Supervised Learning

Contents

- **Basic concepts**
- Decision tree induction
- Evaluation of classifiers
- Naïve Bayes classifier
- Support vector machines
- K-nearest neighbor classifier

An example application

- An emergency room in a hospital measures 17 variables (e.g., blood pressure, age, etc) of newly admitted patients.
- A decision is needed: whether to put a new patient in an intensive-care unit.
- Due to the high cost of ICU, those patients who may survive less than a month are given higher priority.
- Problem: to predict high-risk patients and discriminate them from low-risk patients.

Another application

- A credit card company receives thousands of applications for new cards. Each application contains information about an applicant,
  - age
  - Marital status
  - annual salary
  - outstanding debts
  - credit rating
  - etc.
- Problem: to decide whether an application should approved, or to classify applications into two categories, approved and not approved.

Machine learning and our focus

- Like human learning from past experiences.
- A computer does not have “experiences”.
- A computer system learns from data, which represent some “past experiences” of an application domain.
- Our focus: learn a target function that can be used to predict the values of a discrete class attribute, e.g., approve or not-approved, and high-risk or low risk.
- The task is commonly called: Classification (supervised learning)

The data and the goal

- Data: A set of data records (also called examples, instances or cases) described by
  - *k* attributes: A_1, A_2, … A_k.
  - a class: Each example is labelled with a pre-defined class.
- Goal: To learn a classification model from the data that can be used to predict the classes of new (future, or test) cases/instances.

An example: data (loan application)

Approved or not

ID	Age	Has_Job	Own_House	Credit_Rating	Class
1	young	false	false	fair	**No**
2	young	false	false	good	**No**
3	young	true	false	good	**Yes**
4	young	true	true	fair	**Yes**
5	young	false	false	fair	**No**
6	middle	false	false	fair	**No**
7	middle	false	false	good	**No**
8	middle	true	true	good	**Yes**
9	middle	false	true	excellent	**Yes**
10	middle	false	true	excellent	**Yes**
11	old	false	true	excellent	**Yes**
12	old	false	true	good	**Yes**
13	old	true	false	good	**Yes**
14	old	true	false	excellent	**Yes**
15	old	false	false	fair	**No**

An example: the learning task

- Learn a classification model from the data
- Use the model to classify future loan applications into
  - Yes (approved) and
  - No (not approved)
- What is the class for following case/instance?

Age	Has_Job	Own_house	Credit-Rating	Class
young	false	false	good	?

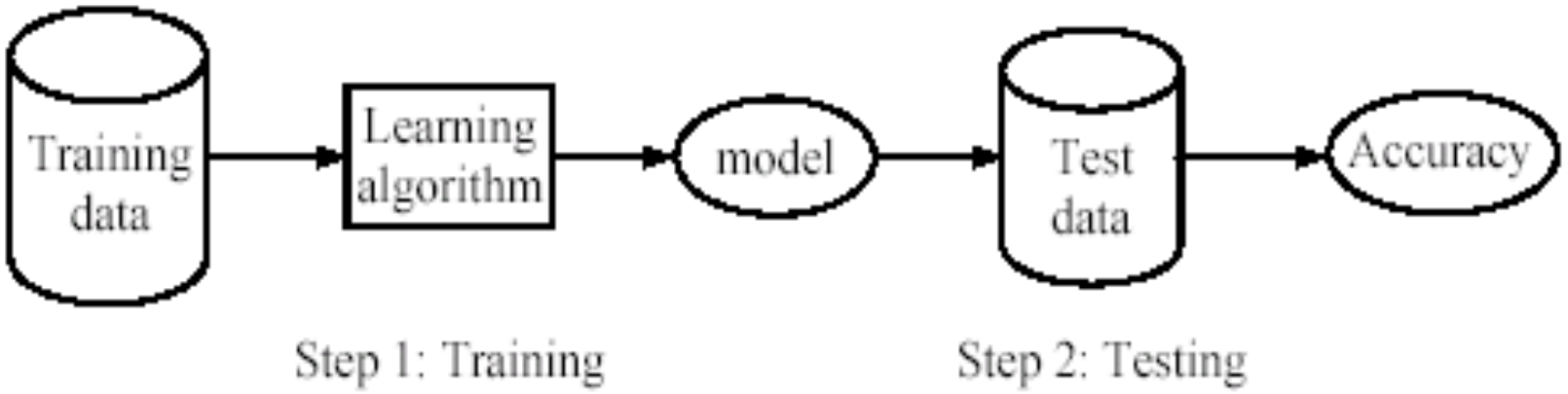
Supervised vs. unsupervised Learning

- Supervised learning: classification is seen as supervised learning from examples.
  - Supervision: The data (observations, measurements, etc.) are labeled with pre-defined classes. It is like that a "teacher" gives the classes (supervision).
  - Test data are classified into these classes too.
- Unsupervised learning (clustering)
  - Class labels of the data are unknown
  - Given a set of data, the task is to establish the existence of classes or clusters in the data

Supervised learning process: two steps

- Learning (training): Learn a model using the training data
- Testing: Test the model using unseen test data to assess the model accuracy

$$Accuracy = \frac{\text{Number of correct classifications}}{\text{Total number of test cases}},$$



What do we mean by learning?

- Given
  - a data set *D*,
  - a task *T*, and
  - a performance measure *M*,

  a computer system is said to **learn** from *D* to perform the task *T* if after learning the system's performance on *T* improves as measured by *M*.
- In other words, the learned model helps the system to perform *T* better as compared to no learning.

An example

- Data: Loan application data
- Task: Predict whether a loan should be approved or not.
- Performance measure: accuracy.

No learning: classify all future applications (test data) to the majority class (i.e., Yes):

Accuracy = 9/15 = 60%.

- We can do better than 60% with learning.

Fundamental assumption of learning

Assumption: The distribution of training examples is identical to the distribution of test examples (including future unseen examples).

- In practice, this assumption is often violated to certain degree.
- Strong violations will clearly result in poor classification accuracy.
- To achieve good accuracy on the test data, training examples must be sufficiently representative of the test data.

Road Map

- Basic concepts
- **Decision tree induction**
- Evaluation of classifiers
- Naïve Bayes
- Support vector machines
- K-nearest neighbor

Introduction

- Decision tree learning is one of the most widely used techniques for classification.
  - Its classification accuracy is competitive with other methods, and
  - it is very efficient.
- The classification model is a tree, called decision tree.
- C4.5 by Ross Quinlan is perhaps the best known system. It can be downloaded from the Web.

The loan data (reproduced)

Approved or not

ID	Age	Has_Job	Own_House	Credit_Rating	Class
1	young	false	false	fair	**No**
2	young	false	false	good	**No**
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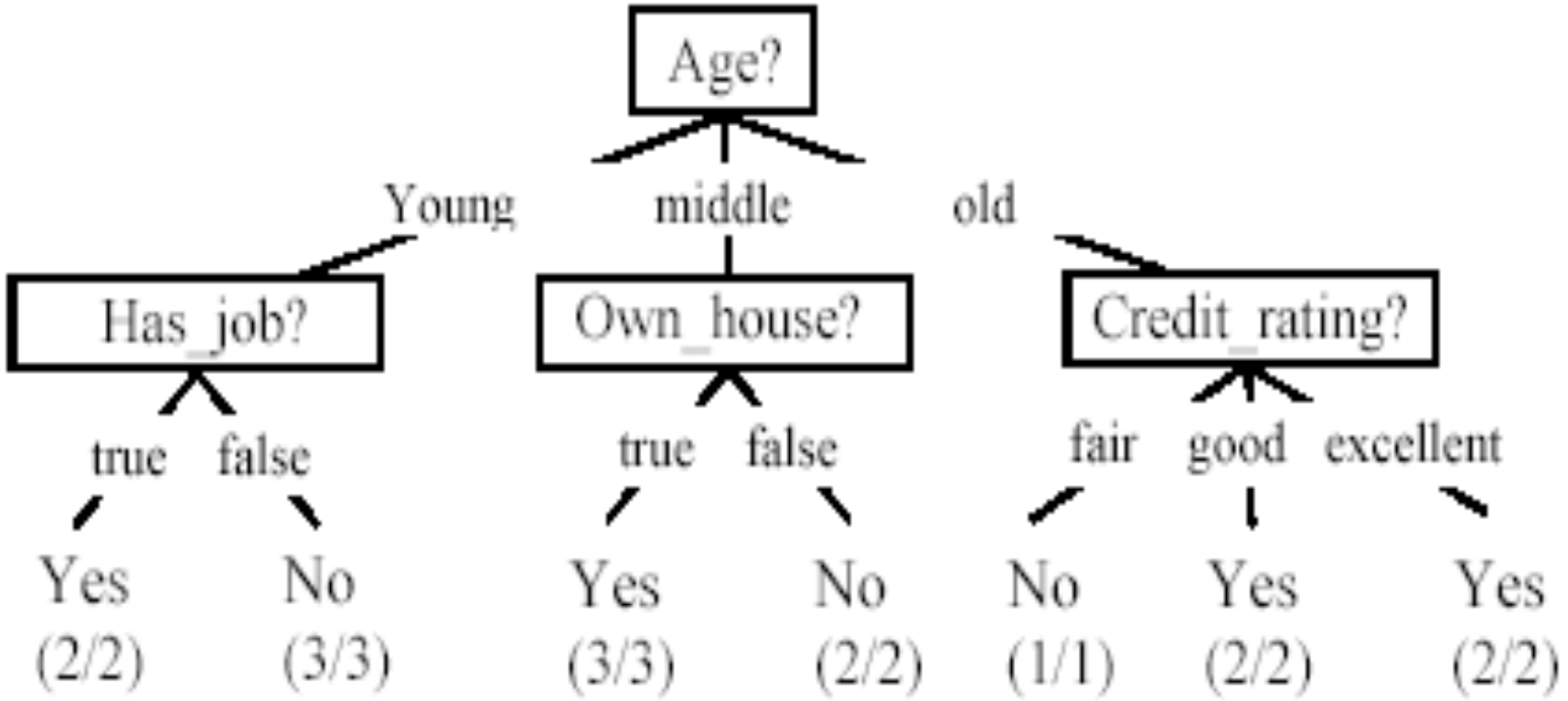
12	old	false	true	good	**Yes**
13	old	true	false	good	**Yes**
14	old	true	false	excellent	**Yes**
15	old	false	false	fair	**No**

