Classification
Lecture 2: Methods

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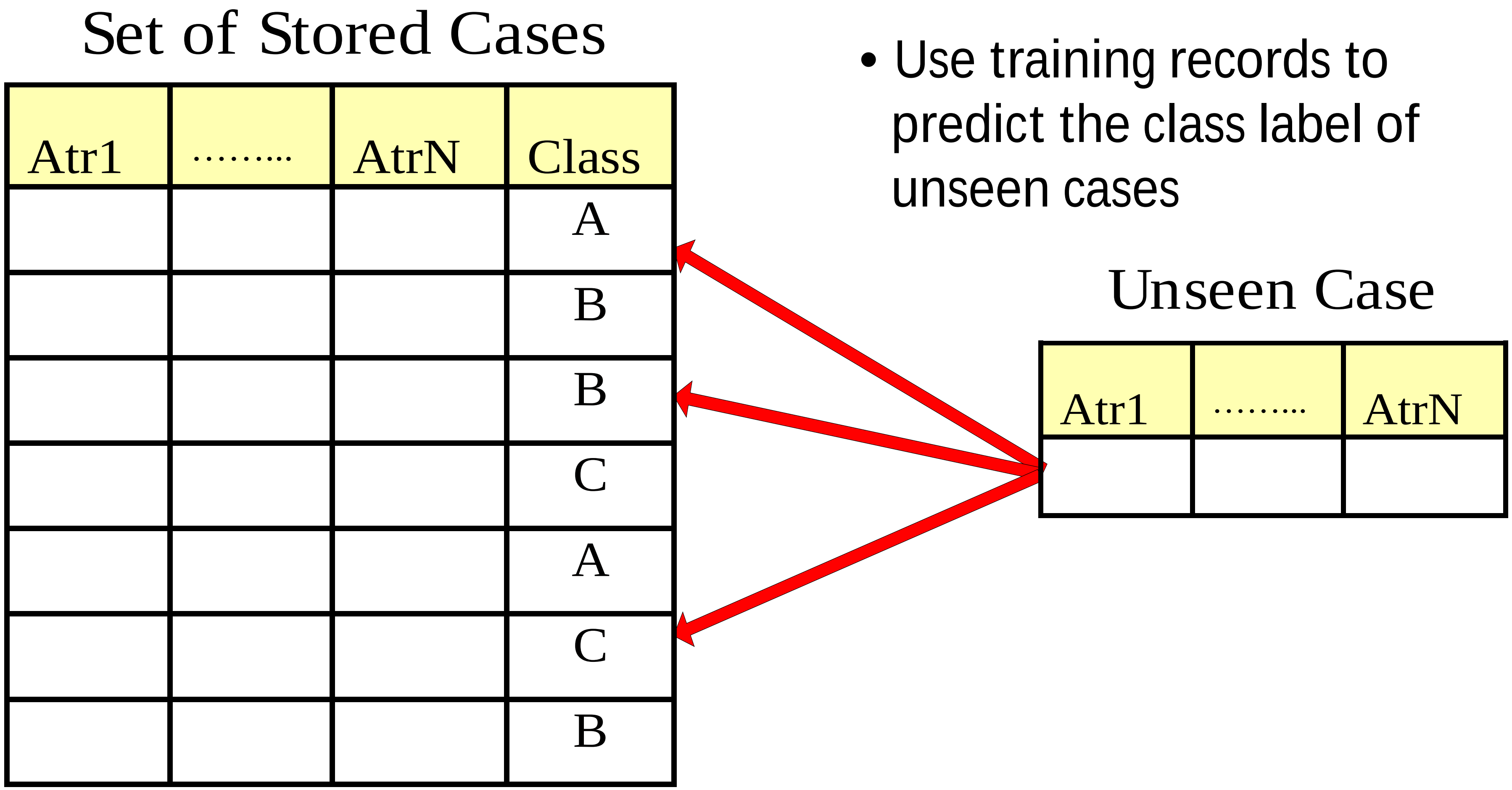
Outline

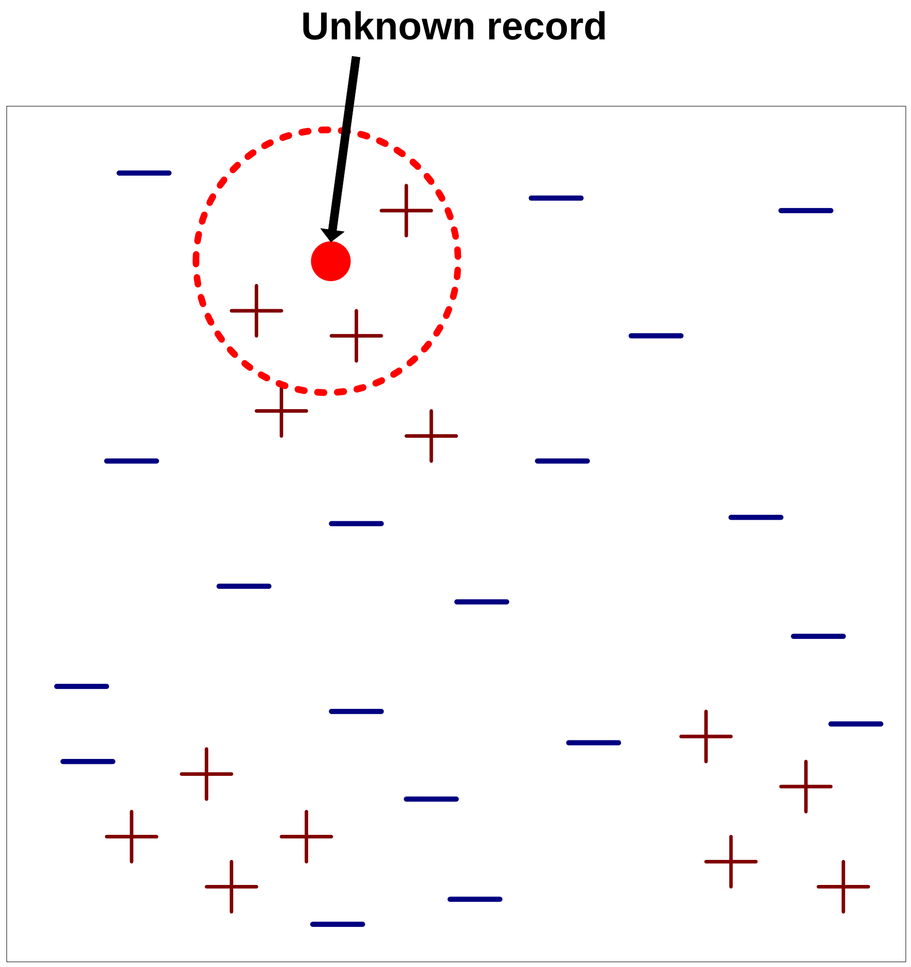
- **Basics**
  - Problem, goal, evaluation
- **Methods**
  - Decision Tree
  - Naïve Bayes
  - Nearest Neighbor
  - Rule-based Classification
  - Logistic Regression
  - Support Vector Machines
  - Ensemble methods
  - ………
- **Advanced topics**
  - Multi-view Learning
  - Semi-supervised Learning
  - Transfer Learning
  - ……

Nearest Neighbor Classifiers

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



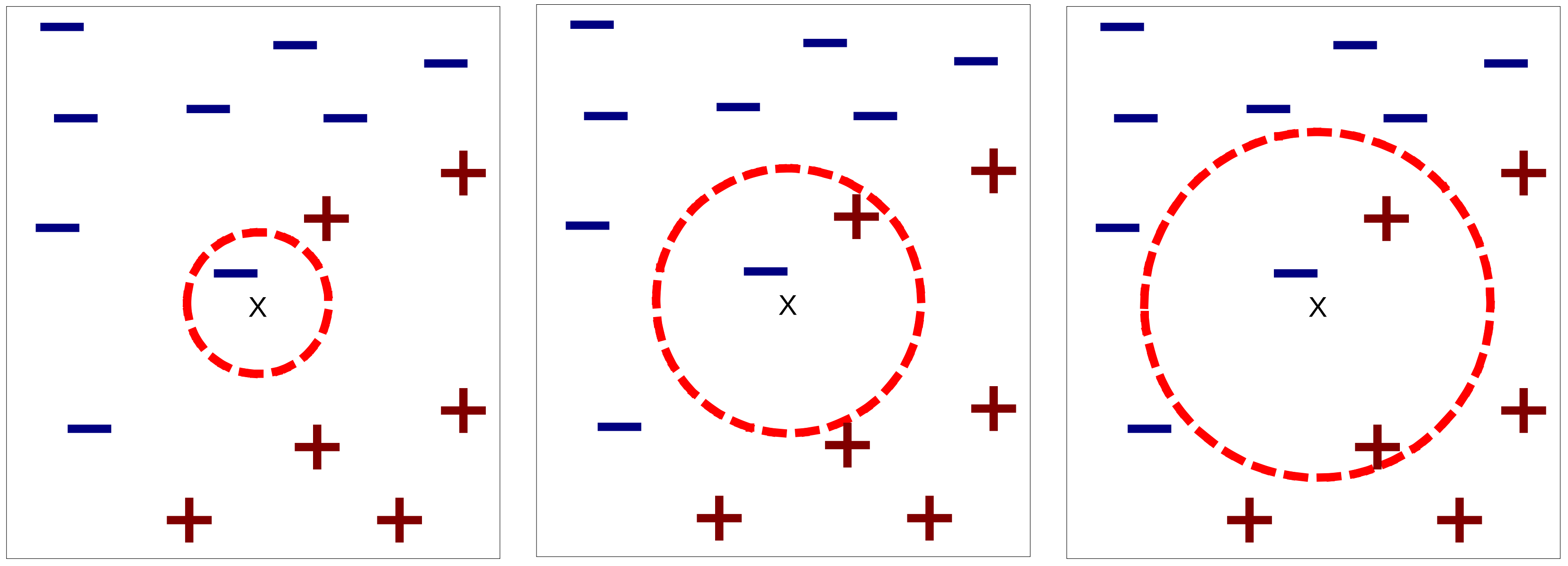
Nearest-Neighbor Classifiers



- 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)

Definition of Nearest Neighbor

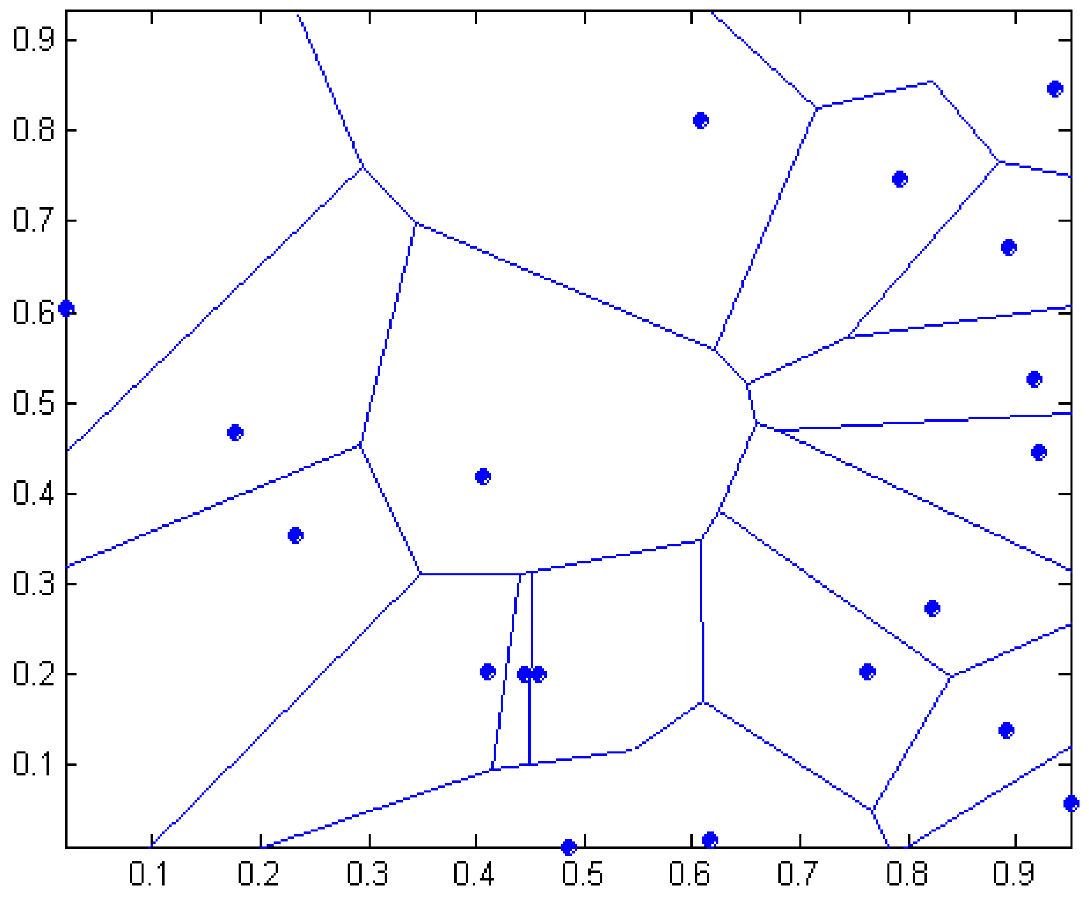


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

1 nearest-neighbor

Voronoi Diagram



Nearest Neighbor Classification

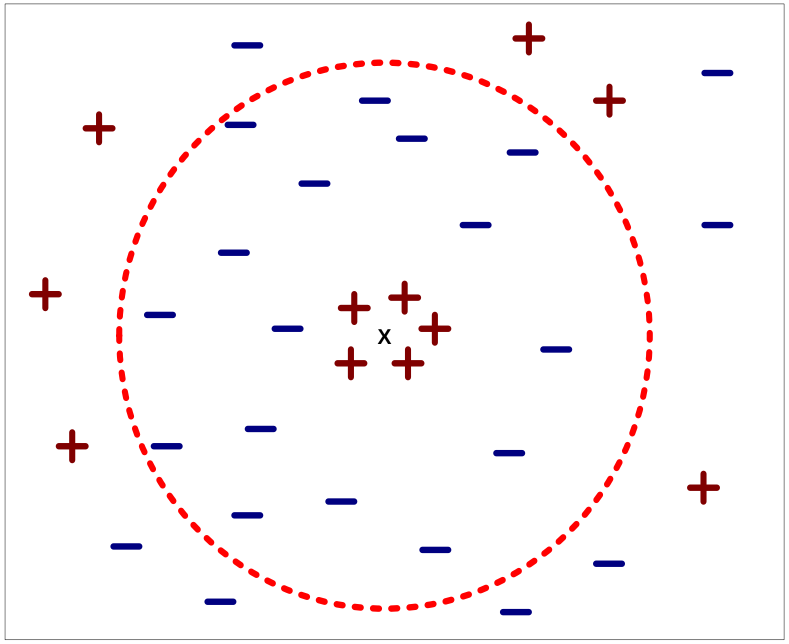
- Compute distance between two points:
  - Euclidean distance

