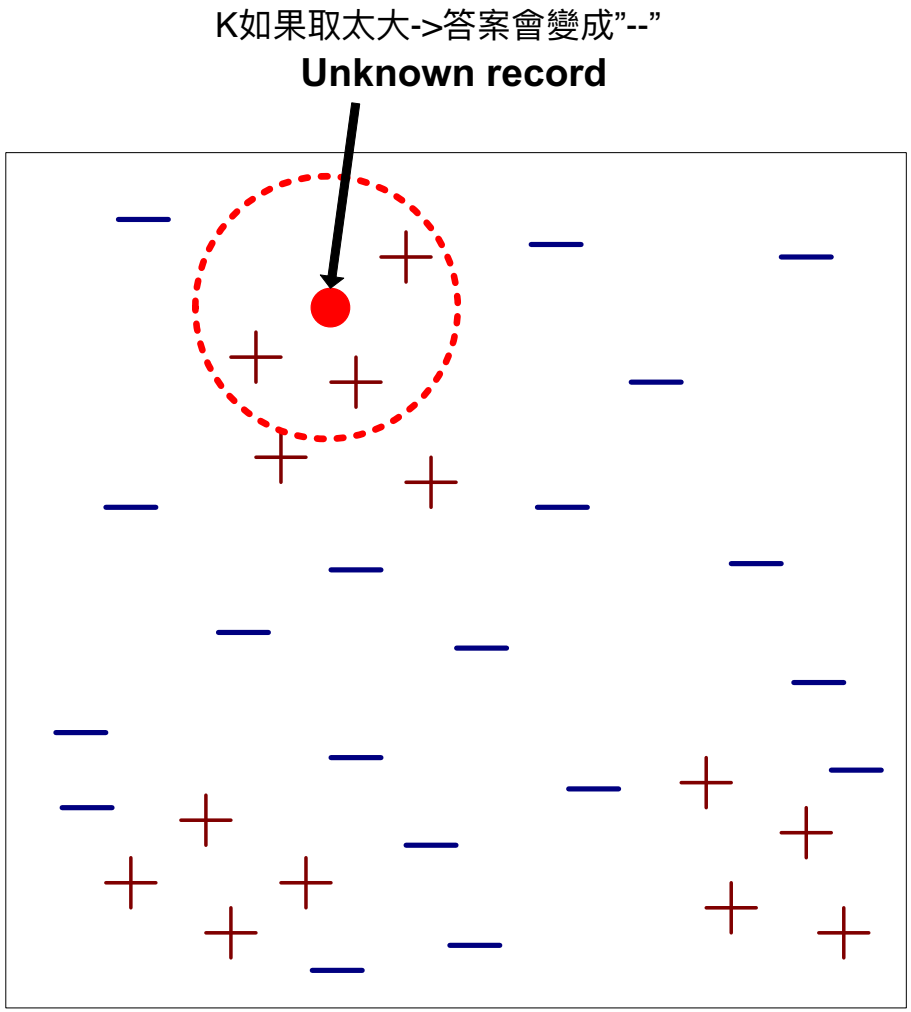
KNN

Nearest Neighbor Classifiers

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it's probably a duck



Nearest-Neighbor Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric to compute distance between records
  - The value of *k*, the number of nearest neighbors to retrieve

- To classify an unknown record:
  - Compute distance to other training records
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Nearest Neighbor Classification

- k-NN classifiers are lazy learners
  - It does not build models explicitly
- Compute distance between two points:
  - Euclidean distance

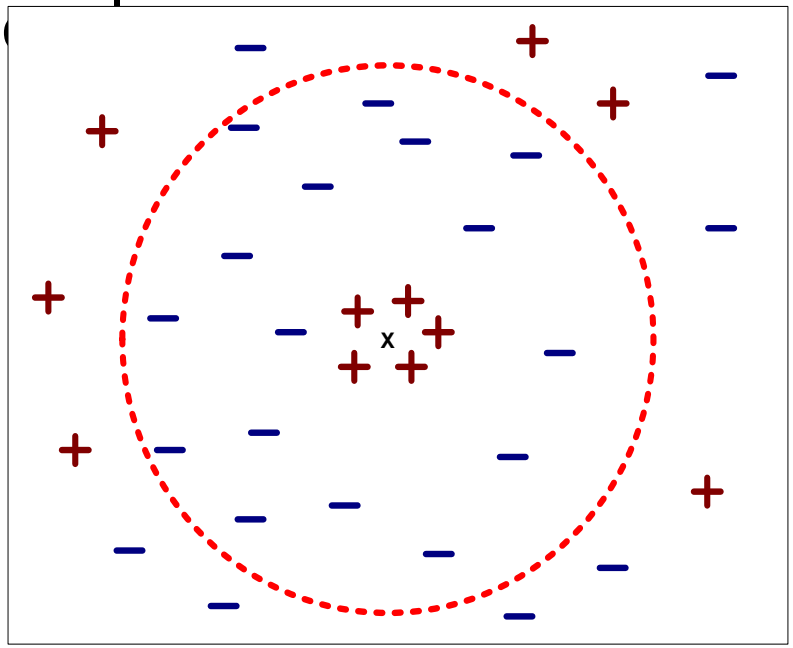
$$d(p,q) = \sqrt{\sum_i (p_i - q_i)^2}$$

