DATA MINING
LECTURE 10

Classification

k-nearest neighbor classifier
Naïve Bayes
Logistic Regression
Support Vector Machines

NEAREST NEIGHBOR CLASSIFICATION

Instance-Based Classifiers

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

Set of Stored Cases

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

Unseen Case

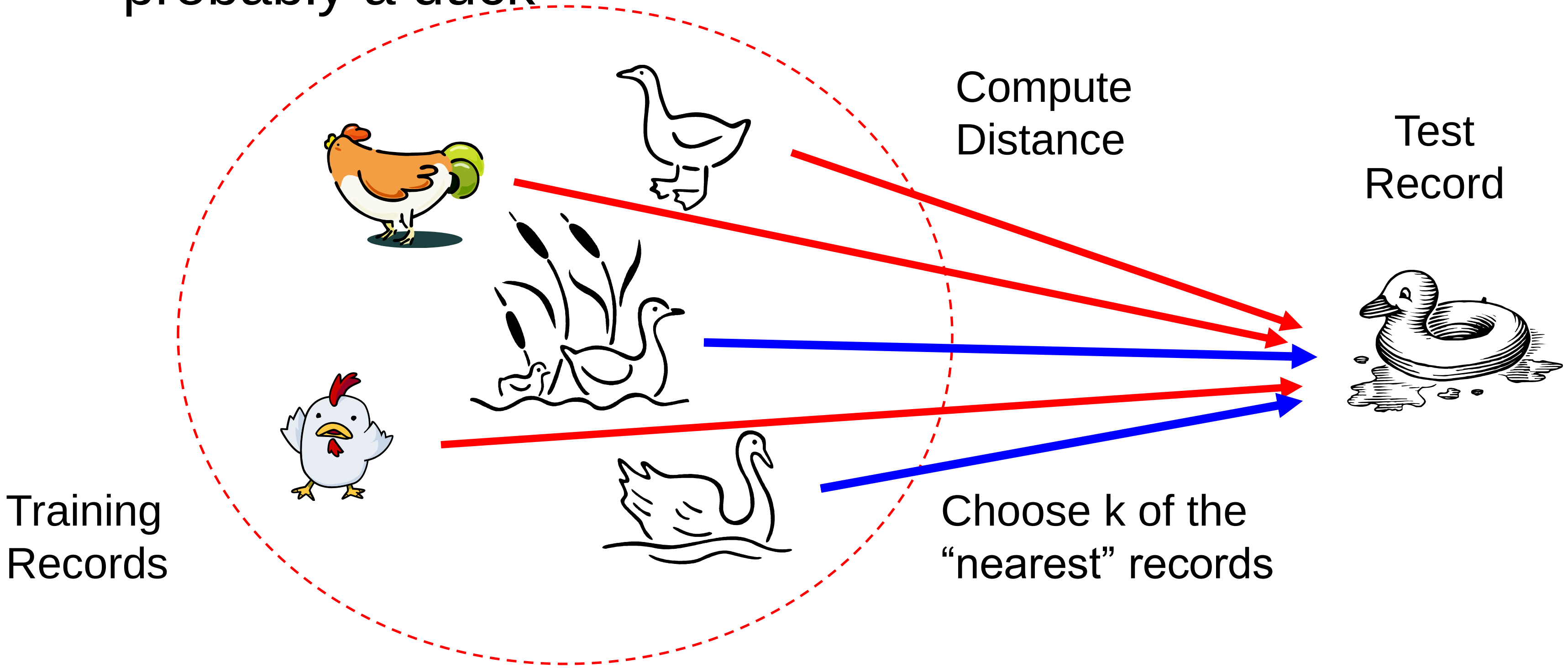
Atr1	………	AtrN

Instance Based Classifiers