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

- 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 other classes



Nearest Neighbor Classification

- **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

- **k-NN classifiers are lazy learners**
  - It does not build models explicitly
  - Different from eager learners such as decision tree induction
  - Classifying unknown records are relatively expensive

Bayesian Classification

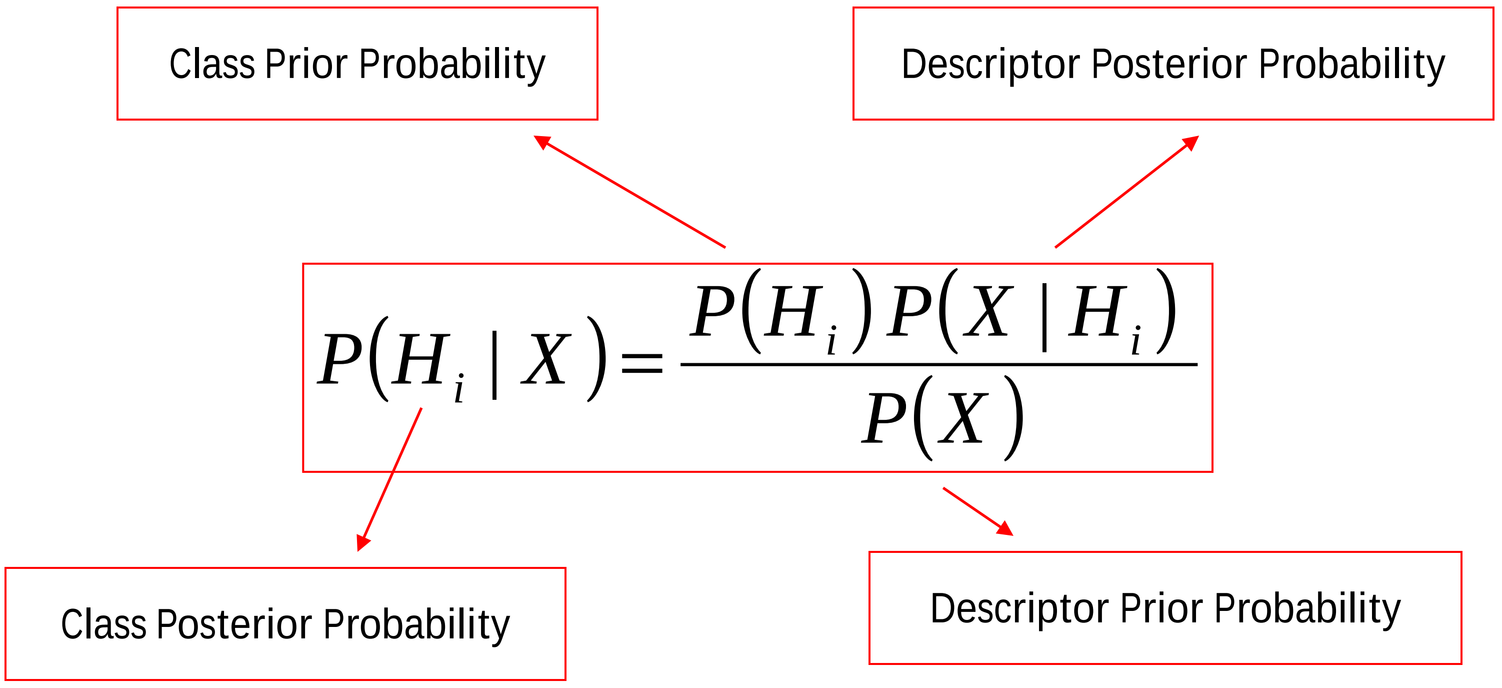
- Bayesian classifier vs. decision tree
  - Decision tree: predict the class label
  - Bayesian classifier: statistical classifier; predict class membership probabilities
- Based on Bayes theorem; estimate *posterior* probability
- Naïve Bayesian classifier:
  - Simple classifier that assumes attribute independence
  - Efficient when applied to large databases
  - Comparable in performance to decision trees

Posterior Probability

- Let X be a data sample whose class label is unknown
- Let H_i be the hypothesis that X belongs to a particular class C_i
- $P(H_i|X)$ is *posteriori* probability of H conditioned on X
  - Probability that data example X belongs to class C_i given the attribute values of X
  - e.g., given X=(age:31…40, income: medium, student: yes, credit: fair), what is the probability X buys computer?

Bayes Theorem

- To classify means to determine the highest $P(H_i|X)$ among all classes $C_1,\ldots C_m$
  - If $P(H_1|X)>P(H_0|X)$, then X buys computer
  - If $P(H_0|X)>P(H_1|X)$, then X does not buy computer
  - Calculate $P(H_i|X)$ using the Bayes theorem


Class Prior Probability
Descriptor Posterior Probability
Class Posterior Probability
Descriptor Prior Probability

$$P(H_i \mid X) = \frac{P(H_i)\,P(X \mid H_i)}{P(X)}$$

Class Prior Probability

- P(H_i) is *class prior* probability that X belongs to a particular class C_i
  - Can be estimated by n_i/n from training data samples
  - n is the total number of training data samples
  - n_i is the number of training data samples of class C_i

	Age	Income	Student	Credit	Buys_computer
P1	31…40	high	no	fair	no
P2	<=30	high	no	excellent	no
P3	31…40	high	no	fair	yes
P4	>40	medium	no	fair	yes
P5	>40	low	yes	fair	yes
P6	>40	low	yes	excellent	no
P7	31…40	low	yes	excellent	yes
P8	<=30	medium	no	fair	no
P9	<=30	low	yes	fair	yes
P10	>40	medium	yes	fair	yes

H1: Buys_computer=yes
H0: Buys_computer=no
P(H1)=6/10 = 0.6
P(H0)=4/10 = 0.4

$$P(H_i|X)=\frac{P(X|H_i)P(H_i)}{P(X)}$$

Descriptor Prior Probability

- P(X) is *prior* probability of X
  - Probability that observe the attribute values of X
  - Suppose $X= (x_1, x_2,..., x_d)$ and they are independent, then $P(X) =P(x_1)\ P(x_2)\ ...\ P(x_d)$
  - $P(x_j)=n_j/n$, where
  - n_j is number of training examples having value x_j for attribute A_j
  - n is the total number of training examples
  - Constant for all classes

	Age	Income	Student	Credit	Buys_computer
P1	31···40	high	no	fair	no
P2	<=30	high	no	excellent	no
P3	31···40	high	no	fair	yes
P4	>40	medium	no	fair	yes
P5	>40	low	yes	fair	yes
P6	>40	Low	yes	excellent	No
P7	31···40	low	yes	excellent	yes
P8	<=30	medium	no	fair	no
P9	<=30	low	yes	fair	yes
P10	>40	medium	yes	fair	yes

- X=(age:31…40, income: medium, student: yes, credit: fair)
- P(age=31…40)=3/10   P(income=medium)=3/10
  P(student=yes)=5/10   P(credit=fair)=7/10

$$P(H_i|X)=\frac{P(X|H_i)P(H_i)}{P(X)}$$

- P(X)=P(age=31…40) ×P(income=medium) ×P(student=yes) ×P(credit=fair)
  =0.3 ×0.3 ×0.5 ×0.7 = 0.0315

Descriptor Posterior Probability

- $P(X|H_i)$ is *posterior* probability of X given H_i
  - Probability that observe X in class C_i
  - Assume $X=(x_1, x_2,..., x_d)$ and they are independent, then $P(X|H_i) = P(x_1|H_i)\ P(x_2|H_i)\ ...\ P(x_d|H_i)$
  - $P(x_j|H_i)=n_{i,j}/n_i$, where
  - $n_{i,j}$ is number of training examples in class C_i having value x_j for attribute A_j
  - n_i is number of training examples in C_i

	Age	Income	Student	Credit	Buys_computer
P1	31…40	high	no	fair	no
P2	<=30	high	no	excellent	no
P3	31…40	high	no	fair	yes
P4	>40	medium	no	fair	yes
P5	>40	low	yes	fair	yes
P6	>40	low	yes	excellent	no
P7	31…40	low	yes	excellent	yes
P8	<=30	medium	no	fair	no
P9	<=30	low	yes	fair	yes
P10	>40	medium	yes	fair	yes

- X= (age:31…40, income: medium, student: yes, credit: fair)
- H_1 = X buys a computer
- $n_1 = 6$, $n_{11}=2$, $n_{21}=2$, $n_{31}=4$, $n_{41}=5$,
- $P(X|H_1)= \frac{2}{6} \times \frac{2}{6} \times \frac{4}{6} \times \frac{5}{6} = \frac{5}{81} = 0.062$

	Age	Income	Student	Credit	Buys_computer
P1	31···40	high	no	fair	no
P2	<=30	high	no	excellent	no
P3	31···40	high	no	fair	yes
P4	>40	medium	no	fair	yes
P5	>40	low	yes	fair	yes
P6	>40	low	yes	excellent	no
P7	31···40	low	yes	excellent	yes
P8	<=30	medium	no	fair	no
P9	<=30	low	yes	fair	yes
P10	>40	medium	yes	fair	yes

- X= (age:31…40, income: medium, student: yes, credit: fair)
- H_0 = X does not buy a computer
- $n_0 = 4$, $n_{10}=1$, $n_{20}=1$, $n_{31}=1$, $n_{41} = 2$,
- $P(X|H_0)= \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{2}{4} = \frac{1}{128} = 0.0078$

$$P(H_i|X) = \frac{P(X|H_i)P(H_i)}{P(X)}$$

Bayesian Classifier – Basic Equation

$$\underbrace{P(H_i \mid X)}_{\text{Class Posterior Probability}} = \frac{\overbrace{P(H_i)}^{\text{Class Prior Probability}}\,\overbrace{P(X \mid H_i)}^{\text{Descriptor Posterior Probability}}}{\underbrace{P(X)}_{\text{Descriptor Prior Probability}}}$$

To classify means to determine the highest $P(H_i|X)$ among all classes $C_1,\ldots C_m$

$P(X)$ is constant to all classes

Only need to compare $P(H_i)P(X|H_i)$

Weather Dataset Example

$X =< \text{rain, hot, high, false}>$

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	false	N
sunny	hot	high	true	N
overcast	hot	high	false	P
rain	mild	high	false	P
rain	cool	normal	false	P
rain	cool	normal	true	N
overcast	cool	normal	true	P
sunny	mild	high	false	N
sunny	cool	normal	false	P
rain	mild	normal	false	P
sunny	mild	normal	true	P
overcast	mild	high	true	P
overcast	hot	normal	false	P
rain	mild	high	true	N

Weather Dataset Example: Classifying X

- An unseen sample X = <rain, hot, high, false>
- $P(p)\ P(X|p)$

  $= P(p)\ \ P(\text{rain}|p)\ P(\text{hot}|p)\ P(\text{high}|p)\ P(\text{false}|p)$

  $= \text{x/x} \cdot \text{x/x} \cdot \text{x/x} \cdot \text{x/x} \cdot \text{x/x}$
- $P(n)\ P(X|n)$

  $= P(n)\ P(\text{rain}|n)\ P(\text{hot}|n)\ P(\text{high}|n)\ P(\text{false}|n)$

  $= \text{x/x} \cdot \text{x/x} \cdot \text{x/x} \cdot \text{x/x} \cdot \text{x/x}$

Weather Dataset Example

- Given a training set, we can compute probabilities:

$P(H_i)$

P(p) = 9/14	
P(n) = 5/14	

$P(x_j \mid H_i)$

Outlook	P	N
sunny	2/9	3/5
overcast	4/9	0
rain	3/9	2/5

Temperature	P	N
hot	2/9	2/5
mild	4/9	2/5
cool	3/9	1/5

Humidity	P	N
high	3/9	4/5
normal	6/9	1/5

Windy	P	N
true	3/9	3/5
false	6/9	2/5

Weather Dataset Example: Classifying X

- An unseen sample X = <rain, hot, high, false>
- $P(p)\ P(X|p)$
  $= P(p)\ \ P(\text{rain}|p)\ P(\text{hot}|p)\ P(\text{high}|p)\ P(\text{false}|p)$
  $= 9/14 \cdot 3/9 \cdot 2/9 \cdot 3/9 \cdot 6/9 \cdot = 0.010582$
- $P(n)\ P(X|n)$
  $= P(n)\ P(\text{rain}|n)\ P(\text{hot}|n)\ P(\text{high}|n)\ P(\text{false}|n)$
  $= 5/14 \cdot 2/5 \cdot 2/5 \cdot 4/5 \cdot 2/5 = 0.018286$
- Sample X is classified in class n (don’t play)

Avoiding the Zero-Probability Problem

- Descriptor posterior probability goes to 0 if any of probability is 0:

$$P(X \mid H_i) = \prod_{j=1}^{d} P(x_j \mid H_i)$$

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

    Prob(income = low|H) = 1/1003

    Prob(income = medium|H) = 991/1003

    Prob(income = high|H) = 11/1003

Independence Hypothesis

- makes computation possible
- yields optimal classifiers when satisfied
- but is seldom satisfied in practice, as attributes (variables) are often correlated
- Attempts to overcome this limitation:
  – Bayesian networks, that combine Bayesian reasoning with causal relationships between attributes

Logistic Regression Classifier

- **Input distribution**
  - X is n-dimensional feature vector $< X_1 \ldots X_n >$
  - Y is 0 or 1
  - X|Y ~ Gaussian distribution
  - Y ~ Bernoulli distribution
- **Model P(Y|X)**
  - What does P(Y|X) look like?
  - What does P(Y=0|X)/P(Y=1|X) look like?

$$P(Y=1|X) = \frac{P(Y=1)P(X|Y=1)}{P(Y=1)P(X|Y=1) + P(Y=0)P(X|Y=0)}$$

$$= \frac{1}{1 + \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}}$$

$$= \frac{1}{1 + \exp(\ln \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)})}$$

$$= \frac{1}{1 + \exp(\ (\ln \frac{1-\pi}{\pi}) + \boxed{\sum_i \ln \frac{P(X_i|Y=0)}{P(X_i|Y=1)})}}$$

$$P(x \mid y_k) = \frac{1}{\sigma_{ik}\sqrt{2\pi}} \quad e^{\frac{-(x-\mu_{ik})^2}{2\sigma_{ik}^2}}$$

$$\boxed{\sum_i \left(\frac{\mu_{i0} - \mu_{i1}}{\sigma_i^2} X_i + \frac{\mu_{i1}^2 - \mu_{i0}^2)}{2\sigma_i^2} \right)}$$

$$P(Y=1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$P(Y=0|X=<X_1,...X_n>) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$\frac{P(Y=0|X)}{P(Y=1|X)} = exp(w_0+\sum_i w_i X_i)$$

linear classification rule!