Ex:出稱年月日、血型如何計算距離？要predefine、以及一些domine knolwedge

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - Weigh the vote according to distance
    - weight factor, $w = 1/d^2$

Nearest Neighbor Classification…

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from oth



Nearest Neighbor Classification…

資料前處理要小心

- Scaling issues
  - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
  - Example:
    - height of a person may vary from 1.5m to 1.8m
    - weight of a person may vary from 90lb to 300lb
    - income of a person may vary from $10K to $1M

Nearest Neighbor Classification…

- Problem with Euclidean measure:
  - High dimensional data
    - curse of dimensionality
  - Can produce counter-intuitive results

1 1 1 1 1 1 1 1 1 1 1 0		1 0 0 0 0 0 0 0 0 0 0 0	
0 1 1 1 1 1 1 1 1 1 1 1	vs	0 0 0 0 0 0 0 0 0 0 0 1	
d = 1.4142		d = 1.4142	

- Solution: Normalize the vectors to unit length

Bayes Classifier

- A probabilistic framework for solving classification problems
- Conditional Probability:

$$P(C \mid A) = \frac{P(A,C)}{P(A)}$$

$$P(A \mid C) = \frac{P(A,C)}{P(C)}$$

- Bayes theorem:

$$P(C \mid A) = \frac{P(A \mid C)P(C)}{P(A)}$$

Example of Bayes Theorem

- Given:
  - A doctor knows that meningitis causes stiff neck 50% of the time
  - Prior probability of any patient having meningitis is 1/50,000
  - Prior probability of any patient having stiff neck is 1/20

- If a patient has stiff neck, what's the probability he/she has meningitis?

$$P(M \mid S) = \frac{P(S \mid M)P(M)}{P(S)} = \frac{0.5 \times 1/50000}{1/20} = 0.0002$$

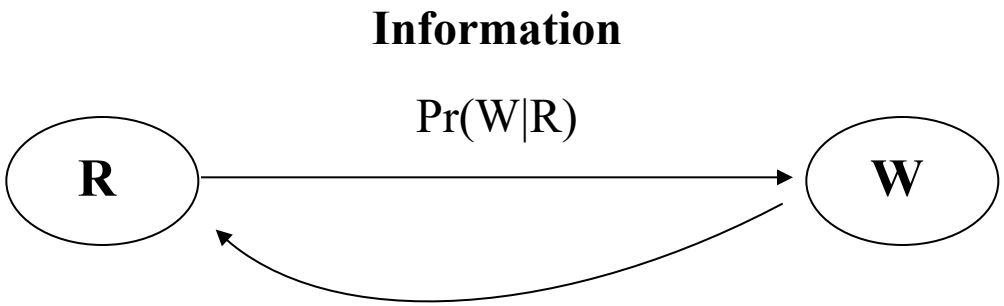
Bayes' Rule

If R= the set of favor news and W="*open source*"?

	R	¬R
W	0.7	0.4
¬W	0.3	0.6

R: It rains

W: The grass is wet



100d	80d	20d
	R	¬R
W	56	8
¬W	24	12

$$\frac{\Pr(W \mid R)\Pr(R)}{\Pr(W)} = \frac{0.7*0.8}{56+8/100} = \frac{0.7*0.8}{0.64}$$

$$\frac{\Pr(W \mid R)\Pr(R)}{\Pr(W)} = \frac{\Pr(W \mid R)\Pr(R)}{\Pr(W \mid R)\Pr(R)+\Pr(W \mid \neg R)\Pr(\neg R)} = \frac{0.7*0.8}{0.7*0.8+0.4*0.2} = \frac{7}{8}$$

Bayesian Classifiers

- Consider each attribute and class label as random variables

- Given a record with attributes (A_1, A_2,…,A_n)
  - Goal is to predict class C
  - Specifically, we want to find the value of C that maximizes P(C| A_1, A_2,…,A_n)

- Can we estimate P(C| A_1, A_2,…,A_n) directly from data?

Bayesian Classifiers

- Approach:
  - compute the posterior probability $P(C \mid A_1, A_2, \ldots, A_n)$ for all values of C using the Bayes theorem

$$P(C \mid A_1 A_2 \ldots A_n) = \frac{P(A_1 A_2 \ldots A_n \mid C) P(C)}{P(A_1 A_2 \ldots A_n)}$$

  - Choose value of C that maximizes
    $P(C \mid A_1, A_2, \ldots, A_n)$
  - Equivalent to choosing value of C that maximizes
    $P(A_1, A_2, \ldots, A_n \mid C)\, P(C)$

- How to estimate $P(A_1, A_2, \ldots, A_n \mid C)$?

Naïve Bayes Classifier

- Assume independence among attributes A_i when class is given:
  - $P(A_1, A_2, \ldots, A_n | C) = P(A_1 | C_j)\, P(A_2 | C_j) \ldots P(A_n | C_j)$
  - Can estimate $P(A_i | C_j)$ for all A_i and C_j.
  - New point is classified to C_j if $P(C_j) \prod P(A_i | C_j)$ is maximal.

How to Estimate Probabilities from Data?