A decision tree from the loan data

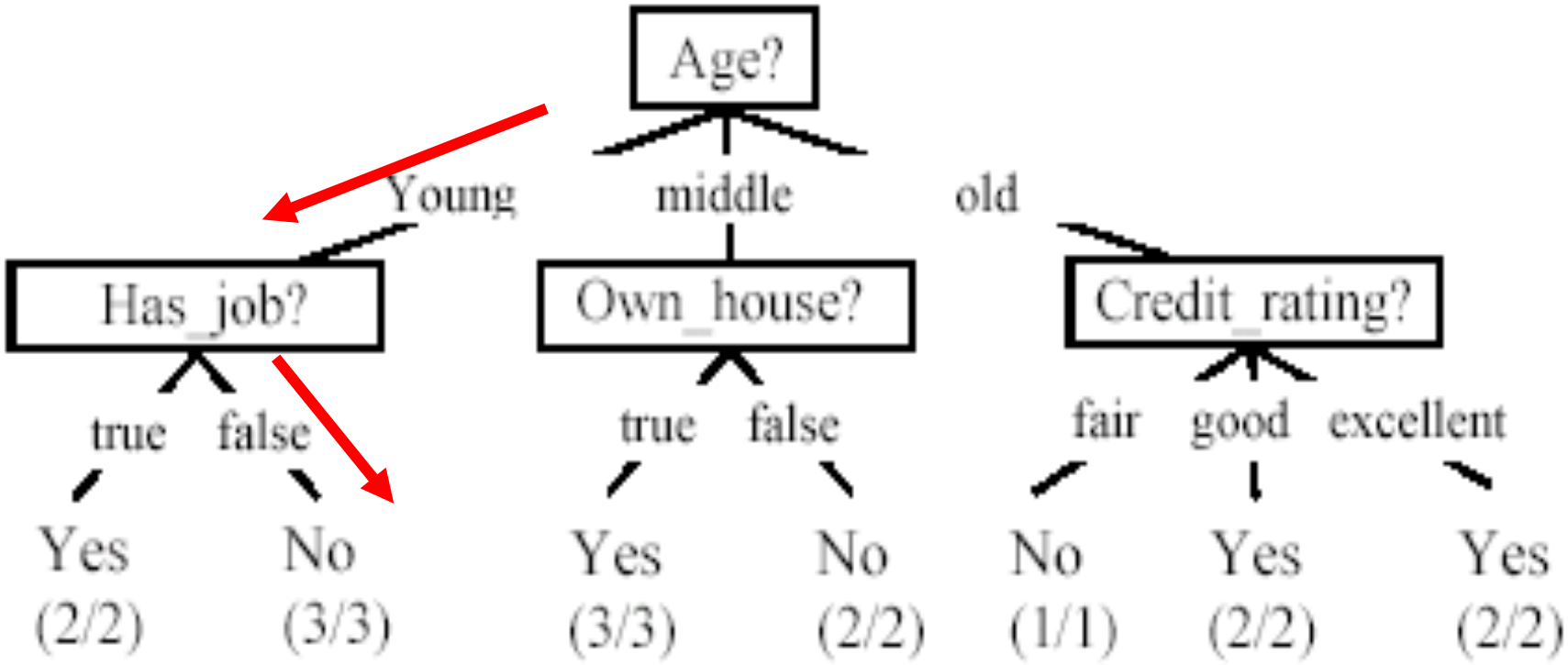
- Decision nodes and leaf nodes (classes)



Use the decision tree

Age	Has_Job	Own_house	Credit-Rating	Class
young	false	false	good	?

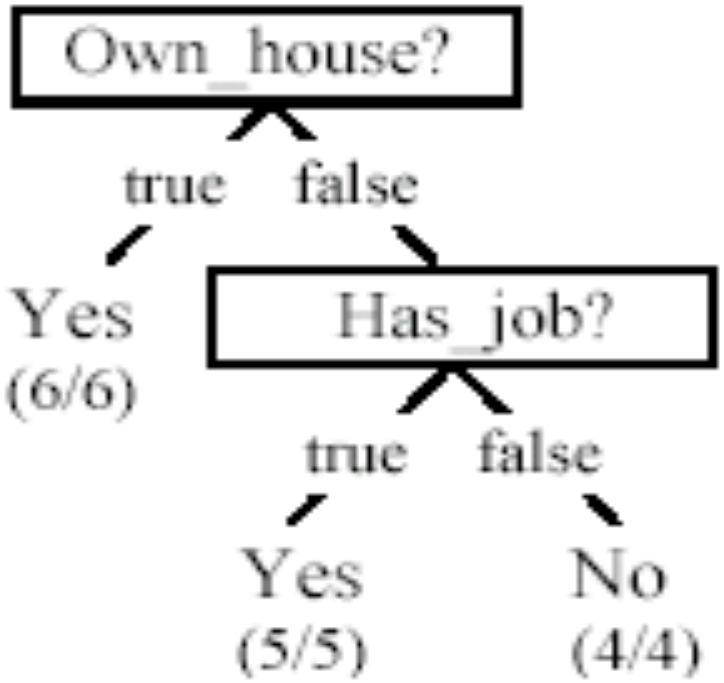
No



Is the decision tree unique?

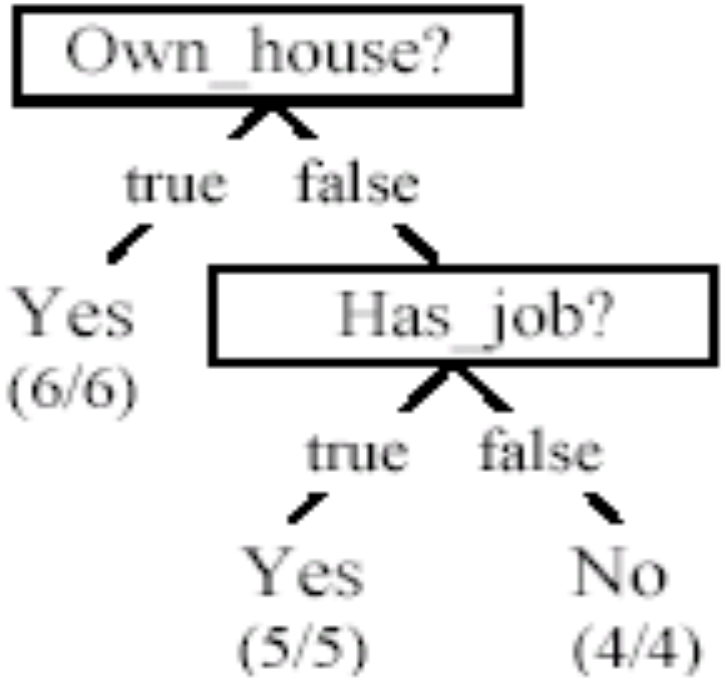
- No. Here is a simpler tree.
- We want smaller tree and accurate tree.
  - Easy to understand and perform better.

- Finding the best tree is NP-hard.
- All current tree building algorithms are heuristic algorithms



From a decision tree to a set of rules

- A decision tree can be converted to a set of rules
- Each path from the root to a leaf is a rule.