implies

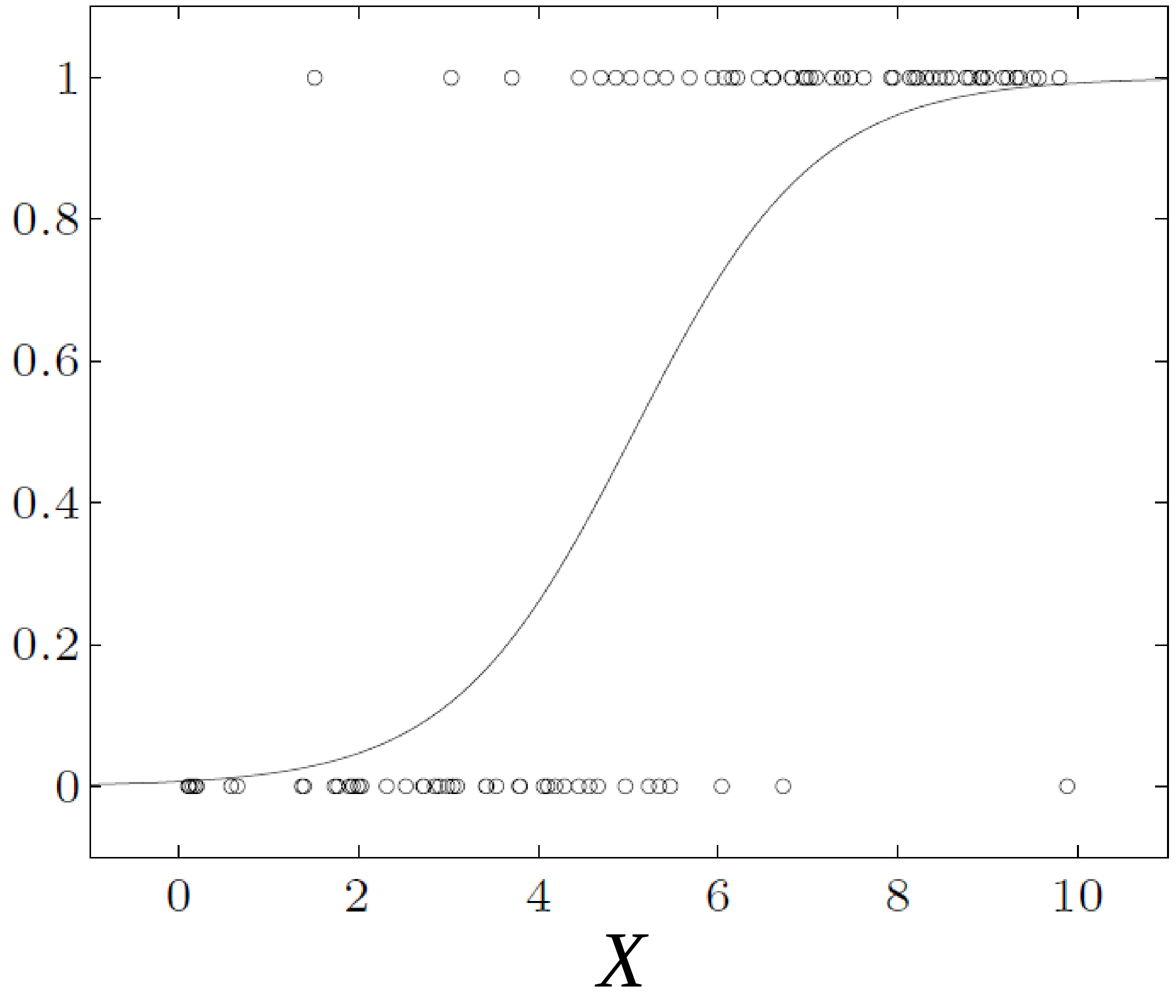
$$\ln \frac{P(Y=0|X)}{P(Y=1|X)} = w_0+\sum_i w_i X_i$$

Log ratio:

Positive—Class 0 Negative—Class 1

Logistic Function

$$P(Y=1|X) = \frac{1}{1+\exp(wX+b)}$$



Training set:

Y=1—P(Y=1|X)=1 Y=0—P(Y=1|X)=0

Maximizing Conditional Likelihood

- Training Set: $\{\langle X^1, Y^1\rangle, \dots \langle X^L, Y^L\rangle\}$
- Find W that maximizes conditional likelihood:

$$\arg\max_W \prod_l P(Y^l | W, X^l)$$

$$P(Y=1|X=<X_1,...X_n>) = \frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

$$P(Y=0|X=<X_1,...X_n>) = \frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

- A concave function in W
- Gradient descent approach to solve it

Rule-Based Classifier

- Classify records by using a collection of "if…then…" rules
- Rule: (*Condition*) ® *y*
  - where
    - *Condition* is a conjunctions of attributes
    - *y* is the class label
  - *LHS*: rule condition
  - *RHS*: rule consequent
  - Examples of classification rules:
    - (Blood Type=Warm) Ù (Lay Eggs=Yes) ® Birds
    - (Taxable Income < 50K) Ù (Refund=Yes) ® Evade=No

Rule-based Classifier (Example)

Name	Blood Type	Give Birth	Can Fly	Live in Water	Class
human	warm	yes	no	no	mammals
python	cold	no	no	no	reptiles
salmon	cold	no	no	yes	fishes
whale	warm	yes	no	yes	mammals
frog	cold	no	no	sometimes	amphibians
komodo	cold	no	no	no	reptiles
bat	warm	yes	yes	no	mammals
pigeon	warm	no	yes	no	birds
cat	warm	yes	no	no	mammals
leopard shark	cold	yes	no	yes	fishes
turtle	cold	no	no	sometimes	reptiles
penguin	warm	no	no	sometimes	birds
porcupine	warm	yes	no	no	mammals
eel	cold	no	no	yes	fishes
salamander	cold	no	no	sometimes	amphibians
gila monster	cold	no	no	no	reptiles
platypus	warm	no	no	no	mammals
owl	warm	no	yes	no	birds
dolphin	warm	yes	no	yes	mammals
eagle	warm	no	yes	no	birds

R1: (Give Birth = no) Ù (Can Fly = yes) ® Birds

R2: (Give Birth = no) Ù (Live in Water = yes) ® Fishes

R3: (Give Birth = yes) Ù (Blood Type = warm) ® Mammals

R4: (Give Birth = no) Ù (Can Fly = no) ® Reptiles

R5: (Live in Water = sometimes) ® Amphibians

Application of Rule-Based Classifier

- A rule *r* covers an instance **x** if the attributes of the instance satisfy the condition of the rule

R1: (Give Birth = no) Ù (Can Fly = yes) ® Birds

R2: (Give Birth = no) Ù (Live in Water = yes) ® Fishes

R3: (Give Birth = yes) Ù (Blood Type = warm) ® Mammals

R4: (Give Birth = no) Ù (Can Fly = no) ® Reptiles

R5: (Live in Water = sometimes) ® Amphibians

Name	Blood Type	Give Birth	Can Fly	Live in Water	Class
hawk	warm	no	yes	no	?
grizzly bear	warm	yes	no	no	?

The rule R1 covers a hawk => Bird

The rule R3 covers the grizzly bear => Mammal

Rule Coverage and Accuracy

- **Coverage of a rule:**
  - Fraction of records that satisfy the condition of a rule
- **Accuracy of a rule:**
  - Fraction of records that satisfy both the LHS and RHS of a rule

Tid	**Refund**	**Marital Status**	**Taxable Income**	**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**

(Status=Single) ® No

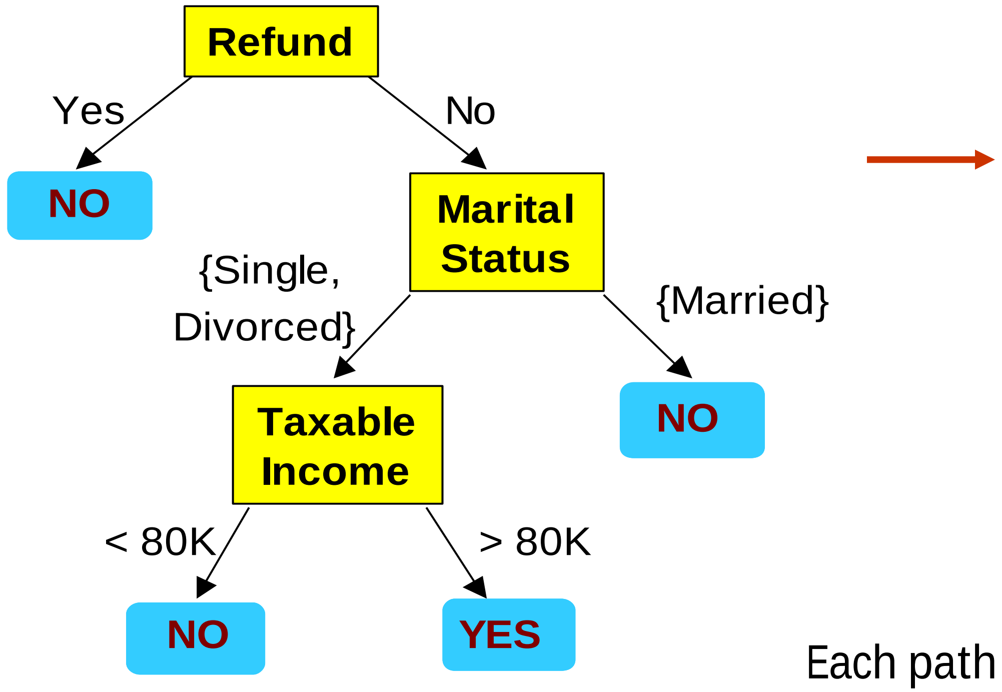
Coverage = 40%, Accuracy = 50%

Characteristics of Rule-Based Classifier

- **Mutually exclusive rules**
  - Classifier contains mutually exclusive rules if the rules are independent of each other
  - Every record is covered by at most one rule

- **Exhaustive rules**
  - Classifier has exhaustive coverage if it accounts for every possible combination of attribute values
  - Each record is covered by at least one rule

From Decision Trees To Rules



Classification Rules

(Refund=Yes) ==> No

(Refund=No, Marital Status={Single,Divorced}, Taxable Income<80K) ==> No

(Refund=No, Marital Status={Single,Divorced}, Taxable Income>80K) ==> Yes

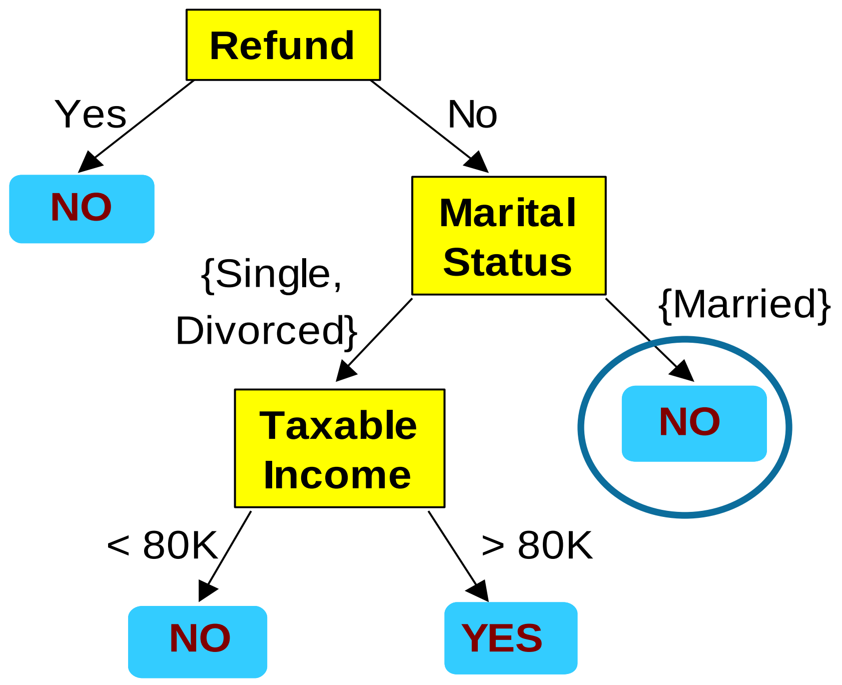
(Refund=No, Marital Status={Married}) ==> No

Each path in the tree forms a rule

Rules are mutually exclusive and exhaustive

Rule set contains as much information as the tree

Rules Can Be Simplified



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

Initial Rule: (Refund=No) Ù (Status=Married) ® No

Simplified Rule: (Status=Married) ® No

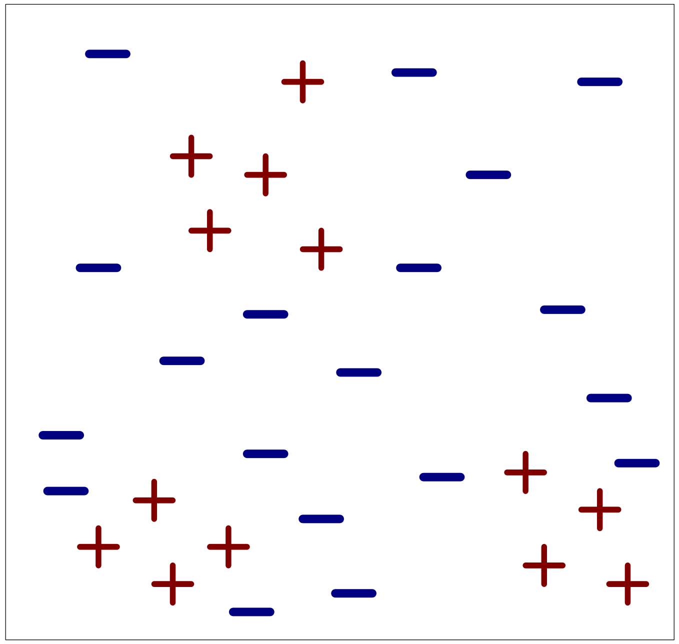
Effect of Rule Simplification

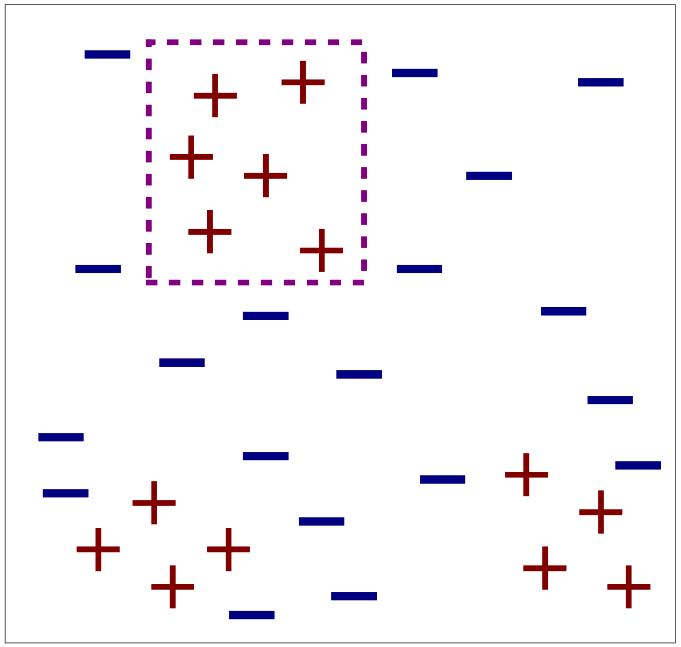
- **Rules are no longer mutually exclusive**
  - A record may trigger more than one rule
  - Solution?
    - Ordered rule set
    - Unordered rule set – use voting schemes
- **Rules are no longer exhaustive**
  - A record may not trigger any rules
  - Solution?
    - Use a default class