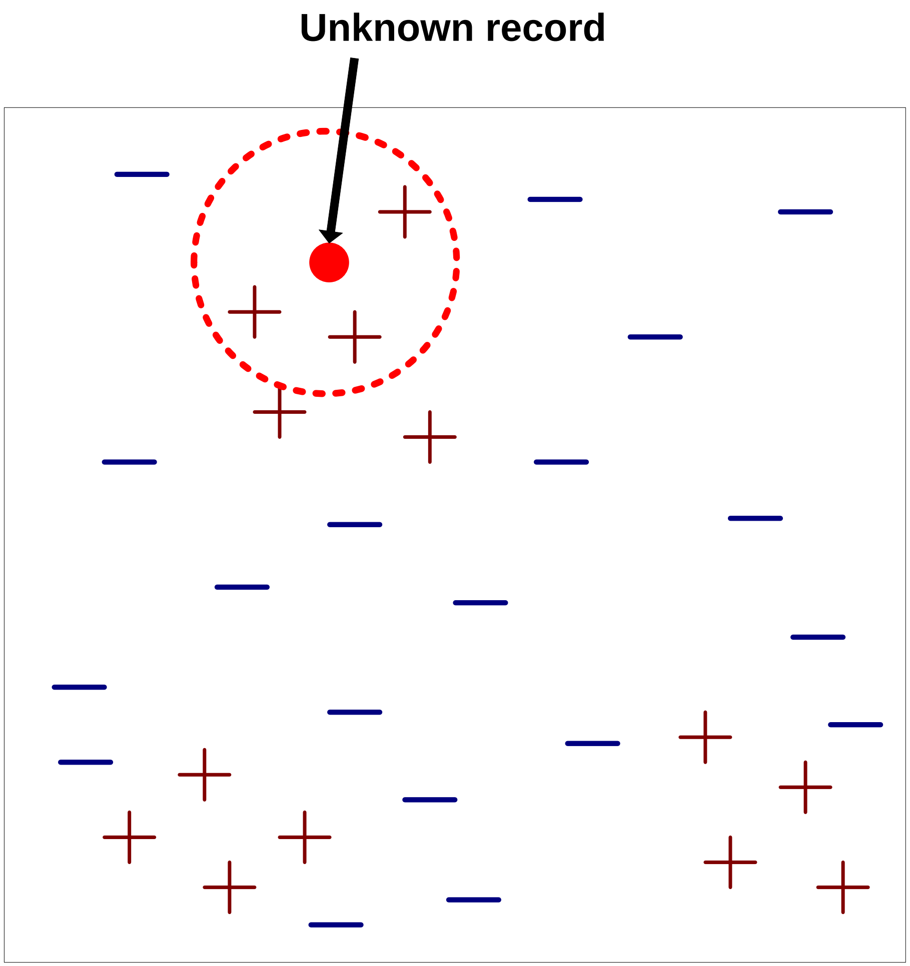
- Examples:
  - Rote-learner
    - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
  - Nearest neighbor
    - Uses k “closest” points (nearest neighbors) for performing classification

Nearest Neighbor Classifiers

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



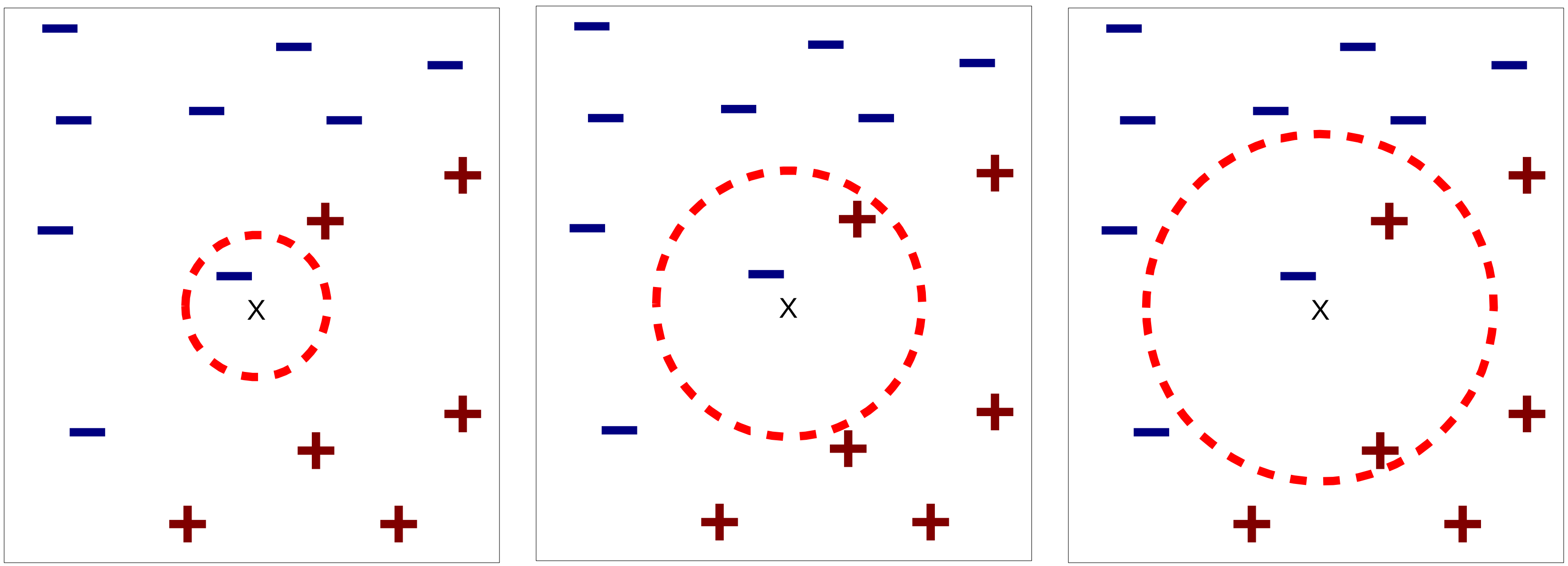
Nearest-Neighbor Classifiers



- 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)