Own_house = true → Class =Yes [sup=6/15, conf=6/6]
Own_house = false, Has_job = true → Class = Yes [sup=5/15, conf=5/5]
Own_house = false, Has_job = false → Class = No [sup=4/15, conf=4/4]

Algorithm for decision tree learning

- Basic algorithm (a greedy **divide-and-conquer** algorithm)
  - Assume attributes are categorical now (continuous attributes can be handled too)
  - Tree is constructed in a top-down recursive manner
  - At start, all the training examples are at the root
  - Examples are partitioned recursively based on selected attributes
  - Attributes are selected on the basis of an impurity function (e.g., information gain)
- Conditions for stopping partitioning
  - All examples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority class is the leaf
  - There are no examples left

Decision tree learning algorithm

. **Algorithm** decisionTree(D, A, T)

```
1    if D contains only training examples of the same class c_j ∈ C then
2        make T a leaf node labeled with class c_j;
3    elseif A = ∅ then
4        make T a leaf node labeled with c_j, which is the most frequent class in D
5    else  // D contains examples belonging to a mixture of classes. We select a single
6          // attribute to partition D into subsets so that each subset is purer
7        p_0 = impurityEval-1(D);
8        for each attribute A_i ∈ {A_1, A_2, ..., A_k} do
9            p_i = impurityEval-2(A_i, D)
10       end
11       Select A_g ∈ {A_1, A_2, ..., A_k} that gives the biggest impurity reduction,
             computed using p_0 − p_i;
12       if p_0 − p_g < threshold then     // A_g does not significantly reduce impurity p_0
13         make T a leaf node labeled with c_j, the most frequent class in D.
14       else                              // A_g is able to reduce impurity p_0
15           Make T a decision node on A_g;
16           Let the possible values of A_g be v_1, v_2, ..., v_m. Partition D into m
                 disjoint subsets D_1, D_2, ..., D_m based on the m values of A_g.
17           for each D_j in {D_1, D_2, ..., D_m} do
18               if D_j ≠ ∅ then
19                   create a branch (edge) node T_j for v_j as a child node of T;
20                   decisionTree(D_j, A-{A_g}, T_j)// A_g is removed
21               end
22           end
23       end
24   end
```

Choose an attribute to partition data

- The *key* to building a decision tree - which attribute to choose in order to branch.
- The objective is to reduce impurity or uncertainty in data as much as possible.
  - A subset of data is pure if all instances belong to the same class.
- The *heuristic* in C4.5 is to choose the attribute with the maximum Information Gain or Gain Ratio based on information theory.

The loan data (reproduced)

Approved or not

ID	Age	Has_Job	Own_House	Credit_Rating	Class
1	young	false	false	fair	**No**
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10	middle	false	true	excellent	**Yes**
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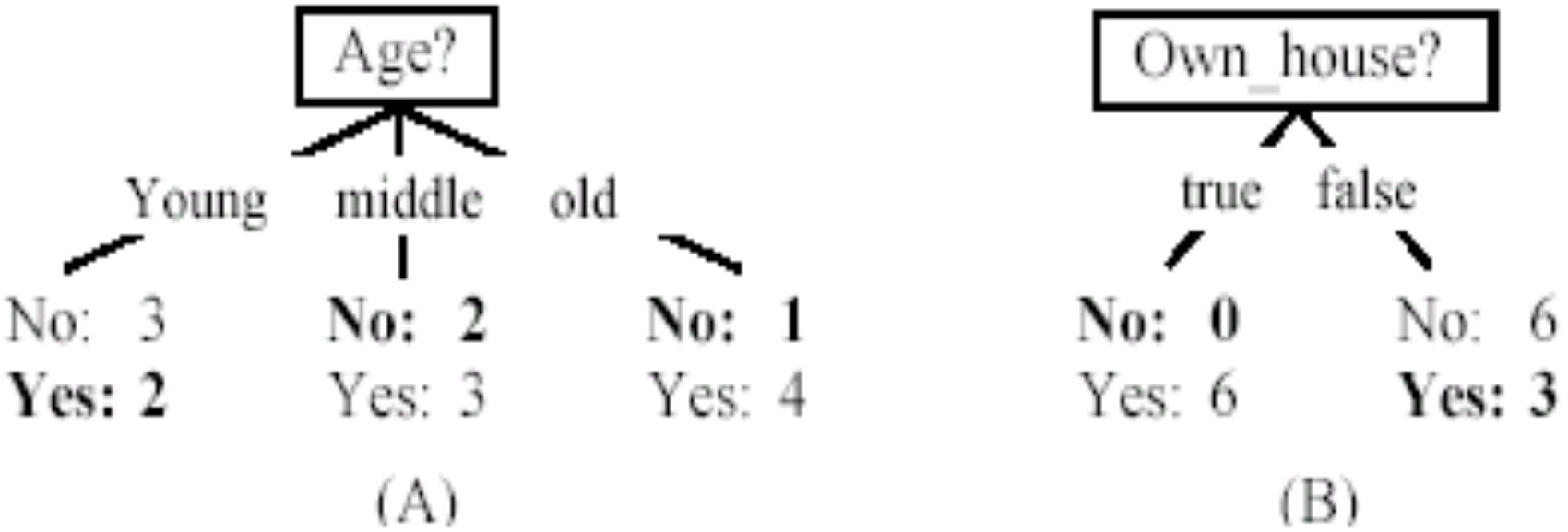
Two possible roots, which is better?



- Fig. (B) seems to be better.

Information theory

- Information theory provides a mathematical basis for measuring the information content.
- To understand the notion of information, think about it as providing the answer to a question, for example, whether a coin will come up heads.
  - If one already has a good guess about the answer, then the actual answer is less informative.
  - If one already knows that the coin is rigged so that it will come with heads with probability 0.99, then a message (advanced information) about the actual outcome of a flip is worth less than it would be for a honest coin (50-50).

Information theory (cont …)

- For a fair (honest) coin, you have no information, and you are willing to pay more (say in terms of $) for advanced information - less you know, the more valuable the information.
- Information theory uses this same intuition, but instead of measuring the value for information in dollars, it measures information contents in **bits**.
- One bit of information is enough to answer a yes/no question about which one has no idea, such as the flip of a fair coin

Information theory: Entropy measure

- The entropy formula,

$$entropy(D) = -\sum_{j=1}^{|C|} \Pr(c_j) \log_2 \Pr(c_j)$$

$$\sum_{j=1}^{|C|} \Pr(c_j) = 1,$$

- $\Pr(c_j)$ is the probability of class c_j in data set D
- We use entropy as a measure of impurity or disorder of data set D. (Or, a measure of information in a tree)

Entropy measure: let us get a feeling

1. The data set D has 50% positive examples ($\Pr(positive) = 0.5$) and 50% negative examples ($\Pr(negative) = 0.5$).

$$entropy(D) = -0.5 \times \log_2 0.5 - 0.5 \times \log_2 0.5 = 1$$

2. The data set D has 20% positive examples ($\Pr(positive) = 0.2$) and 80% negative examples ($\Pr(negative) = 0.8$).

$$entropy(D) = -0.2 \times \log_2 0.2 - 0.8 \times \log_2 0.8 = 0.722$$

3. The data set D has 100% positive examples ($\Pr(positive) = 1$) and no negative examples, ($\Pr(negative) = 0$).

$$entropy(D) = -1 \times \log_2 1 - 0 \times \log_2 0 = 0$$

- As the data become purer and purer, the entropy value becomes smaller and smaller. This is useful to us!

Information gain

- Given a set of examples *D*, we first compute its entropy:

$$entropy(D) = -\sum_{j=1}^{|C|} \Pr(c_j) \log_2 \Pr(c_j)$$

- If we make attribute A_i, with v values, the root of the current tree, this will partition *D* into v subsets D_1, D_2 …, D_v . The expected entropy if A_i is used as the current root:

$$entropy_{A_i}(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times entropy(D_j)$$

Information gain (cont …)

- Information gained by selecting attribute A_i to branch or to partition the data is

$$gain(D, A_i) = entropy(D) - entropy_{A_i}(D)$$

- We choose the attribute with the highest gain to branch/split the current tree.