Learn Rules from Data: Sequential Covering

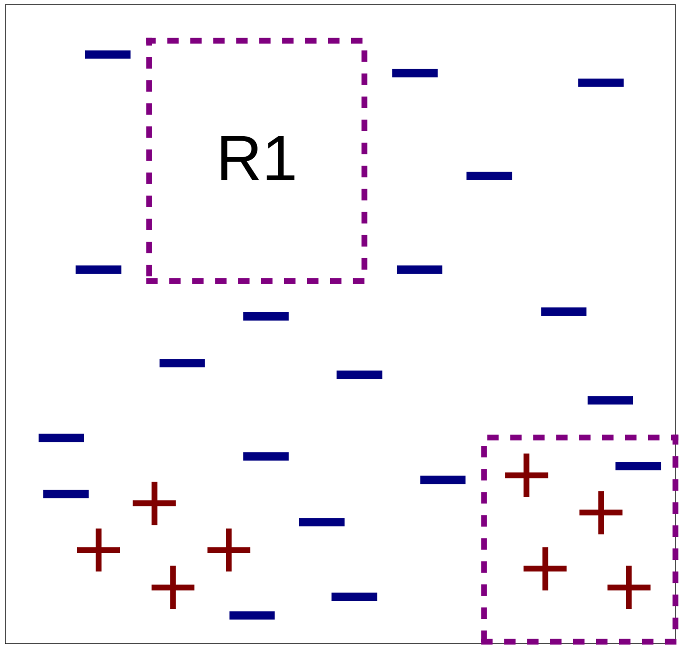
1. Start from an empty rule
2. Grow a rule using the Learn-One-Rule function
3. Remove training records covered by the rule
4. Repeat Step (2) and (3) until stopping criterion is met

Example of Sequential Covering

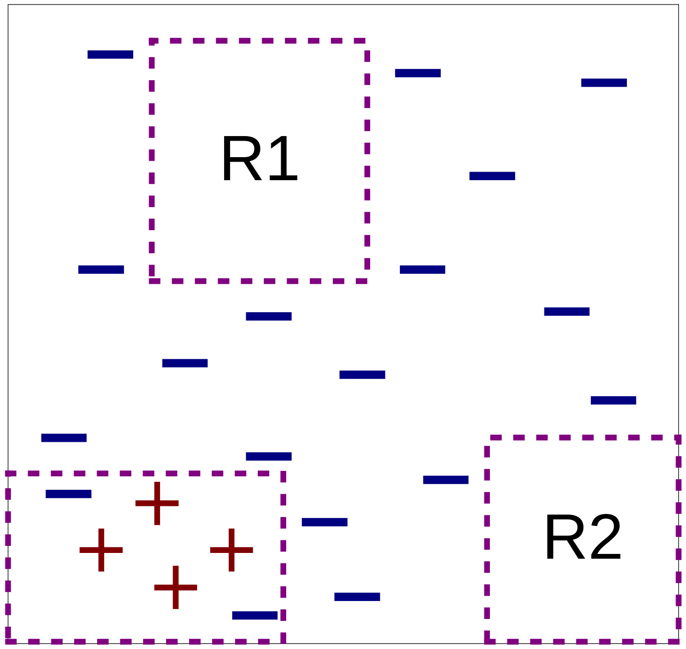

(i) Original Data


(ii) Step 1

Example of Sequential Covering...



(iii) Step 2



(iv) Step 3

How to Learn-One-Rule?

- Start with the *most general rule* possible: condition = empty
- *Adding new attributes* by adopting a greedy depth-first strategy
  - Picks the one that most improves the rule quality
- Rule-Quality measures: consider both coverage and accuracy
  - Foil-gain: assesses info_gain by extending condition

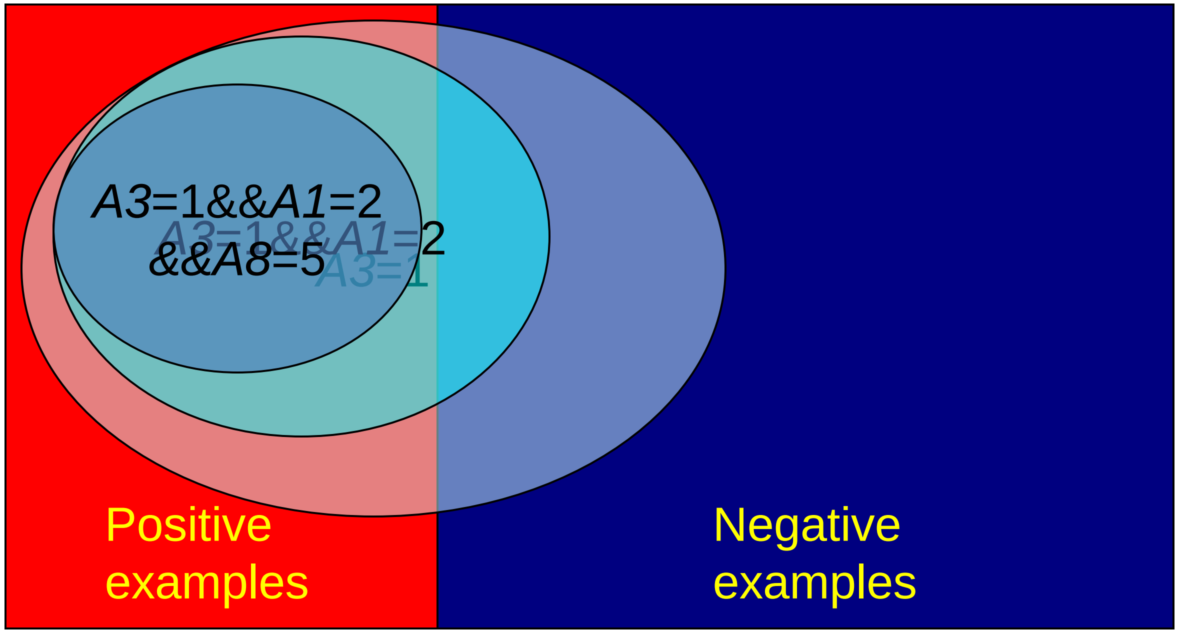
$$FOIL\_Gain = pos' \times \left(\log_2 \frac{pos'}{pos'+neg'} - \log_2 \frac{pos}{pos+neg}\right)$$

    - favors rules that have high accuracy and cover many positive tuples

Rule Generation

- **To generate a rule**

```
while(true)
    find the best predicate p
    if foil-gain(p) > threshold then add p to current rule
    else break
```



Associative Classification

- **Associative classification: Major steps**
  - Mine data to find strong associations between frequent patterns (conjunctions of attribute-value pairs) and class labels
  - Association rules are generated in the form of

    P_1 ^ p_2 … ^ p_l à "A_{class} = C" (conf, sup)
  - Organize the rules to form a rule-based classifier

Associative Classification

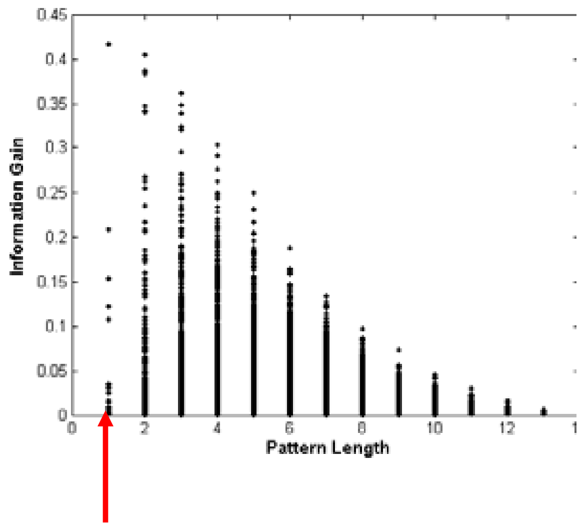
- **Why effective?**
  - It explores highly confident associations among multiple attributes and may overcome some constraints introduced by decision-tree induction, which considers only one attribute at a time
  - Associative classification has been found to be often more accurate than some traditional classification methods, such as C4.5

Associative Classification

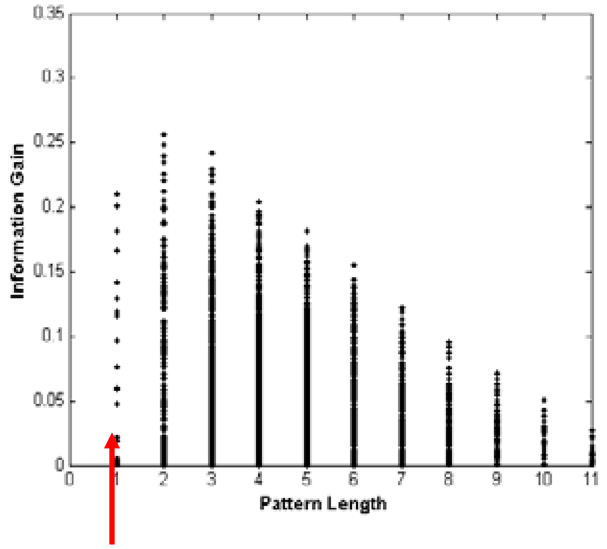
- **Basic idea**
  - Mine possible association rules in the form of
    - Cond-set (a set of attribute-value pairs) à class label
  - Pattern-based approach
    - Mine frequent patterns as candidate condition sets
    - Choose a subset of frequent patterns based on discriminativeness and redundancy

Frequent Pattern vs. Single Feature

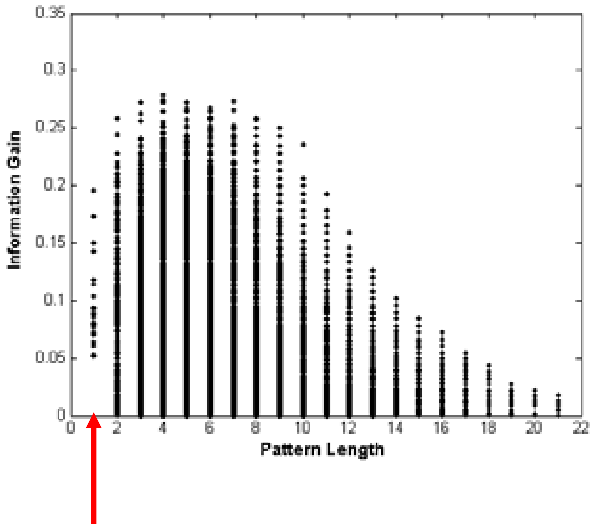
The discriminative power of some frequent patterns is higher than that of single features.



(a) Austral



(b) Cleve



(c) Sonar

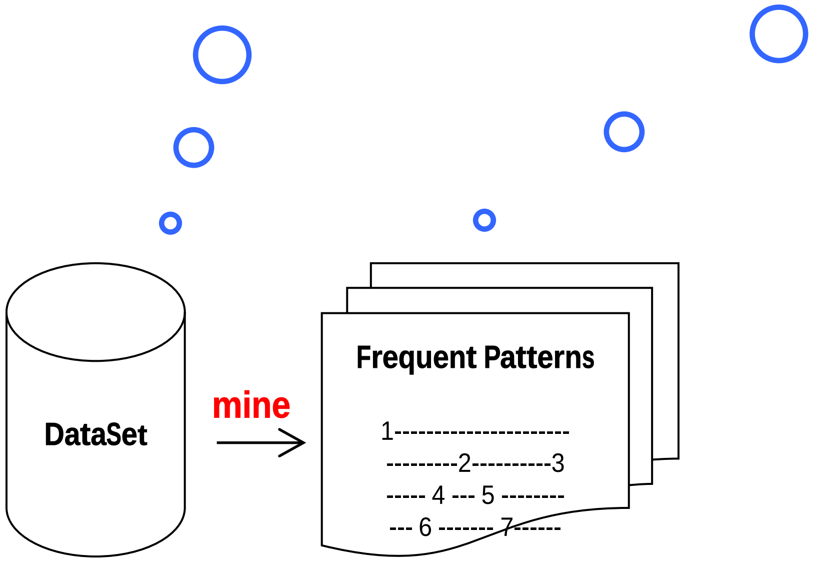
Information Gain vs. Pattern Length

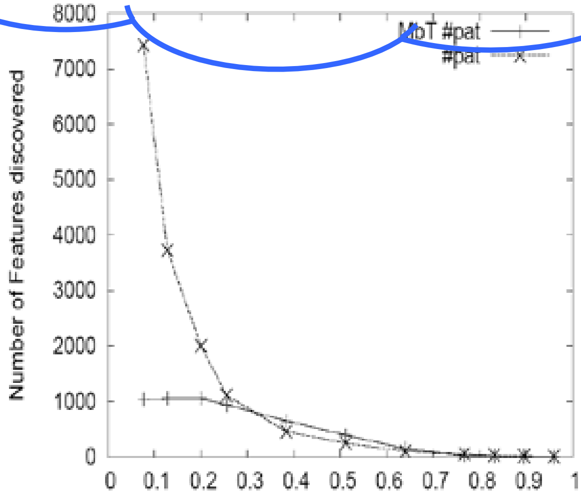
Two Problems

- **Mine step**
  - **combinatorial explosion**

1. exponential explosion

2. patterns not considered if *minsupport* isn't small enough





(a) Number of itemsets mined with varying supports

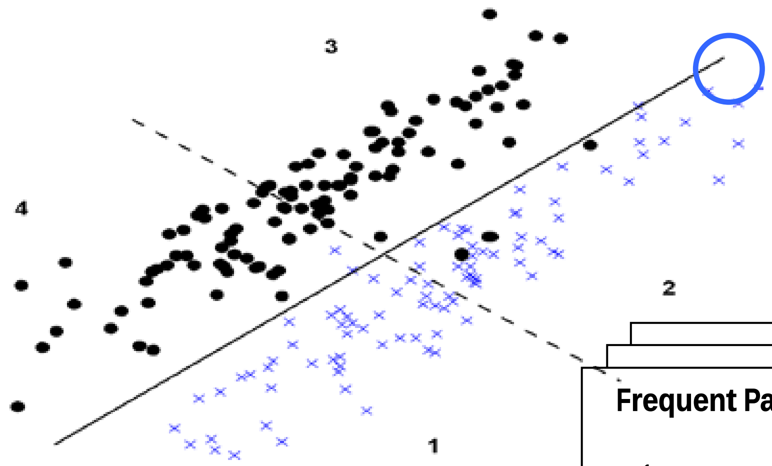
Two Problems

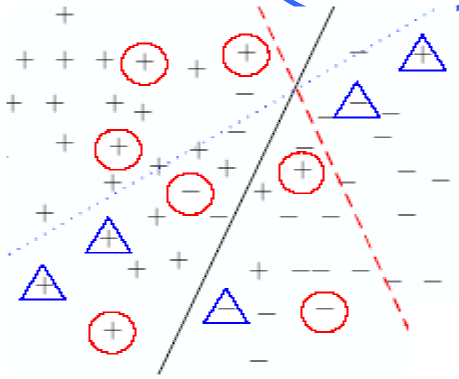
- **Select step**
  - **Issue of discriminative power**