Definition of Nearest Neighbor

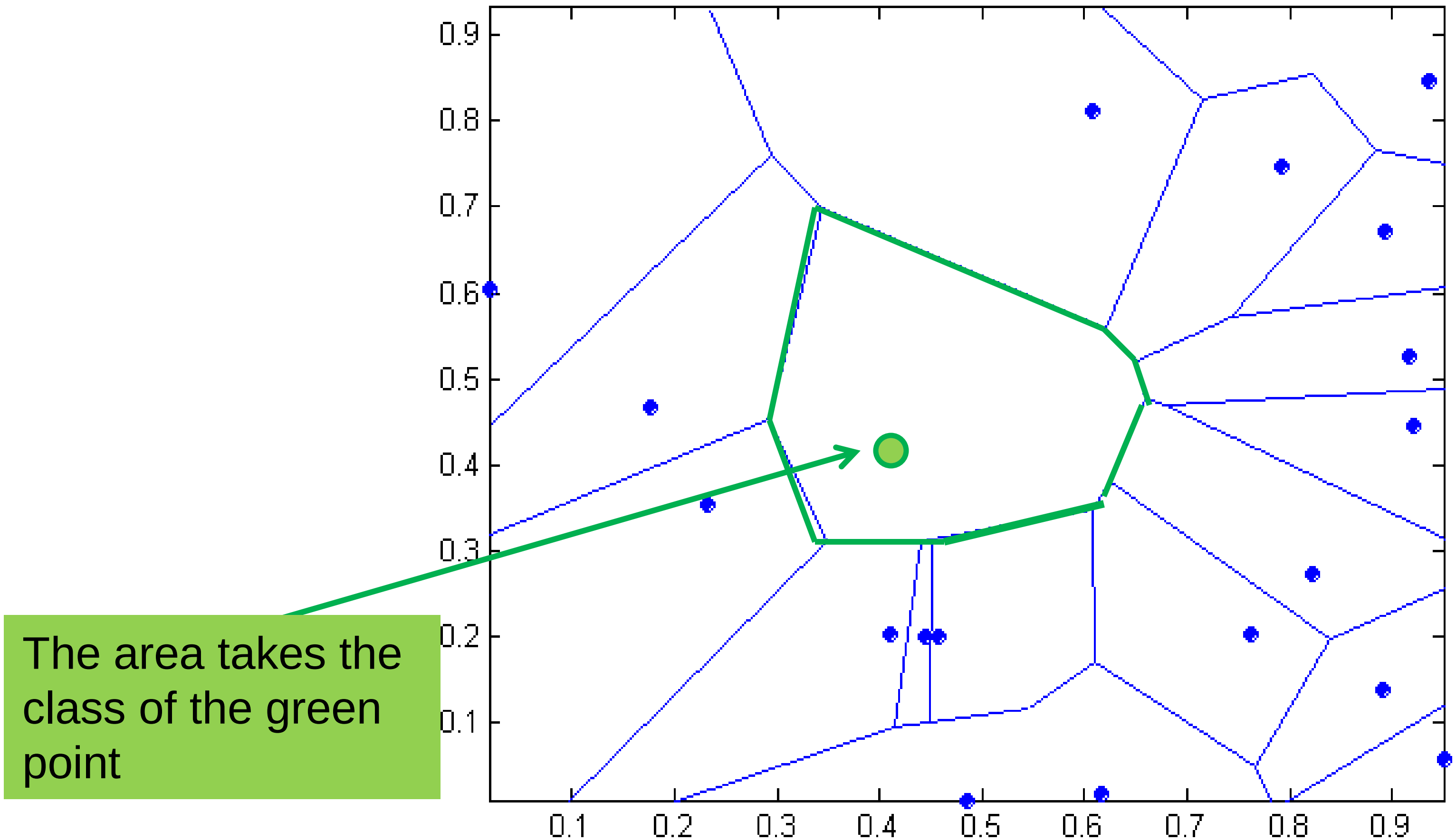


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

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

1 nearest-neighbor

Voronoi Diagram defines the classification boundary



Nearest Neighbor Classification

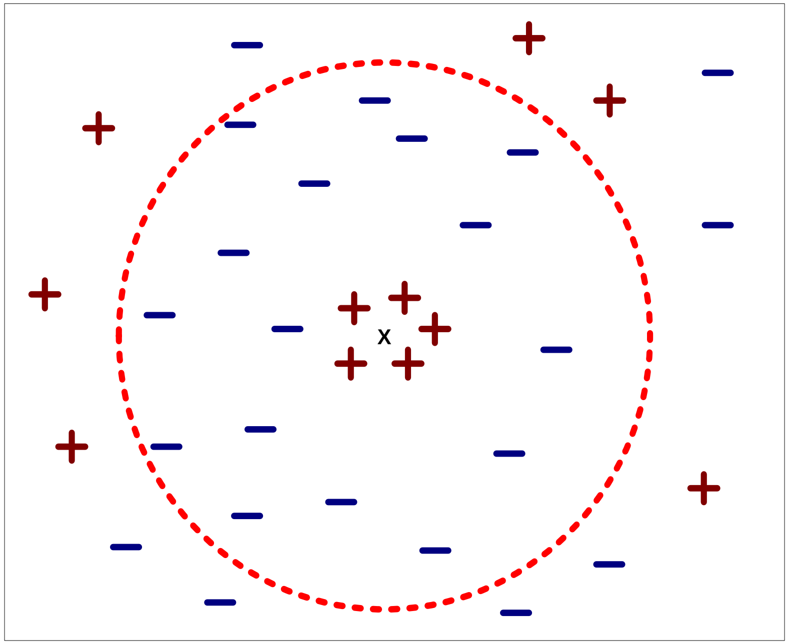
- Compute distance between two points:
  - Euclidean distance

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

- 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…

- 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	vs	1 0 0 0 0 0 0 0 0 0 0 0