An example

$$entropy(D) = \frac{6}{15} \times \log_2 \frac{6}{15} + \frac{9}{15} \times \log_2 \frac{9}{15} = 0.971$$

$$entropy_{Own\_house}(D) = \frac{6}{15} \times entropy(D_1) + \frac{9}{15} \times entropy(D_2)$$

$$= \frac{6}{15} \times 0 + \frac{9}{15} \times 0.918$$

$$= 0.551$$

$$entropy_{Age}(D) = \frac{5}{15} \times entropy(D_1) + \frac{5}{15} \times entropy(D_2) + \frac{5}{15} \times entropy(D_3)$$

$$= \frac{5}{15} \times 0.971 + \frac{5}{15} \times 0.971 + \frac{5}{15} \times 0.722$$

$$= 0.888$$

ID	Age	Has_Job	Own_House	Credit_Rating	Class
1	young	false	false	fair	No
2	young	false	false	excellent	No
3	young	true	false	good	Yes
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5	young	false	false	fair	No
6	middle	false	false	fair	No
7	middle	false	false	good	No
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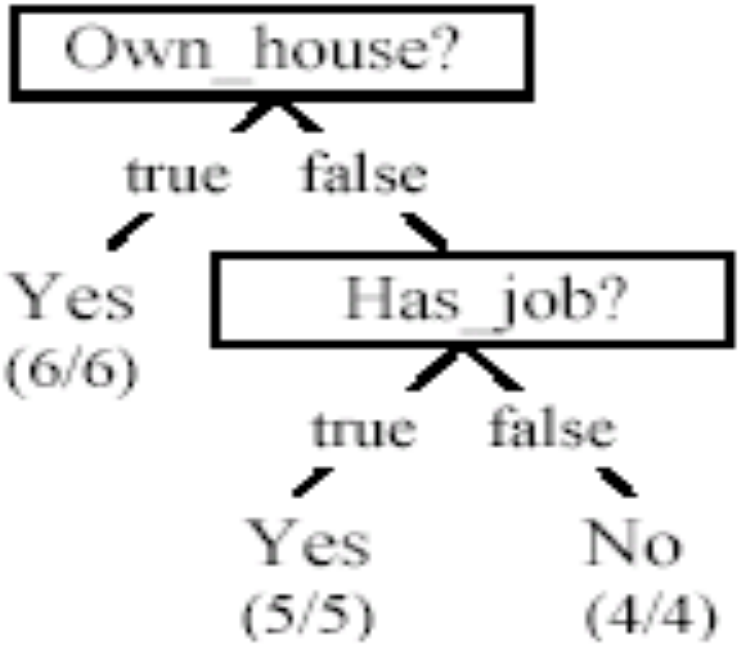
12	old	false	true	good	Yes
13	old	true	false	good	Yes
14	old	true	false	excellent	Yes
15	old	false	false	fair	No

Age	Yes	No	entropy(Di)
young	2	3	0.971
middle	3	2	0.971
old	4	1	0.722

- Own_house is the best choice for the root.

$$gain(D, \text{Age}) = 0.971 - 0.888 = 0.083$$
$$gain(D, \text{Own\_house}) = 0.971 - 0.551 = 0.420$$
$$gain(D, \text{Has\_Job}) = 0.971 - 0.647 = 0.324$$
$$gain(D, \text{Credit\_Rating}) = 0.971 - 0.608 = 0.363$$

We build the final tree

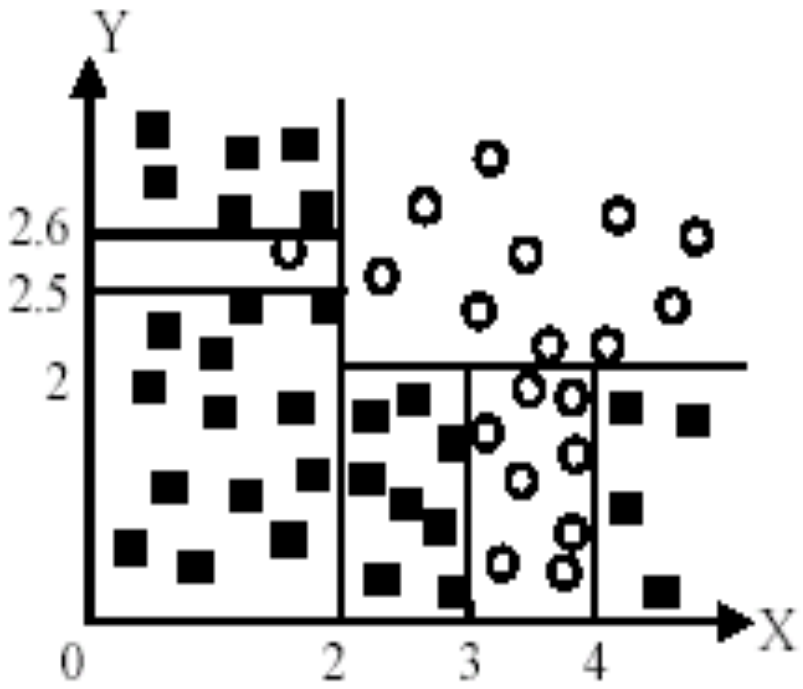


- We can use information gain ratio to evaluate the impurity as well (see the handout)

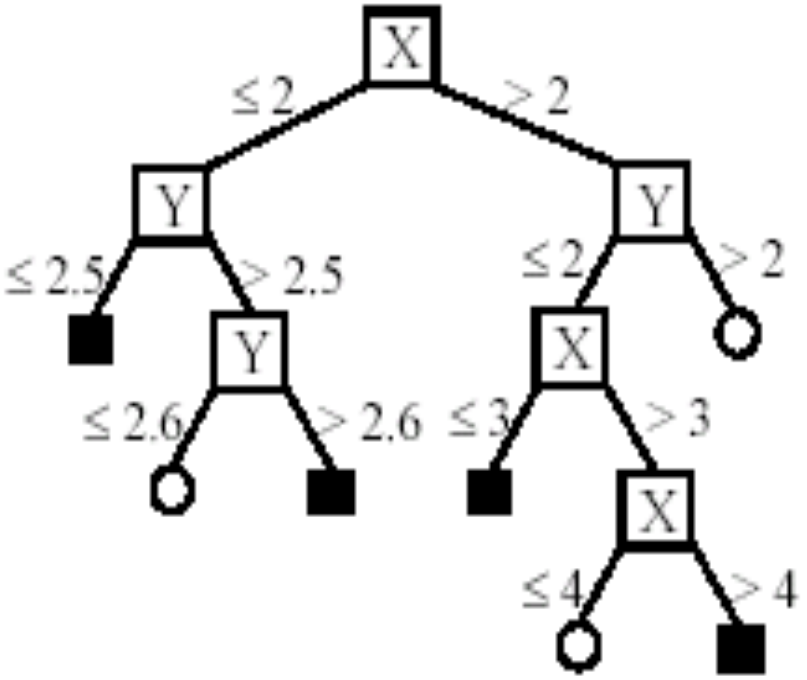
Handling continuous attributes

- Handle continuous attribute by splitting into two intervals (can be more) at each node.
- How to find the best threshold to divide?
  - Use information gain or gain ratio again
  - Sort all the values of an continuous attribute in increasing order $\{v_1, v_2, \ldots, v_r\}$,
  - One possible threshold between two adjacent values v_i and v_{i+1}. Try all possible thresholds and find the one that maximizes the gain (or gain ratio).

An example in a continuous space



(A) A partition of the data space



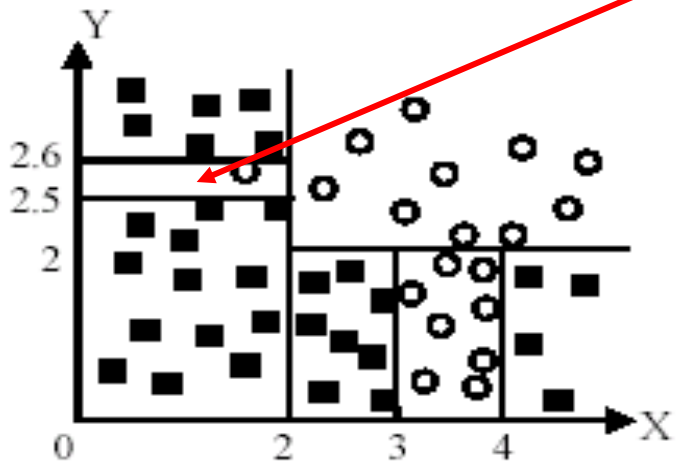
(B). The decision tree

Avoid overfitting in classification

- Overfitting: A tree may overfit the training data
  - Good accuracy on training data but poor on test data
  - Symptoms: tree too deep and too many branches, some may reflect anomalies due to noise or outliers
- Two approaches to avoid overfitting
  - Pre-pruning: Halt tree construction early
    - Difficult to decide because we do not know what may happen subsequently if we keep growing the tree.
  - Post-pruning: Remove branches or sub-trees from a "fully grown" tree.
    - This method is commonly used. C4.5 uses a statistical method to estimates the errors at each node for pruning.
    - A validation set may be used for pruning as well.