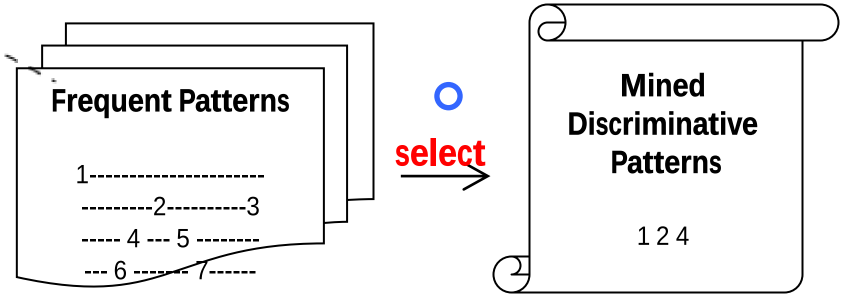
3. InfoGain against the complete dataset, NOT on subset of examples

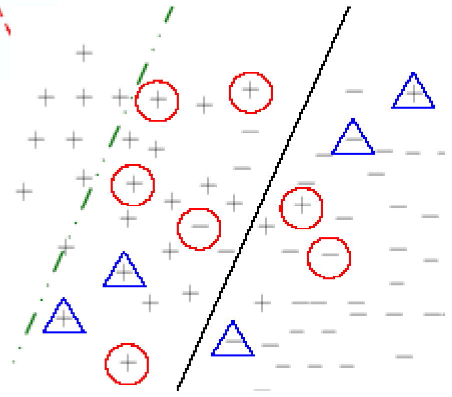
4. Correlation not directly evaluated on their joint predictability

Uncorrelated Patterns $\neq$ higher accuracy



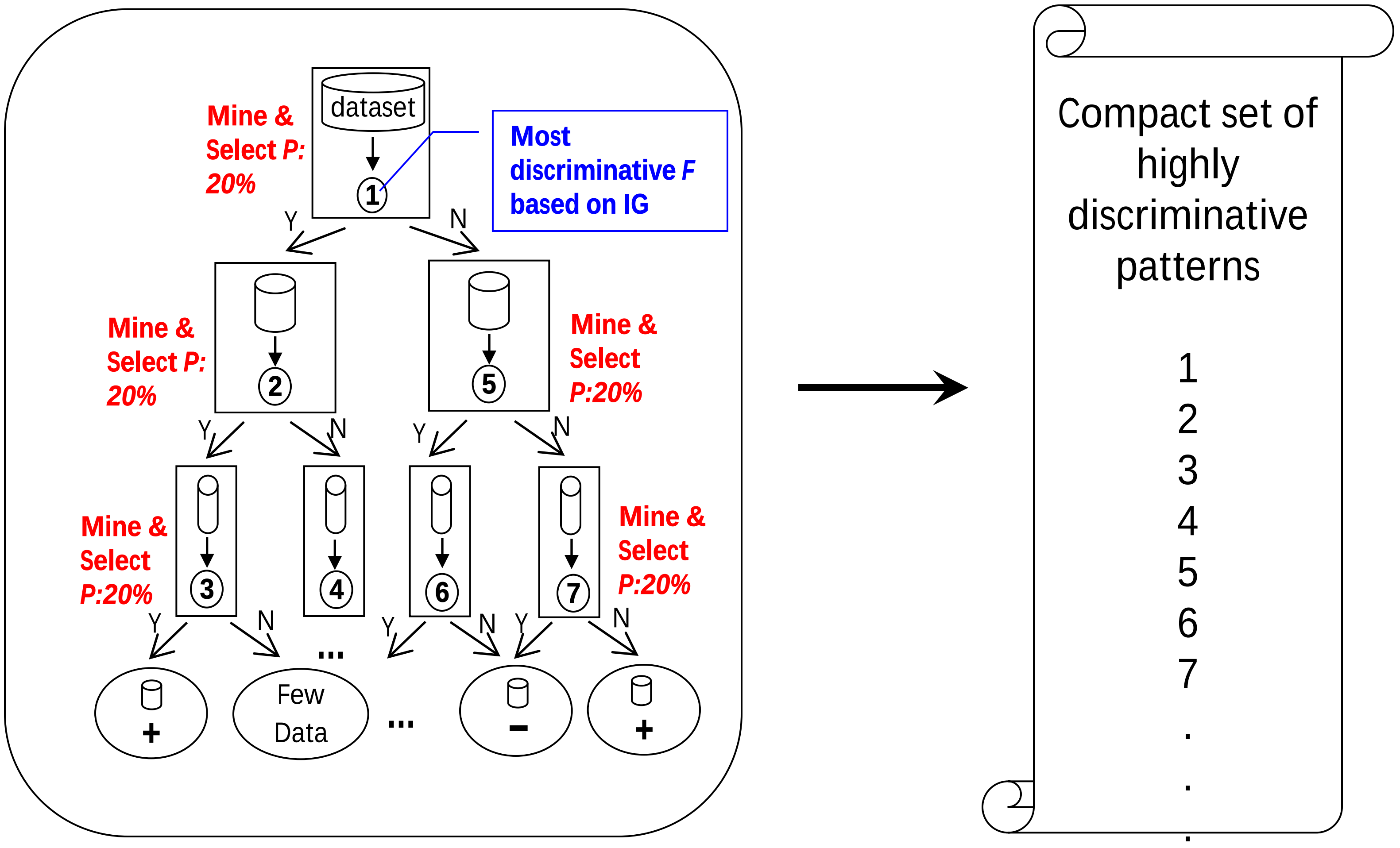






Direct Mining & Selection via Model-based Search Tree

- **Basic Flow**



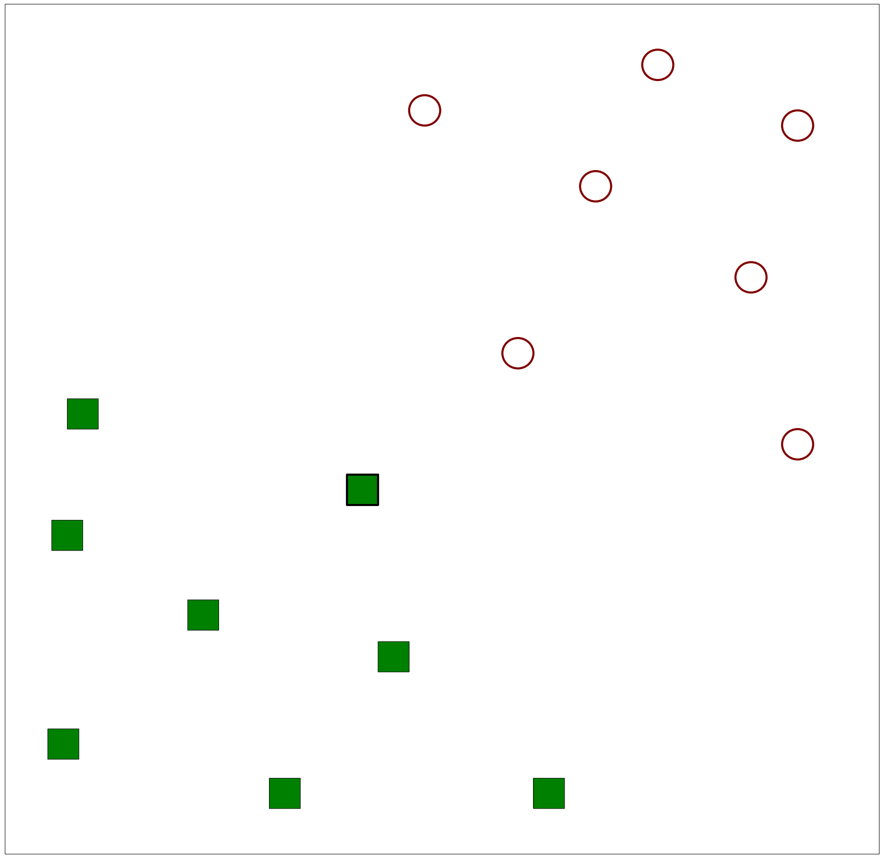
Divide-and-Conquer Based Frequent Pattern Mining

Mined Discriminative Patterns

Advantages of Rule-Based Classifiers

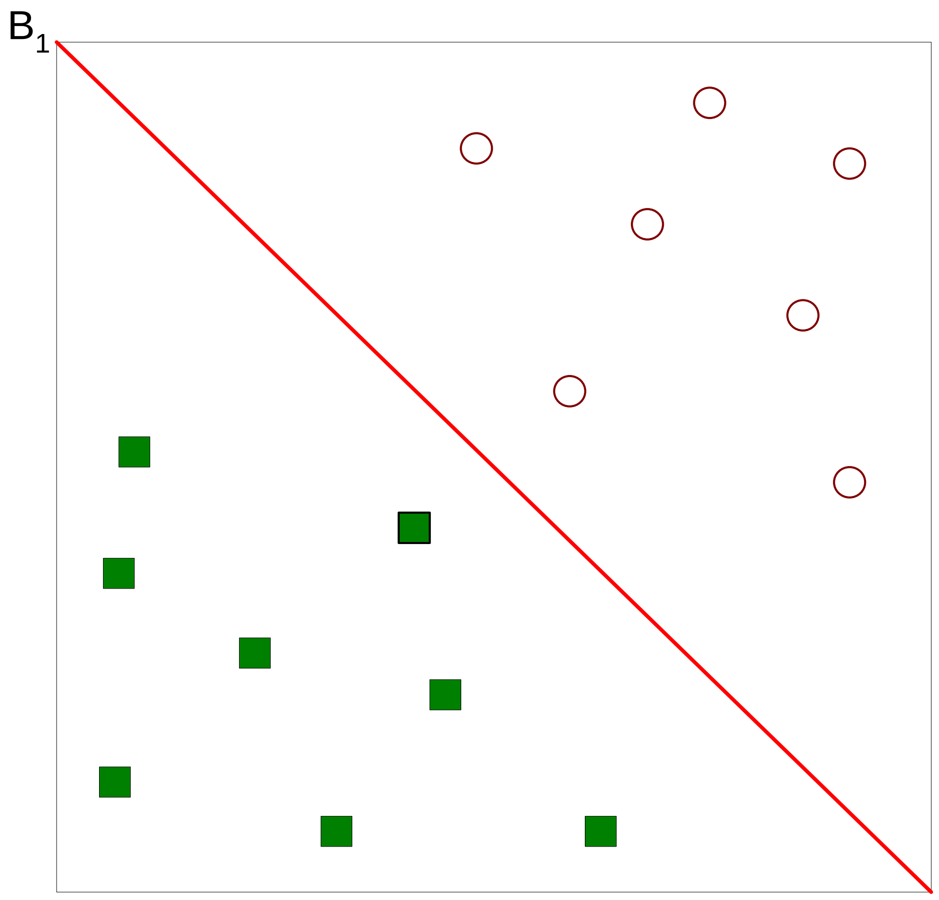
- As highly expressive as decision trees
- Easy to interpret
- Easy to generate
- Can classify new instances rapidly
- Performance comparable to decision trees

Support Vector Machines—An Example



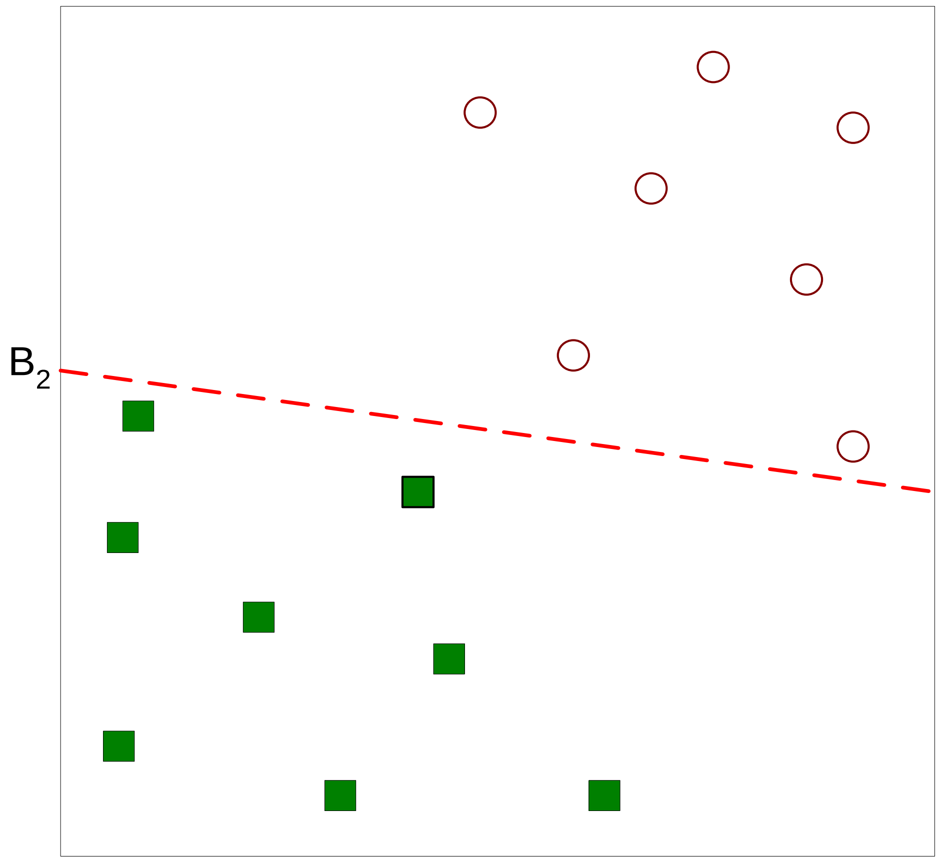
- Find a linear hyperplane (decision boundary) that will separate the data