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Class: $P(C) = N_c/N$
  - e.g., P(No) = 7/10,
    P(Yes) = 3/10

- For discrete attributes:

$$P(A_i \mid C_k) = |A_{ik}| / N_c^k$$

  - where $|A_{ik}|$ is number of instances having attribute A_i and belongs to class C_k
  - Examples:

    P(Status=Married|No) = 4/7
    P(Refund=Yes|Yes)=0

    以前沒有發生過不代表就不會是->
    沒有tranning data, data dias

How to Estimate Probabilities from Data?

- For continuous attributes:
  - Discretize the range into bins
    - one ordinal attribute per bin k
    - violates independence assumption
  - Two-way split: $(A < v)$ or $(A > v)$
    - choose only one of the two splits as new attribute
  - Probability density estimation:
    - Assume attribute follows a normal distribution
    - Use data to estimate parameters of distribution (e.g., mean and standard deviation)
    - Once probability distribution is known, can use it to estimate the conditional probability $P(A_i|c)$

Example of Naïve Bayes Classifier

$$X = (\text{Refund} = \text{No}, \text{Married}, \text{Income} = 120\text{K})$$

naive Bayes Classifier:

P(Refund=Yes|No) = 3/7
P(Refund=No|No) = 4/7
P(Refund=Yes|Yes) = 0
P(Refund=No|Yes) = 1
P(Marital Status=Single|No) = 2/7
P(Marital Status=Divorced|No)=1/7
P(Marital Status=Married|No) = 4/7
P(Marital Status=Single|Yes) = 2/7
P(Marital Status=Divorced|Yes)=1/7
P(Marital Status=Married|Yes) = 0

For taxable income:
If class=No: sample mean=110
sample variance=2975
If class=Yes: sample mean=90
sample variance=25

Given a Test Record:

- P(X|Class=No) = P(Refund=No|Class=No)
  × P(Married| Class=No)
  × P(Income=120K| Class=No)
  = 4/7 × 4/7 × 0.0072 = 0.0024

- P(X|Class=Yes) = P(Refund=No| Class=Yes)
  × P(Married| Class=Yes)
  × P(Income=120K| Class=Yes)
  = 1 × 0 × 1.2 × 10^{-9} = 0

Since P(X|No)P(No) > P(X|Yes)P(Yes)

Therefore P(No|X) > P(Yes|X)
=> Class = No

Naïve Bayes Classifier

- If one of the conditional probability is zero, then the entire expression becomes zero
- Probability estimation:

$$\text{Original}: P(A_i \mid C) = \frac{N_{ic}}{N_c}$$

$$\text{Laplace}: P(A_i \mid C) = \frac{N_{ic} + 1}{N_c + c}$$

$$\text{m-estimate}: P(A_i \mid C) = \frac{N_{ic} + mp}{N_c + m}$$

c: number of classes

p: prior probability

m: parameter

遇到0怎麼辦？
Laplace: 讓大家至少發生一次，本來零的變成一個很小的起始值

Example of Naïve Bayes Classifier

Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
human	yes	no	no	yes	mammals
python	no	no	no	no	non-mammals
salmon	no	no	yes	no	non-mammals
whale	yes	no	yes	no	mammals
frog	no	no	sometimes	yes	non-mammals
komodo	no	no	no	yes	non-mammals
bat	yes	yes	no	yes	mammals
pigeon	no	yes	no	yes	non-mammals
cat	yes	no	no	yes	mammals
leopard shark	yes	no	yes	no	non-mammals
turtle	no	no	sometimes	yes	non-mammals
penguin	no	no	sometimes	yes	non-mammals
porcupine	yes	no	no	yes	mammals
eel	no	no	yes	no	non-mammals
salamander	no	no	sometimes	yes	non-mammals
gila monster	no	no	no	yes	non-mammals
platypus	no	no	no	yes	mammals
owl	no	yes	no	yes	non-mammals
dolphin	yes	no	yes	no	mammals
eagle	no	yes	no	yes	non-mammals

Give Birth	Can Fly	Live in Water	Have Legs	Class
yes	no	yes	no	?

A: attributes

M: mammals

N: non-mammals

$$P(A \mid M) = \frac{6}{7} \times \frac{6}{7} \times \frac{2}{7} \times \frac{2}{7} = 0.06$$

$$P(A \mid N) = \frac{1}{13} \times \frac{10}{13} \times \frac{3}{13} \times \frac{4}{13} = 0.0042$$