An example

Likely to overfit the data



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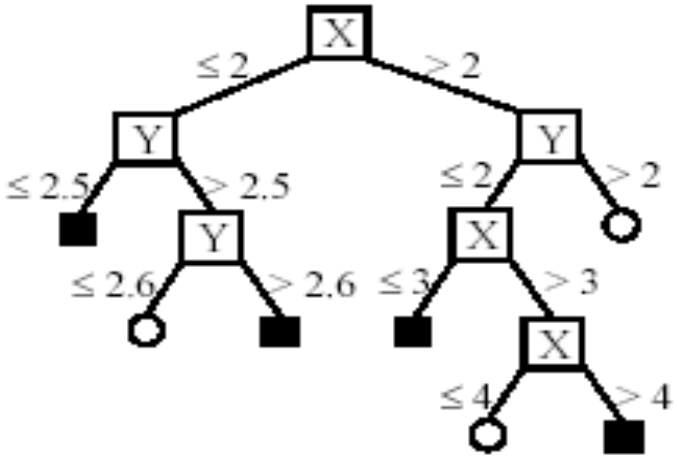
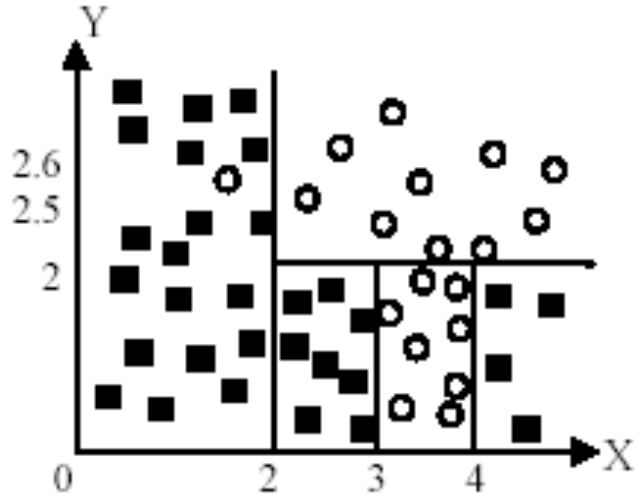
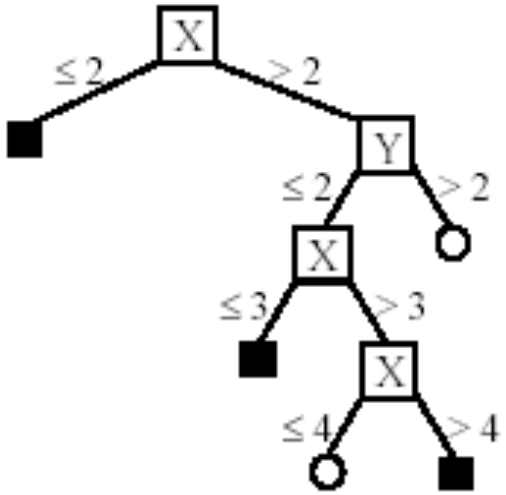


(B). The decision tree





Other issues in decision tree learning

- From tree to rules, and rule pruning
- Handling of miss values
- Handing skewed distributions
- Handling attributes and classes with different costs.
- Attribute construction
- Etc.

Road Map

- Basic concepts
- Decision tree induction
- **Evaluation of classifiers**
- Naïve Bayes classifier
- Support vector machines
- K-nearest neighbor

Evaluating classification methods

- **Predictive accuracy**

$$Accuracy = \frac{\text{Number of correct classifications}}{\text{Total number of test cases}}$$

- Efficiency
  - time to construct the model
  - time to use the model
- Robustness: handling noise and missing values
- Scalability: efficiency in disk-resident databases
- Interpretability:
  - understandable and insight provided by the model
- Compactness of the model: size of the tree, or the number of rules.

Evaluation methods

- **Holdout set**: The available data set *D* is divided into two disjoint subsets,
  - the *training set* D_{train} (for learning a model)
  - the *test set* D_{test} (for testing the model)
- **Important:** training set should not be used in testing and the test set should not be used in learning.
  - Unseen test set provides a unbiased estimate of accuracy.
- The test set is also called the holdout set. (the examples in the original data set *D* are all labeled with classes.)
- This method is mainly used when the data set *D* is large.

Evaluation methods (cont…)

- **n-fold cross-validation**: The available data is partitioned into *n* equal-size disjoint subsets.
- Use each subset as the test set and combine the rest *n*-1 subsets as the training set to learn a classifier.
- The procedure is run *n* times, which give *n* accuracies.
- The final estimated accuracy of learning is the average of the *n* accuracies.
- 10-fold and 5-fold cross-validations are commonly used.
- This method is used when the available data is not large.

Evaluation methods (cont…)

- **Leave-one-out cross-validation**: This method is used when the data set is very small.
- It is a special case of cross-validation
- Each fold of the cross validation has only a single test example and all the rest of the data is used in training.
- If the original data has *m* examples, this is *m*-fold cross-validation

Evaluation methods (cont…)

- **Validation set**: the available data is divided into three subsets,
  - a training set,
  - a validation set and
  - a test set.
- A validation set is used frequently for estimating parameters in learning algorithms.
- In such cases, the values that give the best accuracy on the validation set are used as the final parameter values.
- Cross-validation can be used for parameter estimating as well.

Classification measures

- Accuracy is only one measure (error = 1-accuracy).
- **Accuracy is not suitable in some applications**.
- In text mining, we may only be interested in the documents of a particular topic, which are only a small portion of a big document collection.
- In classification involving skewed or highly imbalanced data, e.g., network intrusion and financial fraud detections, we are interested only in the minority class.
  - High accuracy does not mean any intrusion is detected.
  - E.g., 1% intrusion. Achieve 99% accuracy by doing nothing.
- The class of interest is commonly called the **positive class**, and the rest **negative classes.**

Precision and **recall** measures

- Used in information retrieval and text classification.
- We use a confusion matrix to introduce them.

	Classified Positive	Classified Negative
Actual Positive	TP	FN
Actual Negative	FP	TN

where

TP: the number of correct classifications of the positive examples (**true positive**),

FN: the number of incorrect classifications of positive examples (**false negative**),

FP: the number of incorrect classifications of negative examples (**false positive**), and

TN: the number of correct classifications of negative examples (**true negative**).

Precision and **recall** measures (cont…)

	Classified Positive	Classified Negative
Actual Positive	TP	FN
Actual Negative	FP	TN

$$p = \frac{TP}{TP + FP}. \qquad r = \frac{TP}{TP + FN}.$$

- Precision *p* is the number of correctly classified positive examples divided by the total number of examples that are classified as positive.
- Recall *r* is the number of correctly classified positive examples divided by the total number of actual positive examples in the test set.

An example

	Classified Positive	Classified Negative
Actual Positive	1	99
Actual Negative	0	1000

- This confusion matrix gives
  - precision p = 100% and
  - recall r = 1%

  because we only classified one positive example correctly and no negative examples wrongly.
- Note: precision and recall only measure classification on the positive class.

F_1-value (also called F_1-score)

- It is hard to compare two classifiers using two measures. F_1 score combines precision and recall into one measure

$$F_1 = \frac{2pr}{p + r}$$

F_1-score is the harmonic mean of precision and recall.

$$F_1 = \frac{2}{\frac{1}{p} + \frac{1}{r}}$$

- The harmonic mean of two numbers tends to be closer to the smaller of the two.
- For F_1-value to be large, both *p* and *r* much be large.

Receive operating characteristics curve

- It is commonly called the ROC curve.
- It is a plot of the true positive rate (TPR) against the false positive rate (FPR).
- True positive rate:

$$TPR = \frac{TP}{TP + FN}$$

- False positive rate:

$$FPR = \frac{FP}{TN + FP}$$

Sensitivity and Specificity

- In statistics, there are two other evaluation measures:
  - Sensitivity: Same as TPR
  - Specificity: Also called True Negative Rate (TNR)

$$TNR = \frac{TN}{TN + FP}$$

- Then we have

$$FPR = 1 - specificity$$

Road Map

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Bayesian classification

- Probabilistic view: Supervised learning can naturally be studied from a probabilistic point of view.
- Let A_1 through A_k be attributes with discrete values. The class is C.
- Given a test example *d* with observed attribute values a_1 through a_k.
- Classification is basically to compute the following posteriori probability. The prediction is the class c_j such that

$$\Pr(C = c_j \mid A_1 = a_1, \ldots, A_{|A|} = a_{|A|})$$

is maximal

Apply Bayes' Rule

$$\Pr(C = c_j \mid A_1 = a_1, \ldots, A_{|A|} = a_{|A|})$$

$$= \frac{\Pr(A_1 = a_1, \ldots, A_{|A|} = a_{|A|} \mid C = c_j)\Pr(C = c_j)}{\Pr(A_1 = a_1, \ldots, A_{|A|} = a_{|A|})}$$

$$= \frac{\Pr(A_1 = a_1, \ldots, A_{|A|} = a_{|A|} \mid C = c_j)\Pr(C = c_j)}{\sum_{r=1}^{|C|} \Pr(A_1 = a_1, \ldots, A_{|A|} = a_{|A|} \mid C = c_r)\Pr(C = c_r)}$$

- $\Pr(C=c_j)$ is the class *prior* probability: easy to estimate from the training data.

Computing probabilities

- The denominator $P(A_1=a_1,...,A_k=a_k)$ is irrelevant for decision making since it is the same for every class.
- We only need $P(A_1=a_1,...,A_k=a_k \mid C=c_i)$, which can be written as

  $Pr(A_1=a_1|A_2=a_2,...,A_k=a_k, C=c_j)* Pr(A_2=a_2,...,A_k=a_k |C=c_j)$
- Recursively, the second factor above can be written in the same way, and so on.
- Now an assumption is needed.