Example



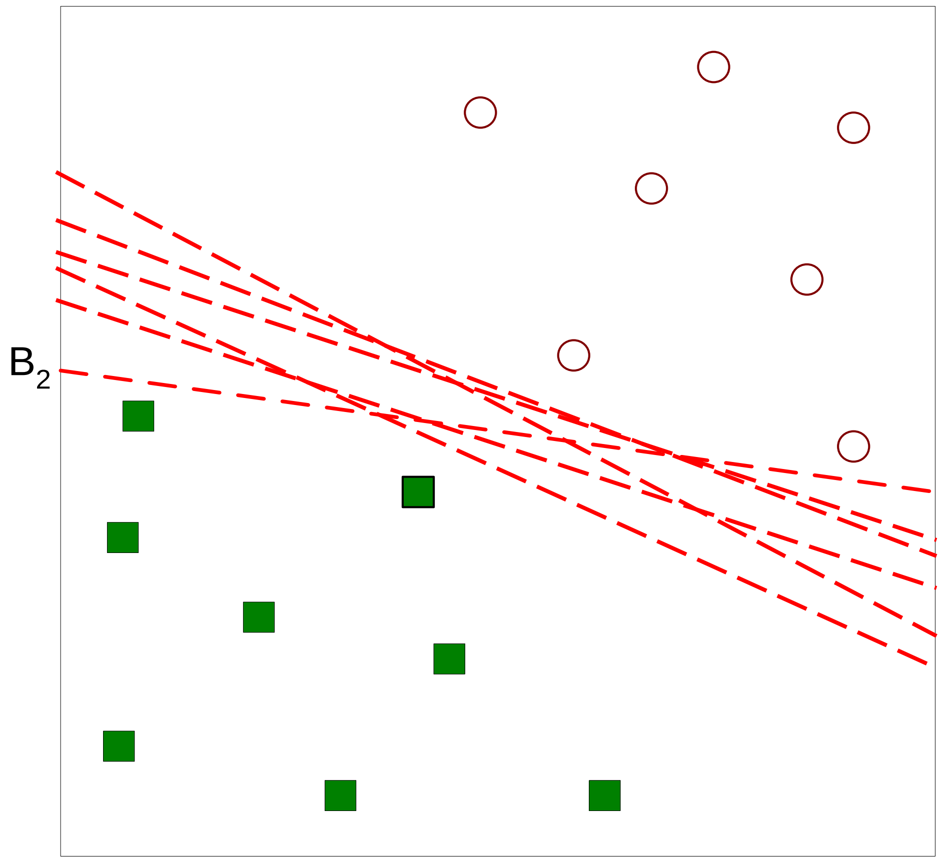
- One Possible Solution

Example



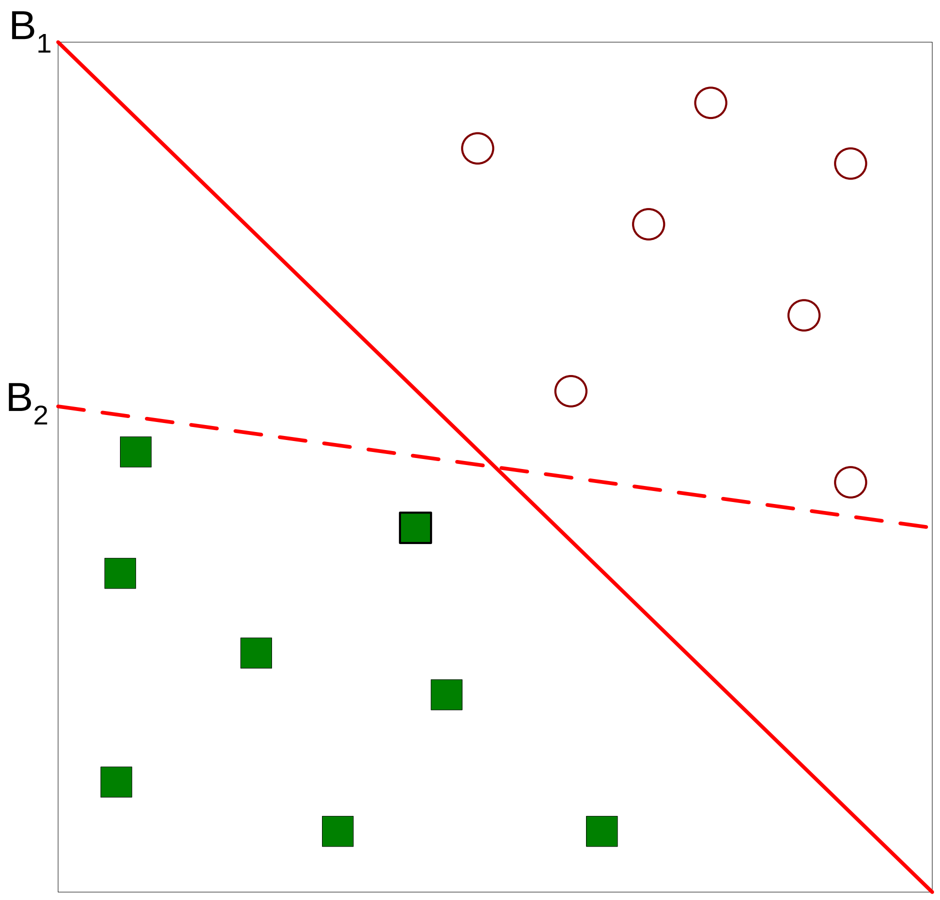
- Another possible solution

Example



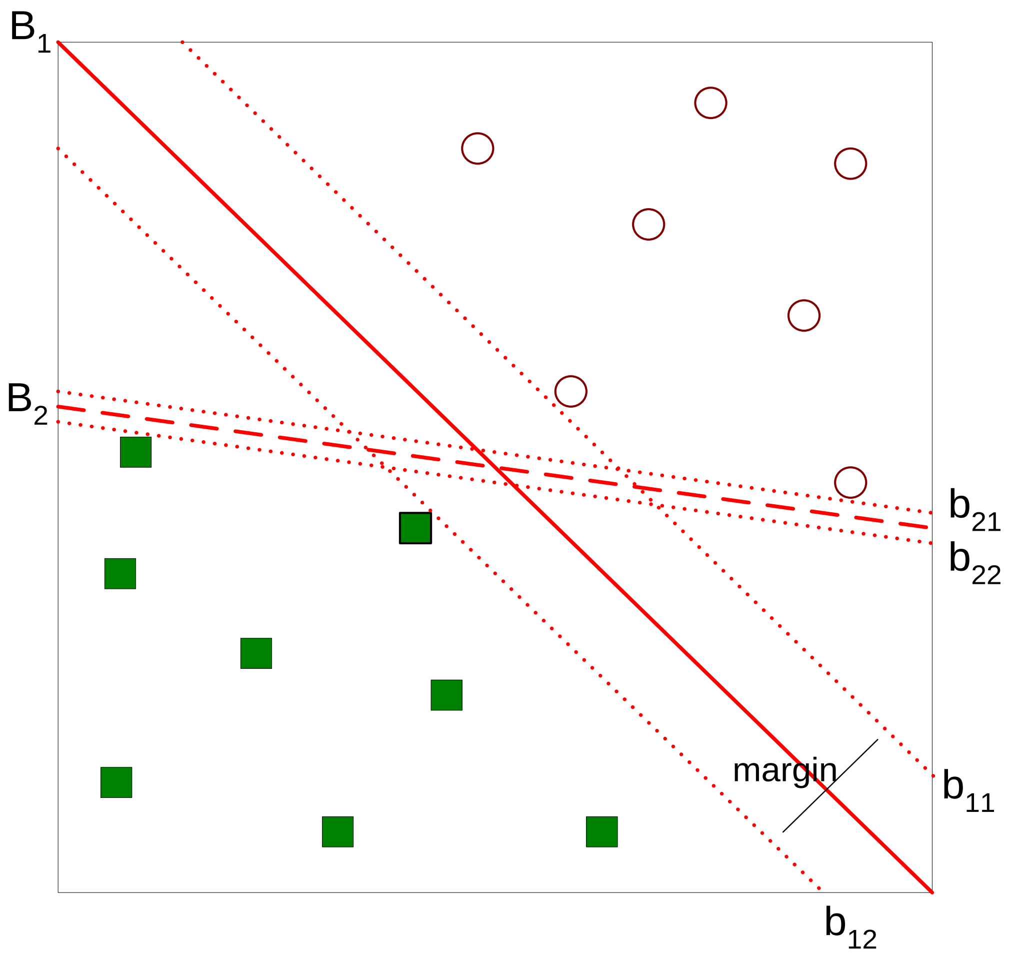
- Other possible solutions

Choosing Decision Boundary



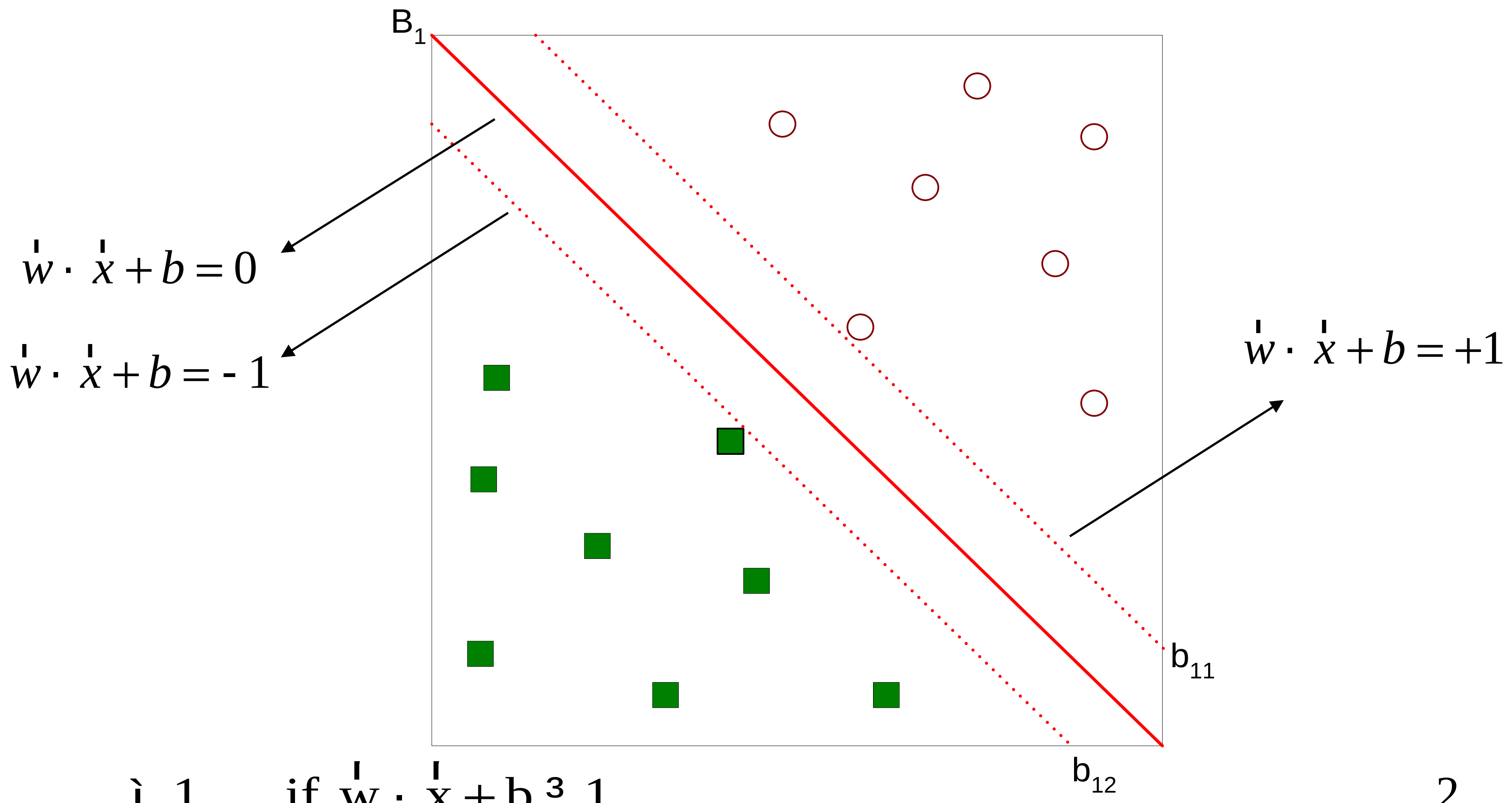
- Which one is better? B1 or B2?
- How do you define better?

Maximize Margin between Classes



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

Formal Definition


B_1
$\vec{w}\cdot\vec{x}+b=0$
$\vec{w}\cdot\vec{x}+b=-1$
$\vec{w}\cdot\vec{x}+b=+1$
b_{11}
b_{12}

$$y=\begin{cases}1 & \text{if } \vec{w}\cdot\vec{x}+b\geq 1\\ -1 & \text{if } \vec{w}\cdot\vec{x}+b\leq -1\end{cases}$$

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

Support Vector Machines

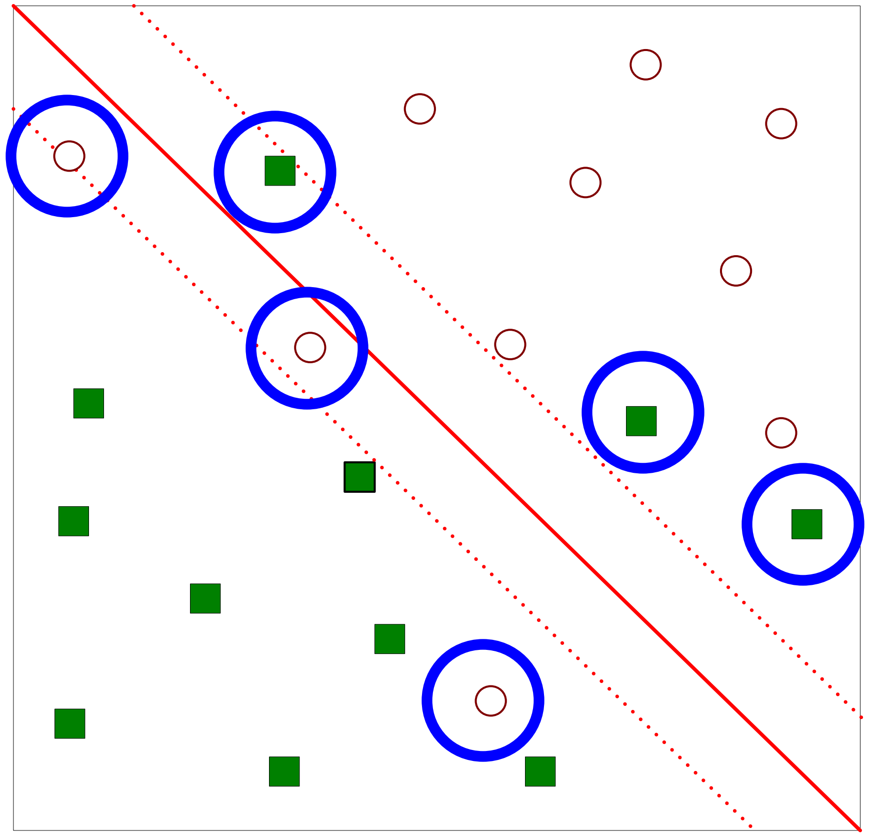
- We want to maximize: $\text{Margin} = \dfrac{2}{\|\vec{w}\|^2}$
  - Which is equivalent to minimizing: $L(w) = \dfrac{\|\vec{w}\|^2}{2}$
  - But subjected to the following constraints:

$$\vec{w} \cdot \vec{x}_i + b \geq 1 \text{ if } y_i = 1$$
$$\vec{w} \cdot \vec{x}_i + b \leq -1 \text{ if } y_i = -1$$

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

Noisy Data

- What if the problem is not linearly separable?