$$P(A \mid M)P(M) = 0.06 \times \frac{7}{20} = 0.021$$

$$P(A \mid N)P(N) = 0.004 \times \frac{13}{20} = 0.0027$$

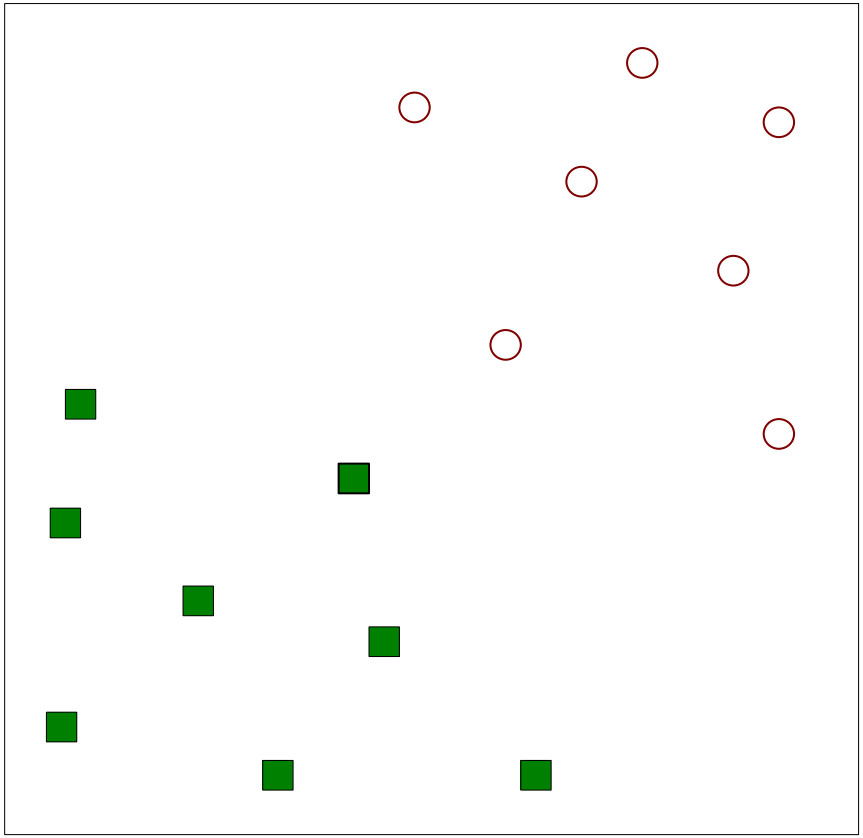
P(A|M)P(M) > P(A|N)P(N)

=> Mammals

Naïve Bayes (Summary)

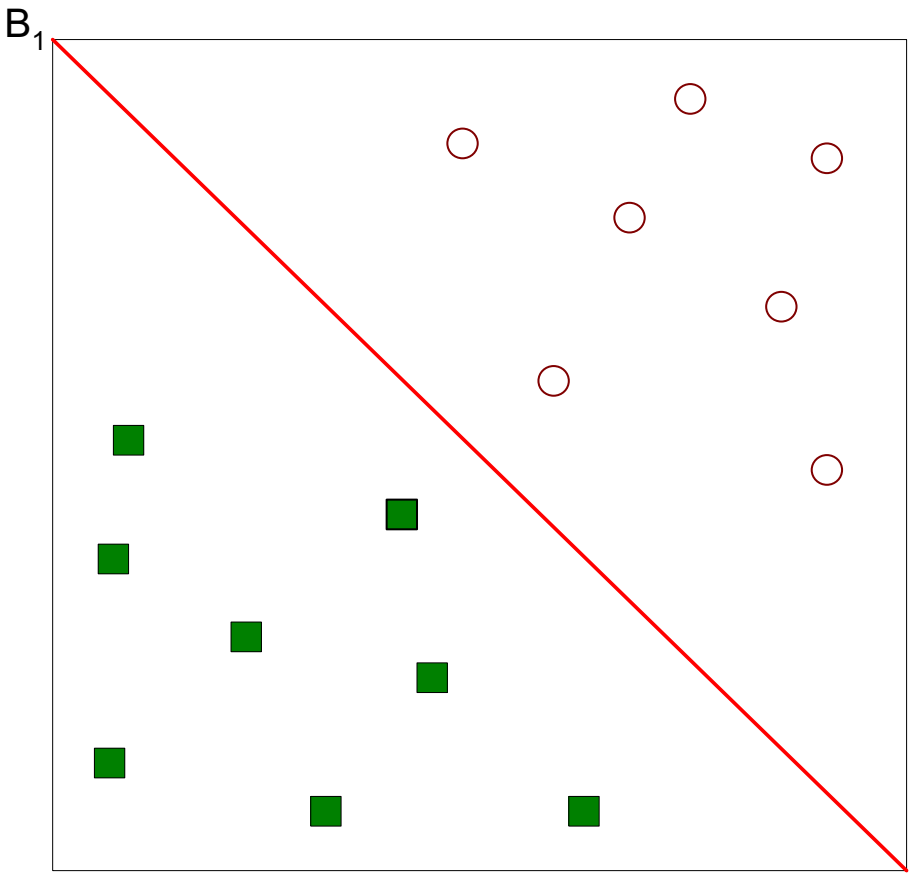
- Robust to isolated noise points
- Handle missing values by ignoring the instance during probability estimate calculations
- Robust to irrelevant attributes
- Independence assumption may not hold for some attributes
  - Use other techniques such as *Bayesian Belief Networks* (BBN)