Conditional independence assumption

- All attributes are conditionally independent given the class $C = c_j$.
- Formally, we assume,

  $\Pr(A_1=a_1 \mid A_2=a_2, ..., A_{|A|}=a_{|A|}, C=c_j) = \Pr(A_1=a_1 \mid C=c_j)$

  and so on for A_2 through $A_{|A|}$. I.e.,

$$\Pr(A_1 = a_1,..., A_{|A|} = a_{|A|} \mid C = c_i) = \prod_{i=1}^{|A|} \Pr(A_i = a_i \mid C = c_j)$$

Final naïve Bayesian classifier

$$\Pr(C = c_j \mid A_1 = a_1, \ldots, A_{|A|} = a_{|A|})$$

$$= \frac{\Pr(C = c_j) \prod_{i=1}^{|A|} \Pr(A_i = a_i \mid C = c_j)}{\sum_{r=1}^{|C|} \Pr(C = c_r) \prod_{i=1}^{|A|} \Pr(A_i = a_i \mid C = c_r)}$$

- We are done!
- How do we estimate $P(A_i = a_i \mid C = c_j)$? Easy!.

Classify a test instance

- If we only need a decision on the most probable class for the test instance, we only need the numerator as its denominator is the same for every class.
- Thus, given a test example, we compute the following to decide the most probable class for the test instance

$$c = \arg\max_{c_j} \Pr(c_j) \prod_{i=1}^{|A|} \Pr(A_i = a_i \mid C = c_j)$$

An example

- Compute all probabilities required for classification

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

$Pr(C = t) = 1/2$, $Pr(C = f) = 1/2$

$Pr(A=m \mid C=t) = 2/5$
$Pr(A=m \mid C=f) = 1/5$
$Pr(B=b \mid C=t) = 1/5$
$Pr(B=b \mid C=f) = 2/5$

$Pr(A=g \mid C=t) = 2/5$
$Pr(A=g \mid C=f) = 2/5$
$Pr(B=s \mid C=t) = 2/5$
$Pr(B=s \mid C=f) = 1/5$

$Pr(A=h \mid C=t) = 1/5$
$Pr(A=h \mid C=n) = 2/5$
$Pr(B=q \mid C=t) = 2/5$
$Pr(B=q \mid C=f) = 2/5$

Now we have a test example:

$A = m \quad B = q \quad C = ?$

An Example (cont …)

- For C = t, we have

$$\Pr(C=t)\prod_{j=1}^{2}\Pr(A_j=a_j\,|\,C=t)=\frac{1}{2}\times\frac{2}{5}\times\frac{2}{5}=\frac{2}{25}$$

- For class C = f, we have

$$\Pr(C=f)\prod_{j=1}^{2}\Pr(A_j=a_j\,|\,C=f)=\frac{1}{2}\times\frac{1}{5}\times\frac{2}{5}=\frac{1}{25}$$

- C = t is more probable. t is the final class.

On naïve Bayesian classifier

- Advantages:
  - Easy to implement
  - Very efficient
  - Good results obtained in many applications
- Disadvantages
  - Assumption: class conditional independence, therefore loss of accuracy when the assumption is seriously violated (those highly correlated data sets)

Road Map

- Basic concepts
- Decision tree induction
- Evaluation of classifiers
- Naïve Bayesian classification
- **Support vector machines**
- K-nearest neighbor

Introduction

- Support vector machines were invented by V. Vapnik and his co-workers in 1970s in Russia and became known to the West in 1992.
- SVMs are linear classifiers that find a hyperplane to separate two class of data, positive and negative.
- Kernel functions are used for nonlinear separation.
- SVM not only has a rigorous theoretical foundation, but also performs classification more accurately than most other methods in applications, especially for high dimensional data.
- It is perhaps the best classifier for text classification.

Basic concepts

- Let the set of training examples D be

  $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_r, y_r)\}$,

  where $\mathbf{x}_i = (x_1, x_2, \ldots, x_n)$ is an **input vector** in a real-valued space $X \subseteq R^n$ and y_i is its **class label** (output value), $y_i \in \{1, -1\}$.

  1: positive class and -1: negative class.
- SVM finds a linear function of the form (**w**: weight vector)

$$f(\mathbf{x}) = \langle \mathbf{w} \cdot \mathbf{x} \rangle + b$$

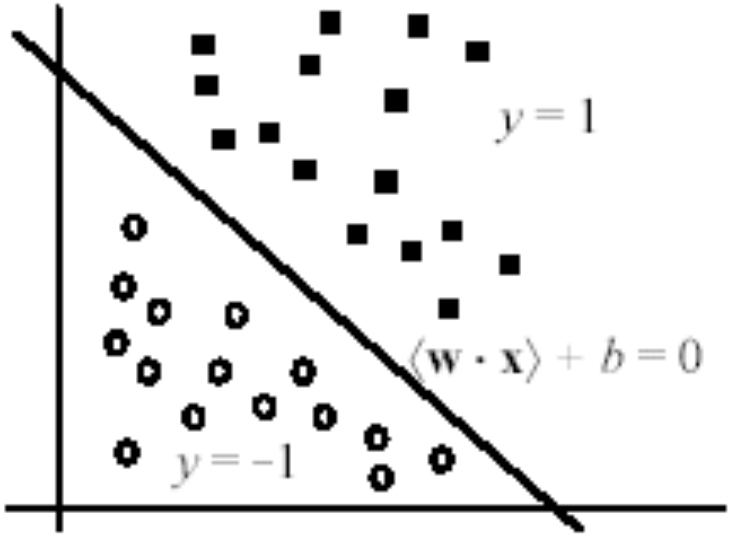
$$y_i = \begin{cases} 1 & if \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 0 \\ -1 & if \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b < 0 \end{cases}$$

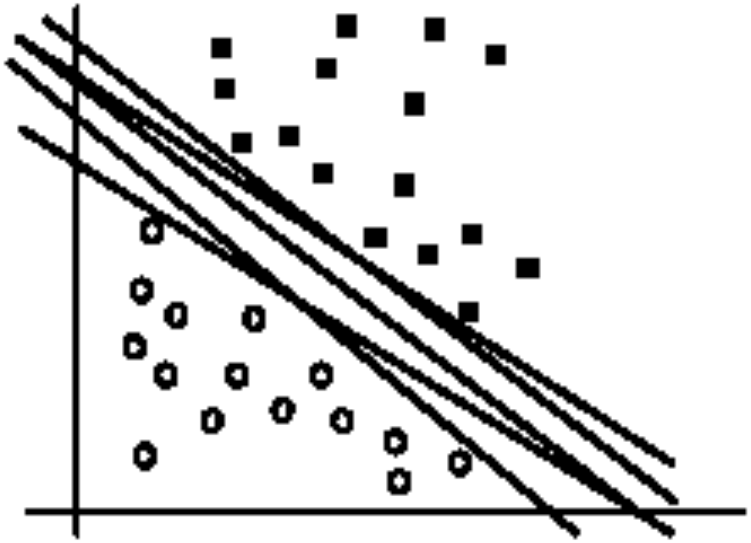
The hyperplane

- The hyperplane that separates positive and negative training data is

$$\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$$

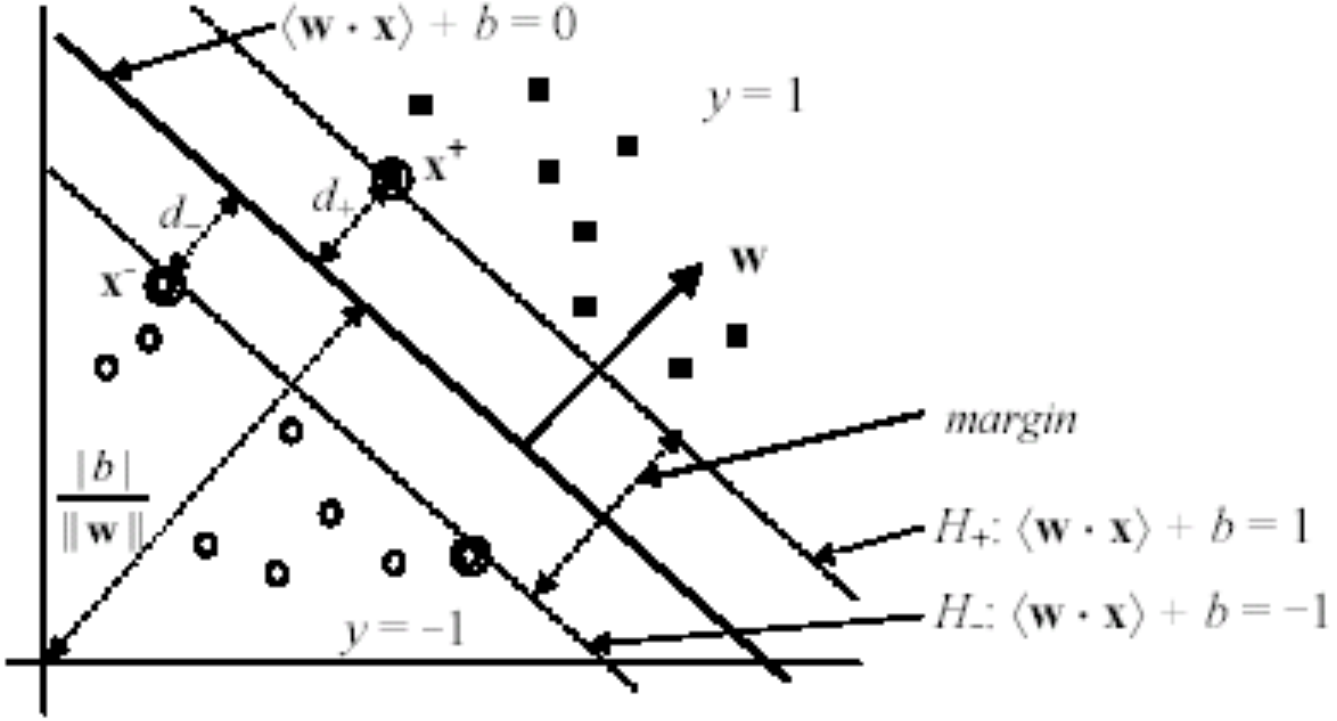
- It is also called the decision boundary (surface).
- So many possible hyperplanes, which one to choose?