Slack Variables

- What if the problem is not linearly separable?
  - Introduce slack variables
    - Need to minimize:

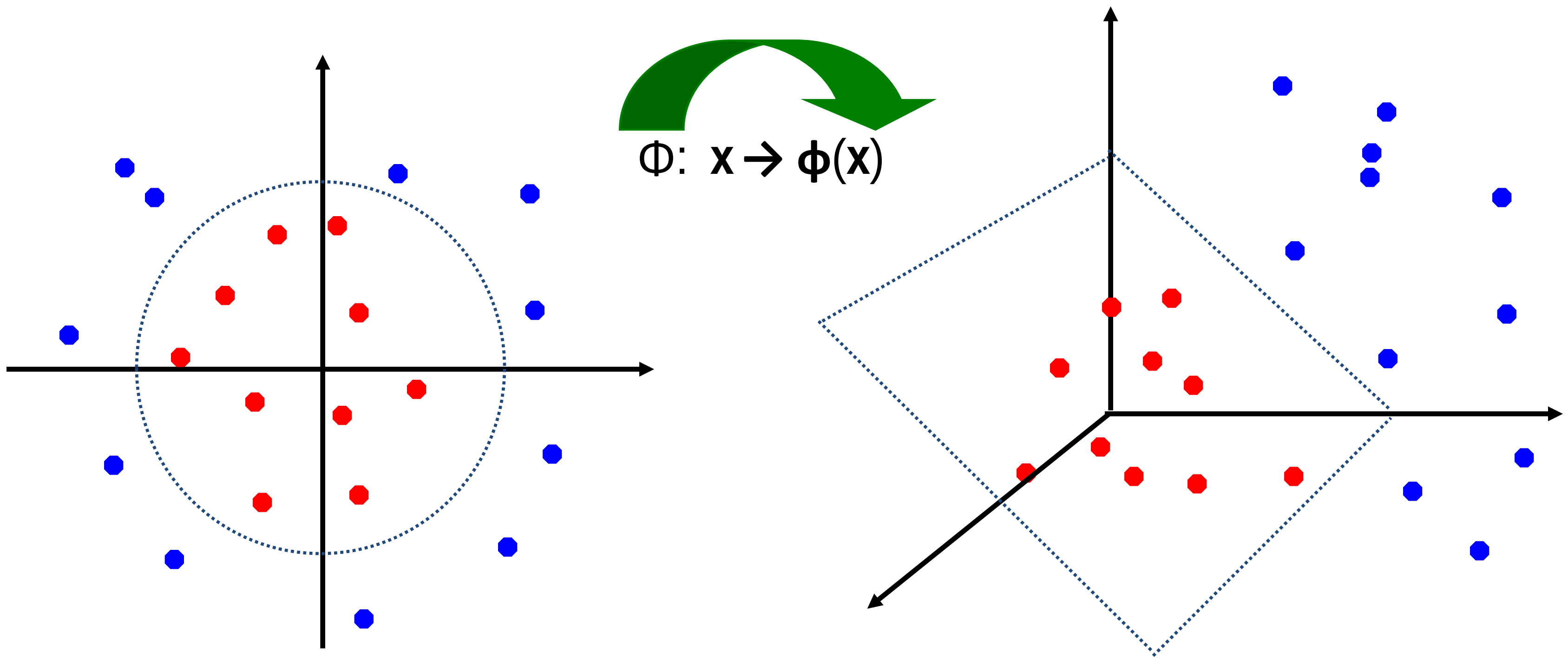
$$L(\vec{w}) = \frac{\|\vec{w}\|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k\right)$$

    - Subject to:

$$\vec{w} \cdot \vec{x}_i + b \geq 1 - \xi_i \quad \text{if } y_i = 1$$
$$\vec{w} \cdot \vec{x}_i + b \leq -1 + \xi_i \quad \text{if } y_i = -1$$

Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is linearly separable:



Ensemble Learning

- **Problem**
  - Given a data set $D=\{x_1,x_2,\ldots,x_n\}$ and their corresponding labels $L=\{l_1,l_2,\ldots,l_n\}$
  - An ensemble approach computes:
    - A set of classifiers $\{f_1,f_2,\ldots,f_k\}$, each of which maps data to a class label: $f_j(x)=l$
    - A combination of classifiers f^* which minimizes generalization error: $f^*(x)= w_1f_1(x)+ w_2f_2(x)+\ldots+ w_kf_k(x)$

Generating Base Classifiers

- **Sampling training examples**
  - Train k classifiers on k subsets drawn from the training set
- **Using different learning models**
  - Use all the training examples, but apply different learning algorithms
- **Sampling features**
  - Train k classifiers on k subsets of features drawn from the feature space
- **Learning “randomly”**
  - Introduce randomness into learning procedures

Bagging (1)

- **Bootstrap**
  - Sampling with replacement
  - Contains around 63.2% original records in each sample
- **Bootstrap Aggregation**
  - Train a classifier on each bootstrap sample
  - Use majority voting to determine the class label of ensemble classifier

Bagging (2)

Original Data:

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
y	1	1	1	-1	-1	-1	-1	1	1	1

Bootstrap samples and classifiers:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x	0.1	0.2	0.3	0.4	0.5	0.5	0.9	1	1	1
y	1	1	1	-1	-1	-1	1	1	1	1

x	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x	0.1	0.2	0.5	0.5	0.5	0.7	0.7	0.8	0.9	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

Combine predictions by majority voting

Boosting (1)

- **Principles**
  - Boost a set of weak learners to a strong learner
  - Make records currently misclassified more important

- **Example**
  - Record 4 is hard to classify
  - Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

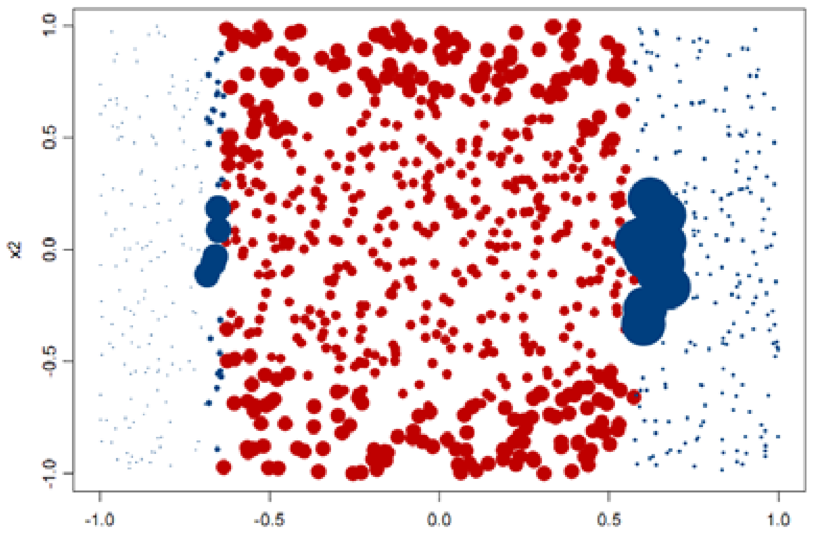
Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

Boosting (2)

- **AdaBoost**
  - Initially, set uniform weights on all the records
  - At each round
    - Create a bootstrap sample based on the weights
    - Train a classifier on the sample and apply it on the original training set
    - Records that are wrongly classified will have their weights increased
    - Records that are classified correctly will have their weights decreased
    - If the error rate is higher than 50%, start over
  - Final prediction is weighted average of all the classifiers with weight representing the training accuracy

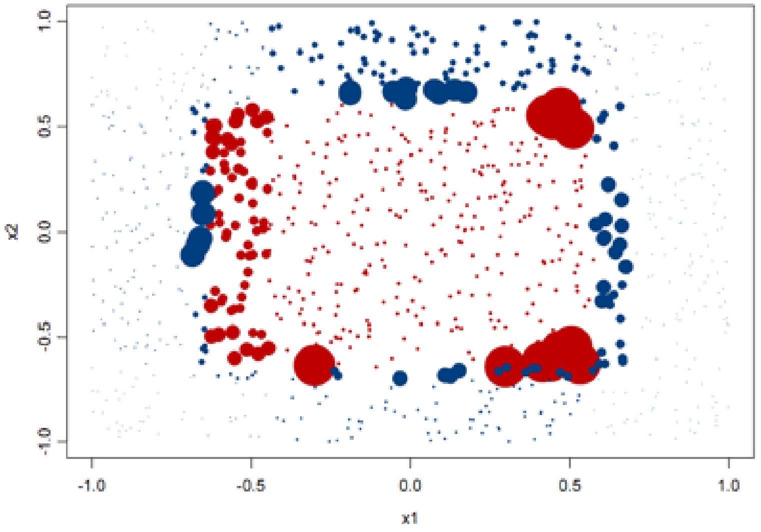
Boosting (3)

- **Determine the weight**
  - For classifier *i*, its error is
$$\varepsilon_i = \frac{\sum_{j=1}^{N} w_j \delta(C_i(x_j) \neq y_j)}{\sum_{j=1}^{N} w_j}$$
  - The classifier's importance is represented as:
$$\alpha_i = \frac{1}{2} \ln\left(\frac{1-\varepsilon_i}{\varepsilon_i}\right)$$
  - The weight of each record is updated as:
$$w_j^{(i+1)} = \frac{w_j^{(i)} \exp\left(-\alpha_i y_j C_i(x_j)\right)}{Z^{(i)}}$$
  - Final combination:
$$C^*(x) = \arg\max_y \sum_{i=1}^{K} \alpha_i \delta\left(C_i(x) = y\right)$$

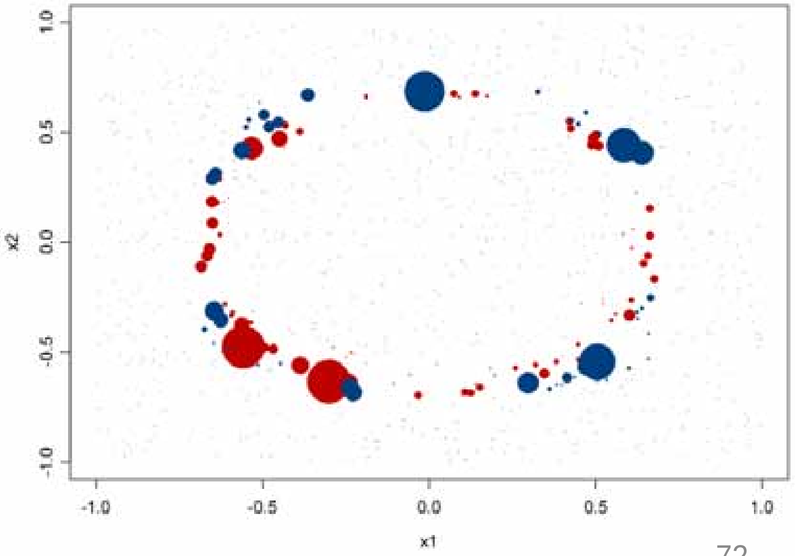


Classifications (colors) and Weights (size) after *1 iteration* Of AdaBoost

3 iterations



20 iterations



Boosting (4)

- **Explanation**
  - Among the classifiers of the form:

$$f(x) = \sum_{i=1}^{K} \alpha_i C_i(x)$$

  - We seek to minimize the exponential loss function:

$$\sum_{j=1}^{N} \exp\left(-y_j f(x_j)\right)$$

  - Not robust in noisy settings

Random Forests (1)

- **Algorithm**
  - Choose *T*—number of trees to grow
  - Choose *m*<*M* (M is the number of total features) —number of features used to calculate the best split at each node (typically 20%)
  - For each tree
    - Choose a training set by choosing *N* times (*N* is the number of training examples) with replacement from the training set
    - For each node, randomly choose *m* features and calculate the best split
    - Fully grown and not pruned
  - Use majority voting among all the trees

Random Forests (2)

- **Discussions**
  - Bagging+random features
  - Improve accuracy
    - Incorporate more diversity and reduce variances
  - Improve efficiency
    - Searching among subsets of features is much faster than searching among the complete set

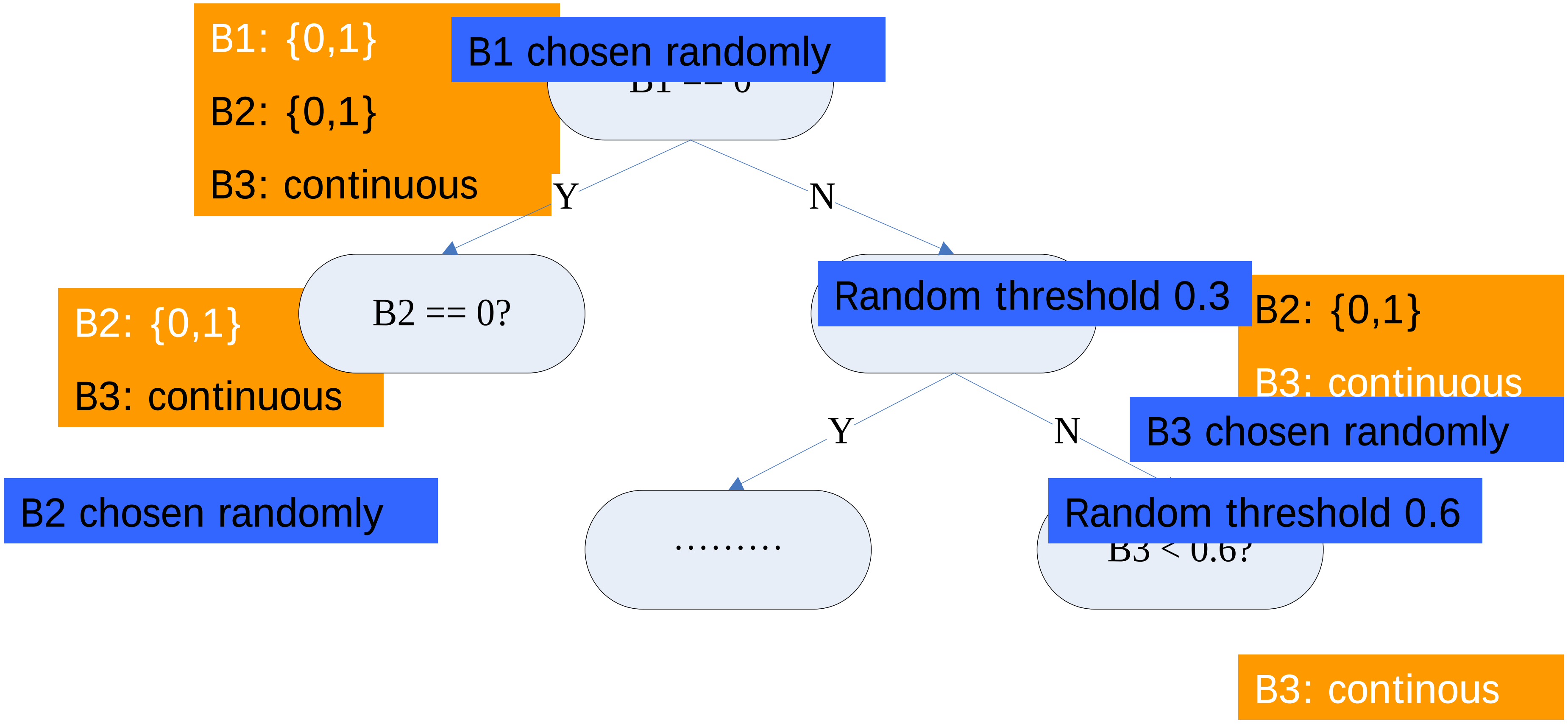
Random Decision Tree (1)