Support Vector Machines



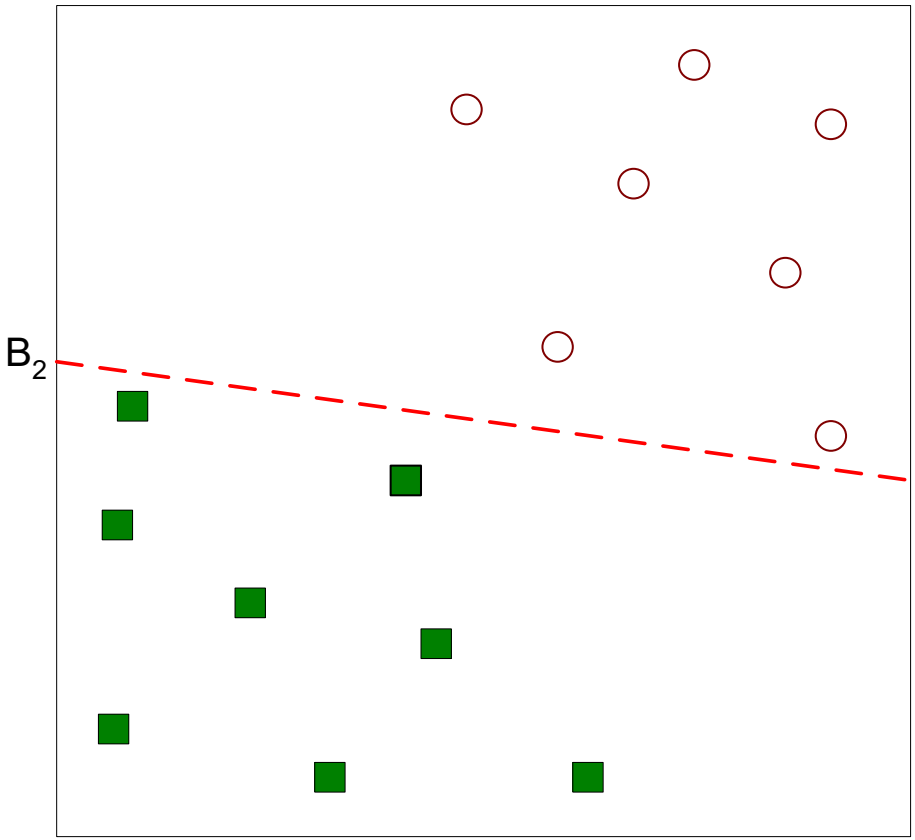
- Find a linear hyperplane (decision boundary) that will separate the data