Maximal margin hyperplane

- SVM looks for the separating hyperplane with the largest margin.
- Machine learning theory says this hyperplane minimizes the error bound



Linear SVM: separable case

- Assume the data are linearly separable.
- Consider a positive data point ($\mathbf{x}^+$, 1) and a negative ($\mathbf{x}^-$, -1) that are closest to the hyperplane

  $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$.
- We define two parallel hyperplanes, H_+ and H_-, that pass through $\mathbf{x}^+$ and $\mathbf{x}^-$ respectively. H_+ and H_- are also parallel to $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$.

$$H_+: \quad \langle \mathbf{w} \cdot \mathbf{x}^+ \rangle + b = 1$$

$$H_-: \quad \langle \mathbf{w} \cdot \mathbf{x}^- \rangle + b = -1$$

$$\text{such that} \quad \begin{cases} \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 1 & \text{if } y_i = 1 \\ \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \leq -1 & \text{if } y_i = -1, \end{cases}$$

Compute the margin

- Now let us compute the distance between the two margin hyperplanes H_+ and H_-. Their distance is the **margin** ($d_+ + d_-$ in the figure).
- Recall from vector space in algebra that the (perpendicular) **distance** from a point $\mathbf{x}_i$ to the hyperplane $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$ is:

$$\frac{|\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b|}{\|\mathbf{w}\|} \tag{36}$$

where $\|\mathbf{w}\|$ is the norm of $\mathbf{w}$,

$$\|\mathbf{w}\| = \sqrt{<\mathbf{w} \cdot \mathbf{w}>} = \sqrt{w_1^2 + w_2^2 + \ldots + w_n^2} \tag{37}$$

Compute the margin (cont …)

- Let us compute d_+.
- Instead of computing the distance from $\mathbf{x}^+$ to the separating hyperplane $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$, we pick up any point $\mathbf{x}_s$ on $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$ and compute the distance from $\mathbf{x}_s$ to $\langle \mathbf{w} \cdot \mathbf{x}^+ \rangle + b = 1$ by applying the distance Eq. (36) and noticing $\langle \mathbf{w} \cdot \mathbf{x}_s \rangle + b = 0$,

$$d_+ = \frac{|\langle \mathbf{w} \cdot \mathbf{x}_s \rangle + b - 1|}{\| \mathbf{w} \|} = \frac{1}{\| \mathbf{w} \|} \tag{38}$$

$$margin = d_+ + d_- = \frac{2}{\| \mathbf{w} \|} \tag{39}$$

An optimization problem!

Definition (Linear SVM: separable case): Given a set of linearly separable training examples,

$$D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_r, y_r)\}$$

Learning is to solve the following constrained minimization problem,

$$\text{Minimize}: \quad \frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} \tag{40}$$

$$\text{Subject to}: \quad y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1, \quad i = 1, 2, \ldots, r$$

$y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 1, \quad i = 1, 2, \ldots, r$ summarizes

$\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 1$ for $y_i = 1$

$\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \leq -1$ for $y_i = -1$.

Solve the constrained minimization

- Standard Lagrangian method

$$L_P = \frac{1}{2}\langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_i [y_i (\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) - 1] \qquad (41)$$

  where $\alpha_i \geq 0$ are the **Lagrange multipliers**.
- Optimization theory says that an optimal solution to (41) must satisfy certain conditions, called **Kuhn-Tucker conditions**, which are necessary (but not sufficient)
- Kuhn-Tucker conditions play a central role in constrained optimization.

How to deal with nonlinear separation?

- The SVM formulations require linear separation.
- Real-life data sets may need nonlinear separation.
- To deal with nonlinear separation, the same formulation and techniques as for the linear case are still used.
- We only transform the input data into another space (usually of a much higher dimension) so that
  - a linear decision boundary can separate positive and negative examples in the transformed space,
- The transformed space is called the **feature space**. The original data space is called the **input space**.

Space transformation

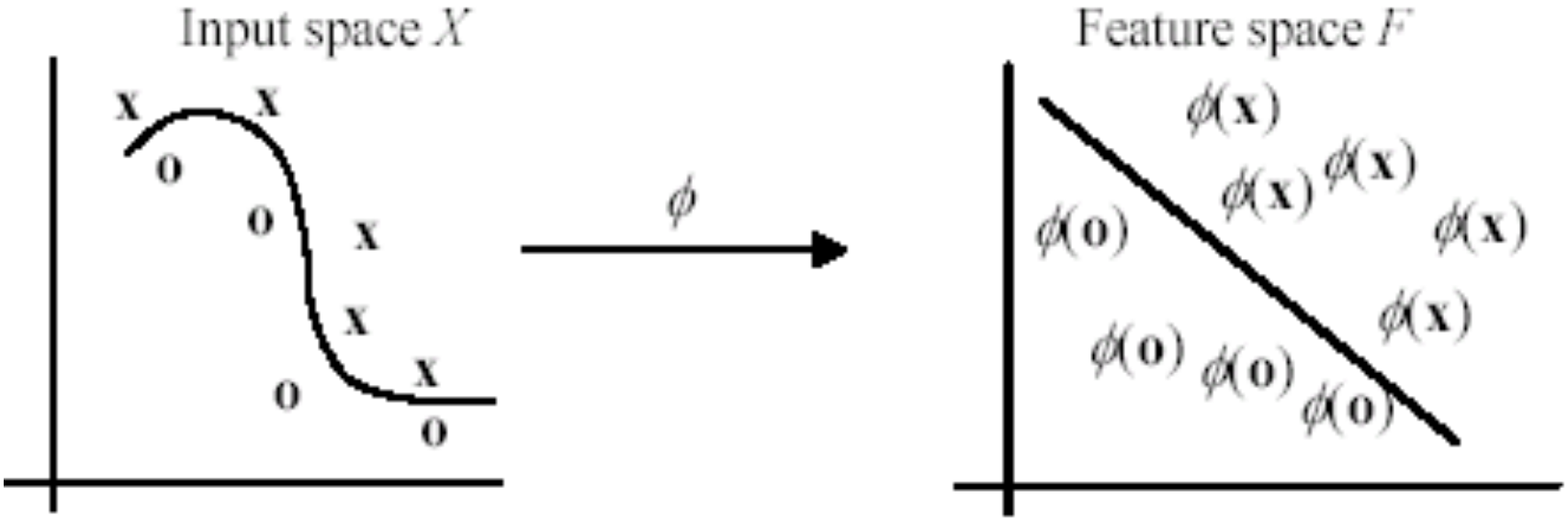
- The basic idea is to map the data in the input space X to a feature space F via a nonlinear mapping ϕ,

$$\begin{aligned} \phi &: X \to F \\ \mathbf{x} &\mapsto \phi(\mathbf{x}) \end{aligned} \tag{76}$$

- After the mapping, the original training data set $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_r, y_r)\}$ becomes:

$$\{(\phi(\mathbf{x}_1), y_1), (\phi(\mathbf{x}_2), y_2), \ldots, (\phi(\mathbf{x}_r), y_r)\} \tag{77}$$

Geometric interpretation



- In this example, the transformed space is also 2-D. But usually, the number of dimensions in the feature space is much higher than that in the input space