- **Single-model learning algorithms**
  - Fix structure of the model, minimize some form of errors, or maximize data likelihood (eg., Logistic regression, Naive Bayes, etc.)
  - Use some “free-form” functions to match the data given some “preference criteria” such as information gain, gini index and MDL. (eg., Decision Tree, Rule-based Classifiers, etc.)
- **Such methods will make mistakes if**
  - Data is insufficient
  - Structure of the model or the preference criteria is inappropriate for the problem
- **Learning as Encoding**
  - Make no assumption about the true model, neither parametric form nor free form
  - Do not prefer one base model over the other, just average them

Random Decision Tree (2)

- **Algorithm**
  - At each node, an un-used feature is chosen randomly
    - A discrete feature is un-used if it has never been chosen previously on a given decision path starting from the root to the current node.
    - A continuous feature can be chosen multiple times on the same decision path, but each time a different threshold value is chosen
  - We stop when one of the following happens:
    - A node becomes too small (<= 3 examples).
    - Or the total height of the tree exceeds some limits, such as the total number of features.
  - Prediction
    - Simple averaging over multiple trees

Random Decision Tree (3)

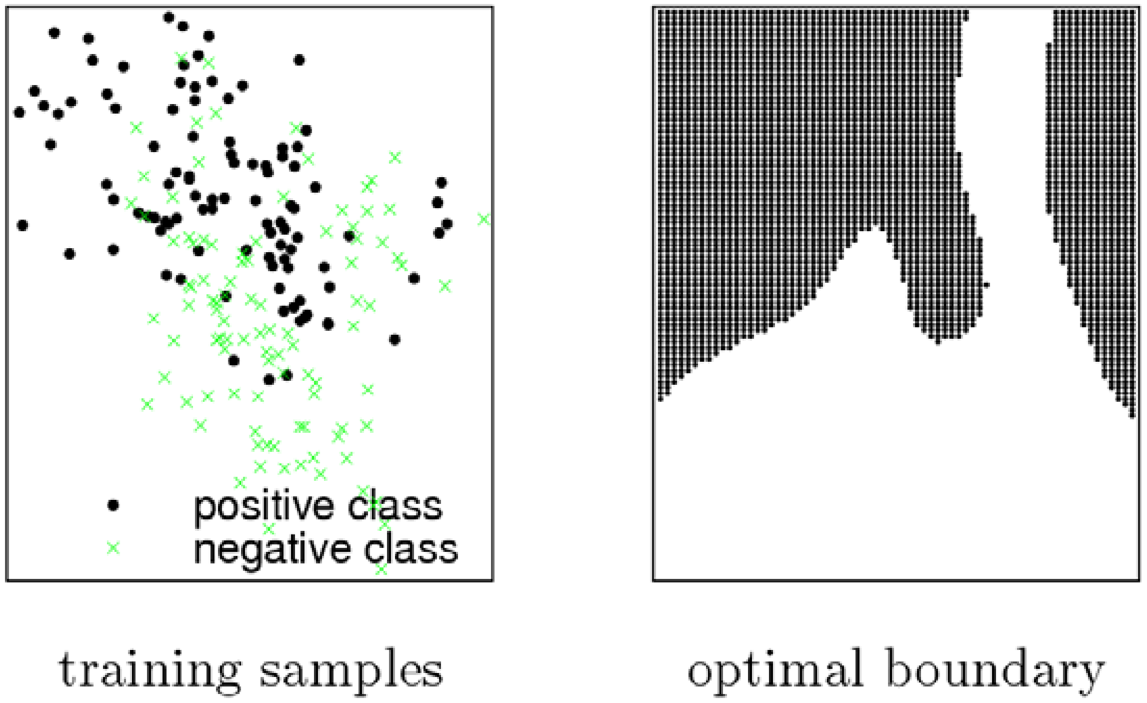


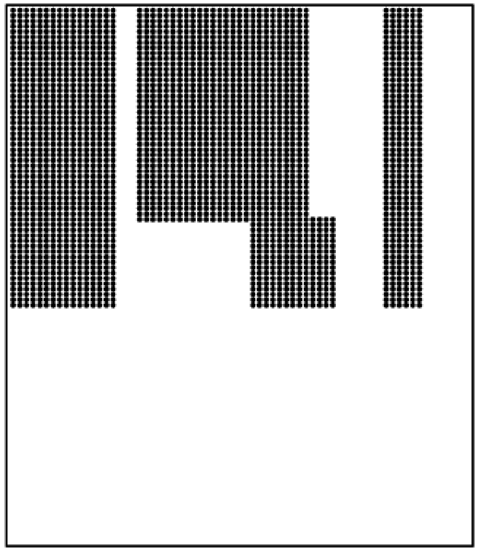
Random Decision Tree (4)

- **Advantages**
  - Training can be very efficient. Particularly true for very large datasets.
    - No cross-validation based estimation of parameters for some parametric methods.
  - Natural multi-class probability.
  - Imposes very little about the structures of the model.

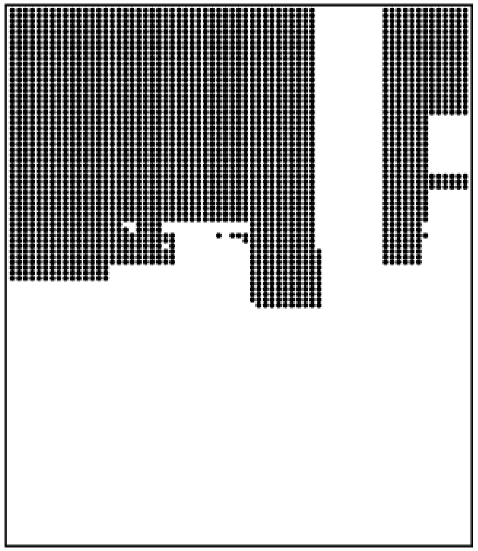
Optimal Decision Boundary

Figure 3.5: Gaussian mixture training samples and optimal boundary.

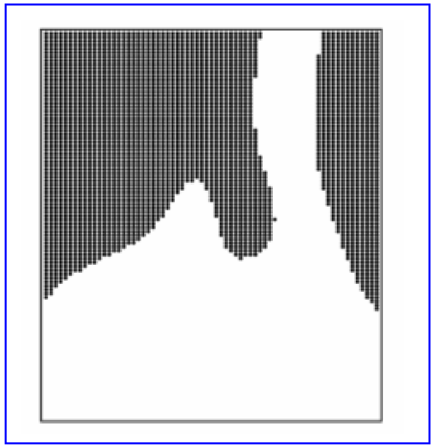


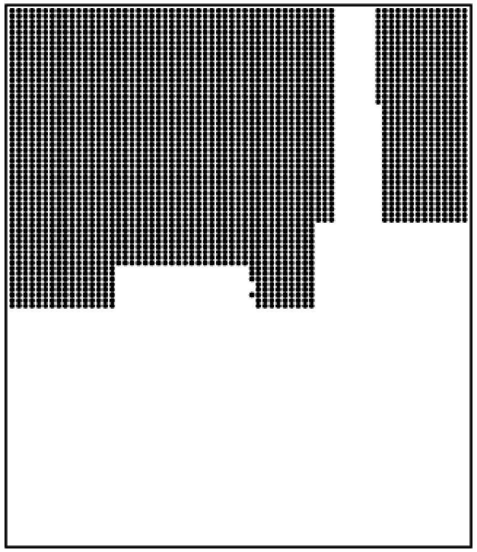


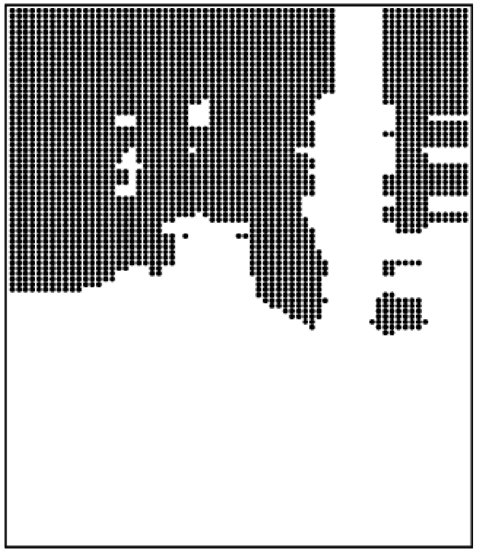
(a) unpruned C4.5



(b) Bagging







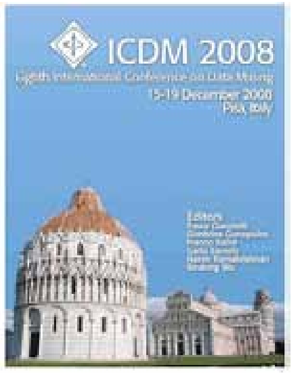
RDT looks like the optimal boundary

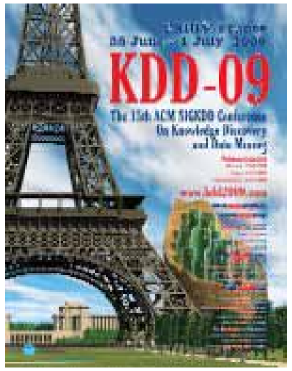
(c) Random Forests

(d) Complete-random tree ensemble

Ensemble Learning--Stories of Success

- Million-dollar prize
  - Improve the baseline movie recommendation approach of Netflix by 10% in accuracy
  - The top submissions all combine several teams and algorithms as an ensemble



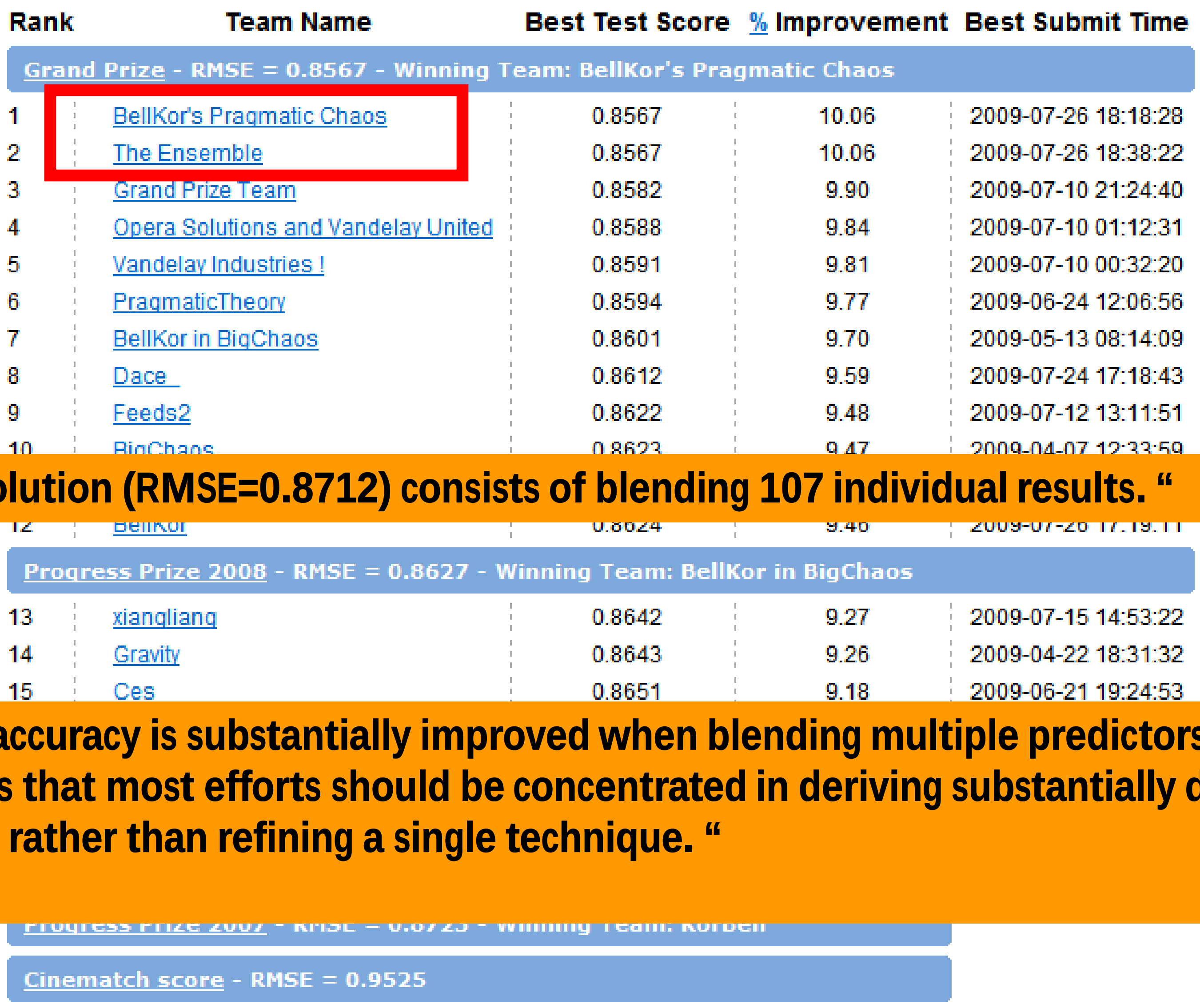


- Data mining competitions
  - Classification problems
  - Winning teams employ an ensemble of classifiers

Netflix Prize

- Supervised learning task
  - Training data is a set of users and ratings (1,2,3,4,5 stars) those users have given to movies.
  - Construct a classifier that given a user and an unrated movie, correctly classifies that movie as either 1, 2, 3, 4, or 5 stars
  - $1 million prize for a 10% improvement over Netflix’s current movie recommender
- Competition
  - At first, single-model methods are developed, and performances are improved
  - However, improvements slowed down
  - Later, individuals and teams merged their results, and significant improvements are observed

Leaderboard



Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace_	0.8612	9.59	2009-07-24 17:18:43
9	Feeds2	0.8622	9.48	2009-07-12 13:11:51
10	BigChaos	0.8623	9.47	2009-04-07 12:33:59
12	BellKor	0.8624	9.46	2009-07-26 17:19:11
Progress Prize 2008 - RMSE = 0.8627 - Winning Team: BellKor in BigChaos				
13	xiangliang	0.8642	9.27	2009-07-15 14:53:22
14	Gravity	0.8643	9.26	2009-04-22 18:31:32
15	Ces	0.8651	9.18	2009-06-21 19:24:53
Progress Prize 2007 - RMSE = 0.8723 - Winning Team: KorBell				
Cinematch score - RMSE = 0.9525				

“Our final solution (RMSE=0.8712) consists of blending 107 individual results. “

“Predictive accuracy is substantially improved when blending multiple predictors. Our experience is that most efforts should be concentrated in deriving substantially different approaches, rather than refining a single technique. “

Take-away Message

- Various classification approaches
  - how they work
  - their strengths and weakness
- Algorithms
  - Decision tree
  - K nearest neighbors
  - Naive Bayes
  - Logistic regression
  - Rule-based classifier
  - SVM
  - Ensemble method