Support Vector Machines



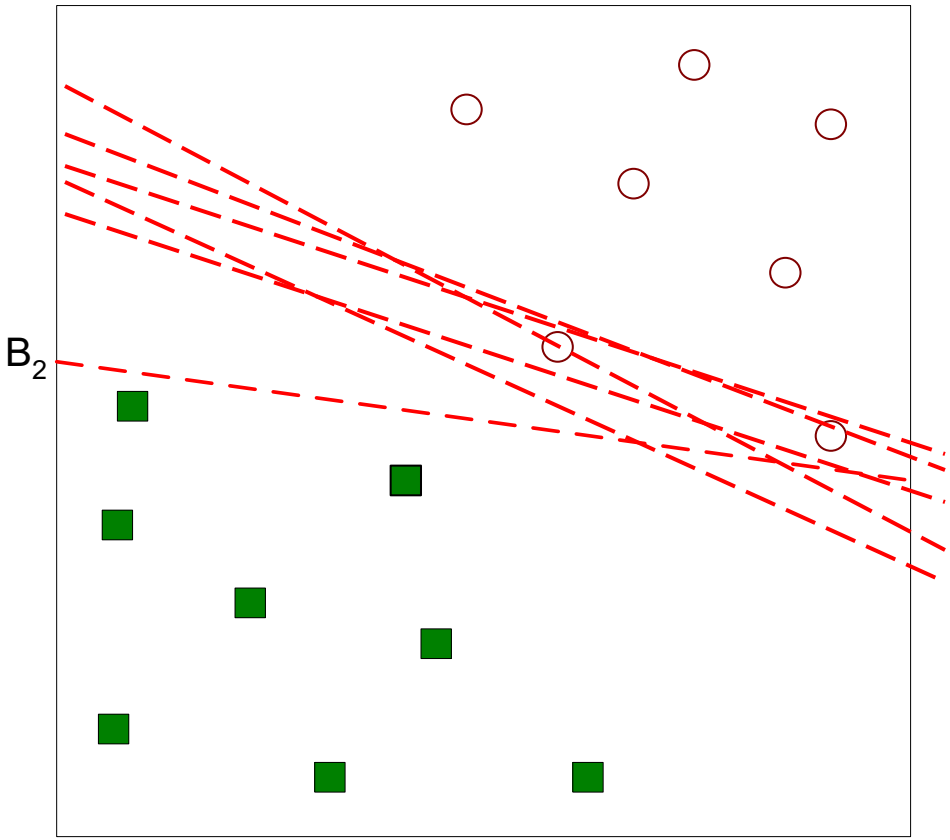
- One Possible Solution

Support Vector Machines



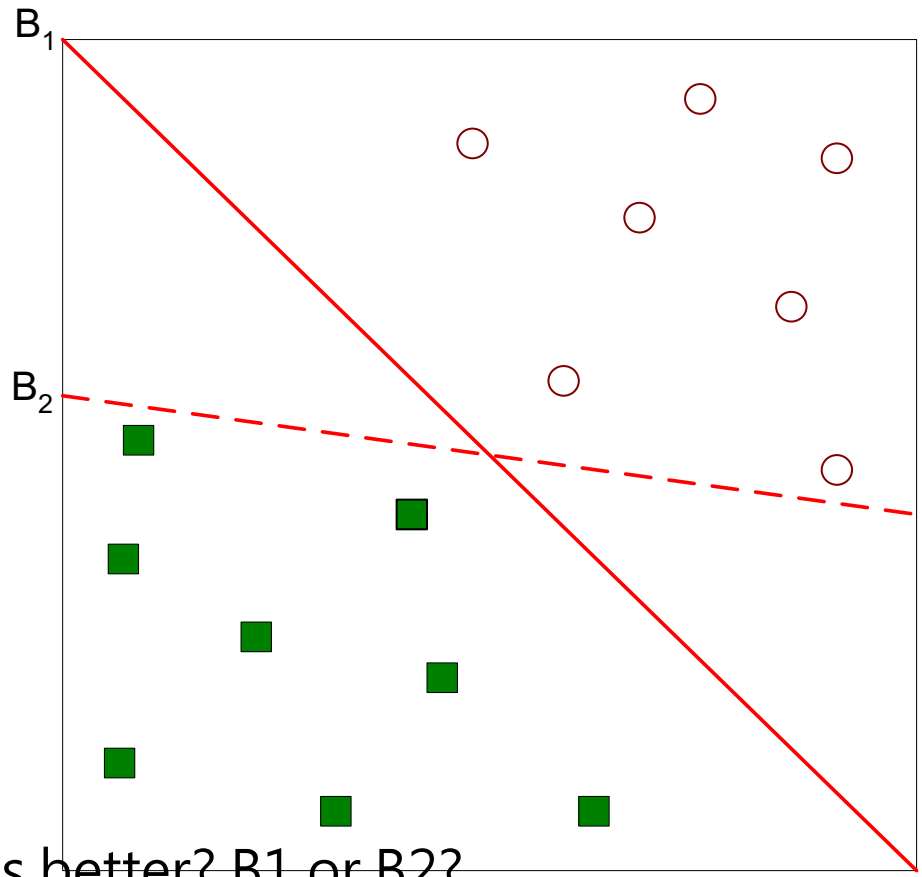
- Another possible solution

Support Vector Machines



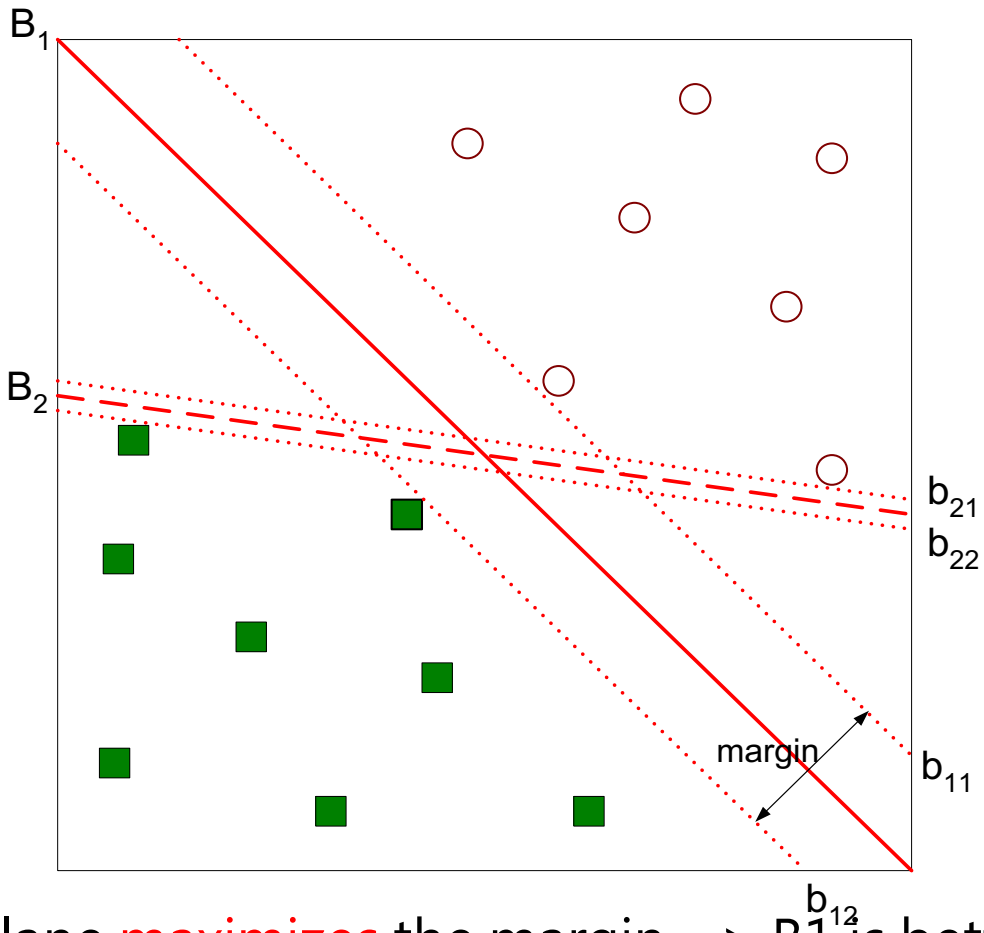
- Other possible solutions

Support Vector Machines



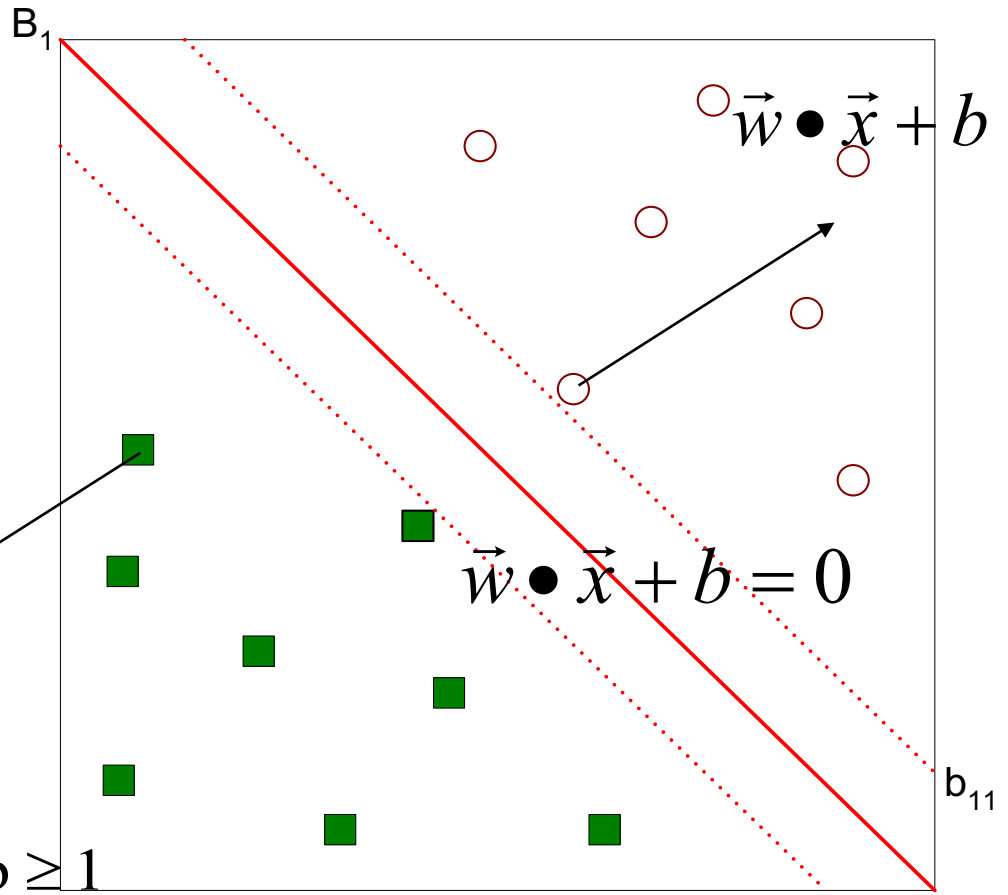
- Which one is better? B1 or B2?
- How do you define better?

Support Vector Machines



- Find hyperplane maximizes the margin => B1 is better than B2

Support Vector Machines