Optimization problem in (61) becomes

With the transformation, the optimization problem in (61) becomes

$$\text{Minimize: } \frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} + C\sum_{i=1}^{r} \xi_i \tag{78}$$

$$\text{Subject to: } y_i(\langle \mathbf{w} \cdot \phi(\mathbf{x}_i) \rangle + b) \geq 1 - \xi_i, \quad i = 1, 2, ..., r$$

$$\xi_i \geq 0, \quad i = 1, 2, ..., r$$

The dual is

$$\text{Maximize: } L_D = \sum_{i=1}^{r} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{r} y_i y_j \alpha_i \alpha_j \langle \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) \rangle. \tag{79}$$

$$\text{Subject to: } \sum_{i=1}^{r} y_i \alpha_i = 0$$

$$0 \leq \alpha_i \leq C, \quad i = 1, 2, ..., r.$$

The final decision rule for classification (testing) is

$$\sum_{i=1}^{r} y_i \alpha_i \langle \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}) \rangle + b \tag{80}$$

An example space transformation

- Suppose our input space is 2-dimensional, and we choose the following transformation (mapping) from 2-D to 3-D:

$$(x_1, x_2) \mapsto ({x_1}^2, {x_2}^2, \sqrt{2}x_1x_2)$$

- The training example ((2, 3), -1) in the input space is transformed to the following in the feature space:

  ((4, 9, 8.5), -1)

Problem with explicit transformation

- The potential problem with this explicit data transformation and then applying the linear SVM is that it may suffer from the curse of dimensionality.
- The number of dimensions in the feature space can be huge with some useful transformations even with reasonable numbers of attributes in the input space.
- This makes it computationally infeasible to handle.
- Fortunately, explicit transformation is not needed.

Kernel functions

- We notice that in the dual formulation both
  - the construction of the optimal hyperplane (79) in *F* and
  - the evaluation of the corresponding decision function (80)

  only require dot products $\langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle$ and never the mapped vector $\phi(\mathbf{x})$ in its explicit form. This is a crucial point.
- Thus, if we have a way to compute the dot product $\langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle$ using the input vectors **x** and **z** directly,
  - no need to know the feature vector $\phi(\mathbf{x})$ or even ϕ itself.
- In SVM, this is done through the use of **kernel functions**, denoted by *K*,

$$K(\mathbf{x}, \mathbf{z}) = \langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle \quad (82)$$

An example kernel function

- Polynomial kernel

$$K(\mathbf{x}, \mathbf{z}) = \langle \mathbf{x} \cdot \mathbf{z} \rangle^d \tag{83}$$

- Let us compute the kernel with degree $d = 2$ in a 2-dimensional space: $\mathbf{x} = (x_1, x_2)$ and $\mathbf{z} = (z_1, z_2)$.

$$\begin{aligned}
\langle \mathbf{x} \cdot \mathbf{z} \rangle^2 &= (x_1 z_1 + x_2 z_2)^2 \\
&= {x_1}^2 {z_1}^2 + 2 x_1 z_1 x_2 z_2 + {x_2}^2 {z_2}^2 \\
&= \langle ({x_1}^2, {x_2}^2, \sqrt{2} x_1 x_2) \cdot ({z_1}^2, {z_2}^2, \sqrt{2} z_1 z_2) \rangle \\
&= \langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle,
\end{aligned} \tag{84}$$

- This shows that the kernel $\langle \mathbf{x} \cdot \mathbf{z} \rangle^2$ is a dot product in a transformed feature space

Kernel trick

- The derivation in (84) is only for illustration purposes.
- We do not need to find the mapping function.
- We can simply apply the kernel function directly by
  - replace all the dot products $\langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle$ in (79) and (80) with the kernel function $K(\mathbf{x}, \mathbf{z})$ (e.g., the polynomial kernel $\langle \mathbf{x} \cdot \mathbf{z} \rangle^d$ in (83)).
- This strategy is called the **kernel trick**.

Is it a kernel function?

- The question is: how do we know whether a function is a kernel without performing the derivation such as that in (84)? I.e,
  - How do we know that a kernel function is indeed a dot product in some feature space?
- This question is answered by a theorem called the Mercer's theorem, which we will not discuss here.

Commonly used kernels

- It is clear that the idea of kernel generalizes the dot product in the input space. This dot product is also a kernel with the feature map being the identity

$$K(\mathbf{x}, \mathbf{z}) = \langle \mathbf{x} \cdot \mathbf{z} \rangle. \tag{85}$$

Commonly used kernels include

$$\text{Polynomial:} \quad K(\mathbf{x}, \mathbf{z}) = (\langle \mathbf{x} \cdot \mathbf{z} \rangle + \theta)^d \tag{86}$$

$$\text{Gaussian RBF:} \quad K(\mathbf{x}, \mathbf{z}) = e^{-\|\mathbf{x}-\mathbf{z}\|^2 / 2\sigma} \tag{87}$$

$$\text{Sigmoidal:} \quad K(\mathbf{x}, \mathbf{z}) = \tanh(k\langle \mathbf{x} \cdot \mathbf{z} \rangle - \delta) \tag{88}$$

where $\theta \in R$, $d \in N$, $\sigma > 0$, and $k, \delta \in R$.

Some other issues in SVM

- SVM works only in a real-valued space. For a categorical attribute, we need to convert its categorical values to numeric values.
- SVM does only two-class classification. For multi-class problems, some strategies can be applied, e.g., one-against-rest, and error-correcting output coding.
- The hyperplane produced by SVM is hard to understand by human users. The matter is made worse by kernels. Thus, SVM is commonly used in applications that do not required human understanding.

Road Map

- Basic concepts
- Decision tree induction
- Evaluation of classifiers
- Naïve Bayesian classification
- Support vector machines
- **K-nearest neighbor**

k-Nearest Neighbor Classification (kNN)

- Unlike all the previous learning methods, kNN does not build model from the training data.
- To classify a test instance *d*, define *k*-neighborhood *P* as *k* nearest neighbors of *d*
- Count number *n* of training instances in *P* that belong to class c_j
- Estimate Pr(c_j|*d*) as *n*/*k*
- No training is needed. Classification time is linear in training set size for each test case.

kNN Algorithm

Algorithm kNN(D, d, k)

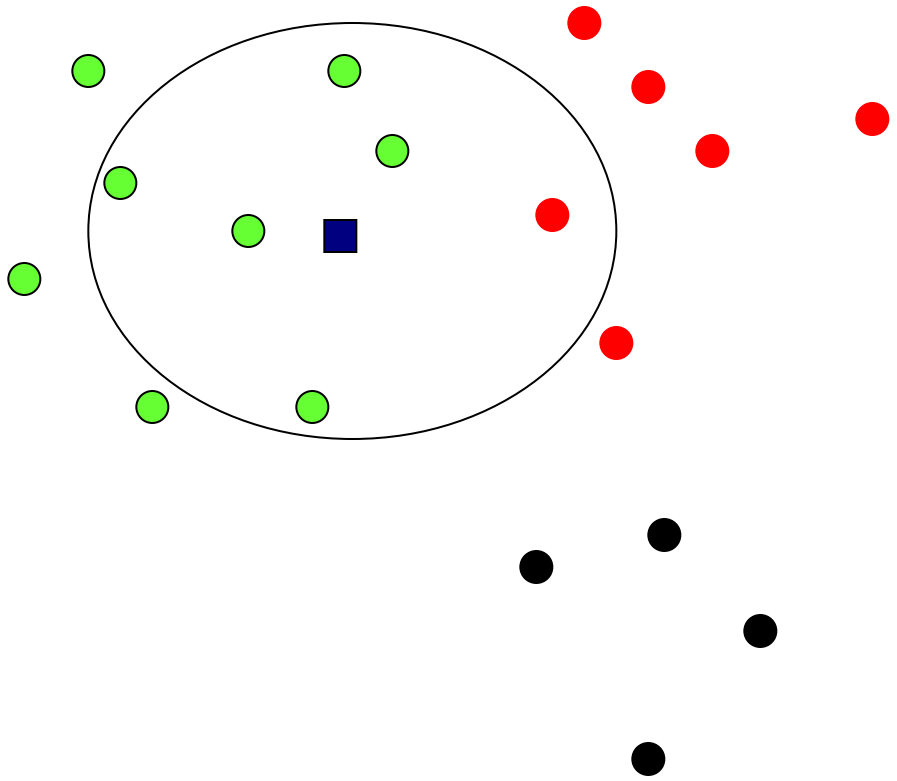
1 Compute the distance between d and every example in D;

2 Choose the k examples in D that are nearest to d, denote the set by P ($\subseteq D$);

3 Assign d the class that is the most frequent class in P (or the majority class);

- k is usually chosen empirically via a validation set or cross-validation by trying a range of k values.
- Distance function is crucial, but depends on applications.

Example: k=6 (6NN)



- Government
- Science
- Arts

A new point ■

Pr(science| ■)?

Discussions

- kNN can deal with complex and arbitrary decision boundaries.
- Despite its simplicity, researchers have shown that the classification accuracy of kNN can be quite strong and in many cases as accurate as those elaborated methods.
- kNN is slow at the classification time
- kNN does not produce an understandable model

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