$$\vec{w} \bullet \vec{x} + b = +1$$

$$\vec{w} \bullet \vec{x} + b = -1$$

$$\vec{w} \bullet \vec{x} + b = 0$$

$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x} + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x} + b \leq -1 \end{cases}$$

$$\text{Margin} = \frac{2}{\| \vec{w} \|^2}$$

Support Vector Machines

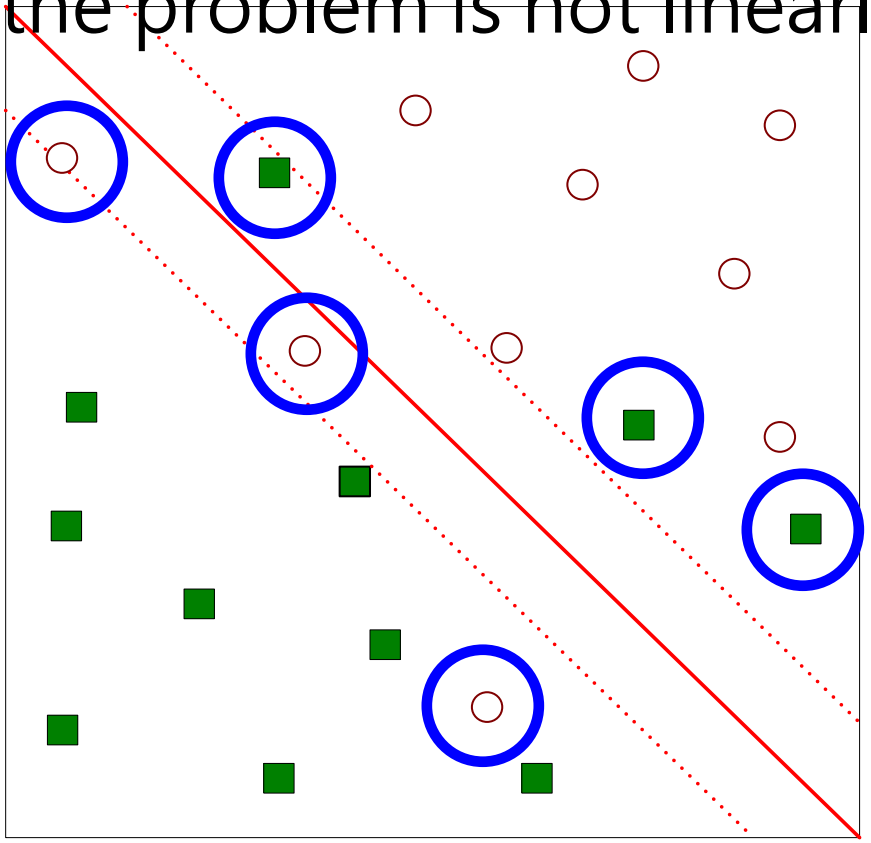
- We want to maximize: $\text{Margin} = \frac{2}{\| \vec{w} \|^2}$
  - Which is equivalent to minimizing: $L(w) = \frac{\| \vec{w} \|^2}{2}$
  - But subjected to the following constraints:

$$f(\vec{x}_i) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x}_i + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x}_i + b \leq -1 \end{cases}$$

    - This is a constrained optimization problem
      - Numerical approaches to solve it (e.g., quadratic programming)

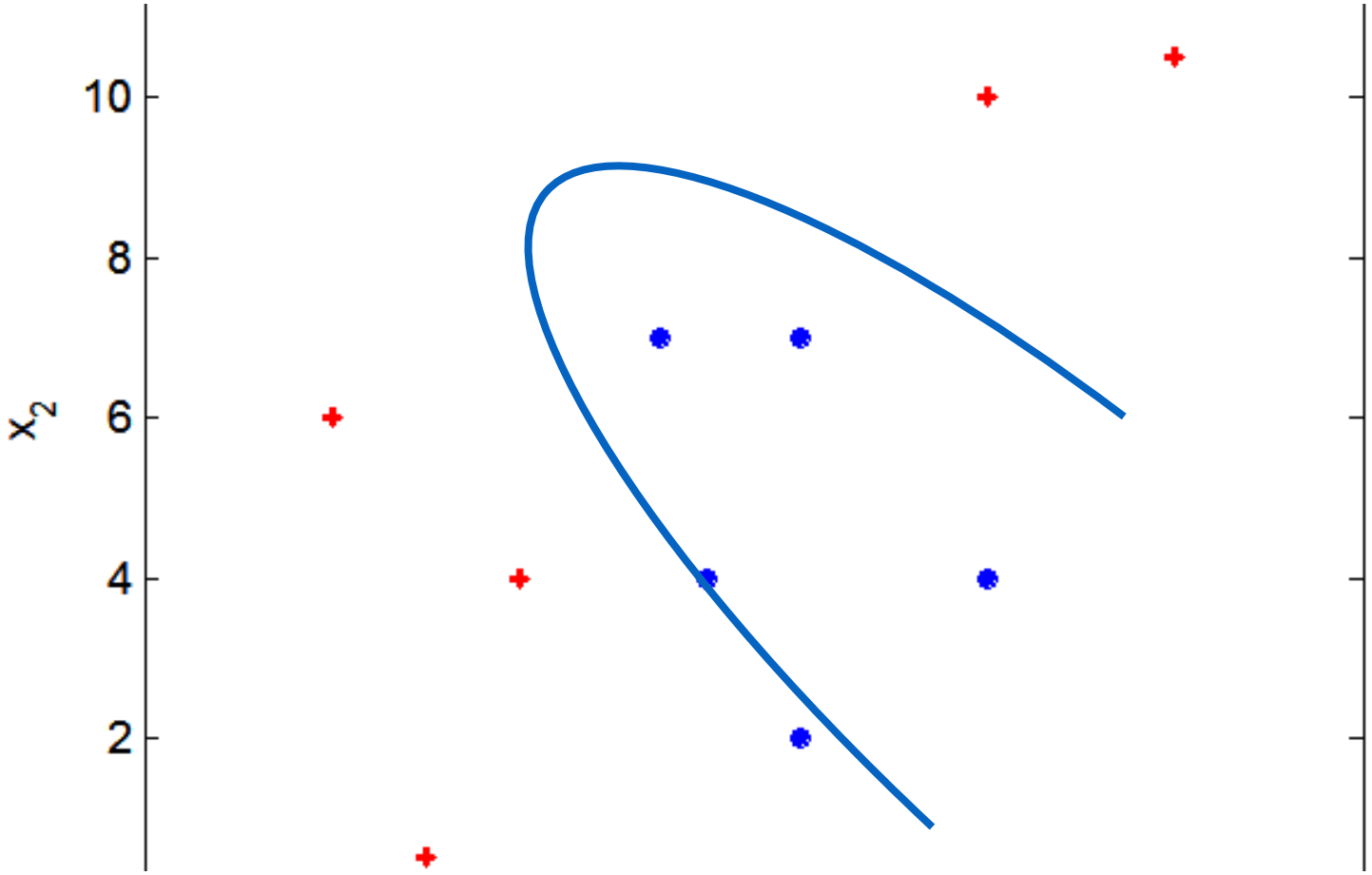
Support Vector Machines

- What if the problem is not linearly separable?



Nonlinear Support Vector Machines

- What if decision boundary is not linear?



Nonlinear Support Vector Machines

- Transform data into higher dimensional space