0 1 1 1 1 1 1 1 1 1 1 1		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

Nearest neighbor Classification…

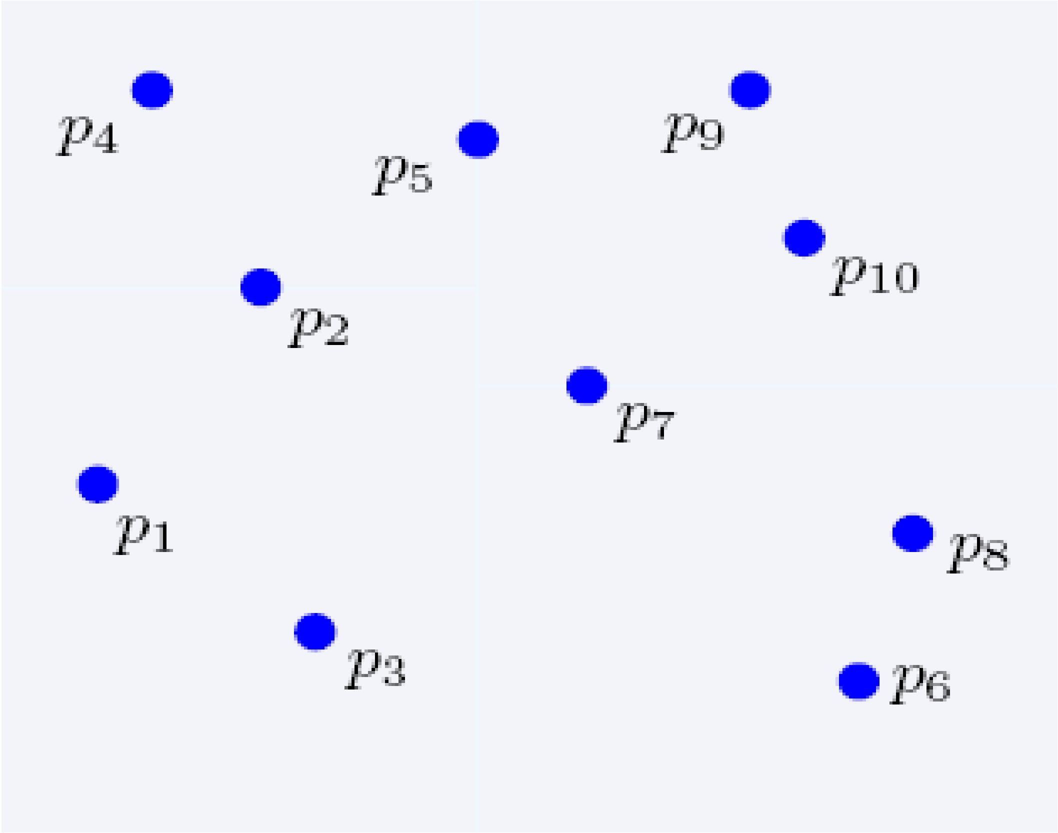
- k-NN classifiers are lazy learners
  - It does not build models explicitly
  - Unlike eager learners such as decision tree induction and rule-based systems
- Classifying unknown records are relatively expensive
  - Naïve algorithm: O(n)
  - Need for structures to retrieve nearest neighbors fast.
    - The Nearest Neighbor Search problem.

Nearest Neighbor Search

- Two-dimensional kd-trees
  - A data structure for answering nearest neighbor queries in R^2

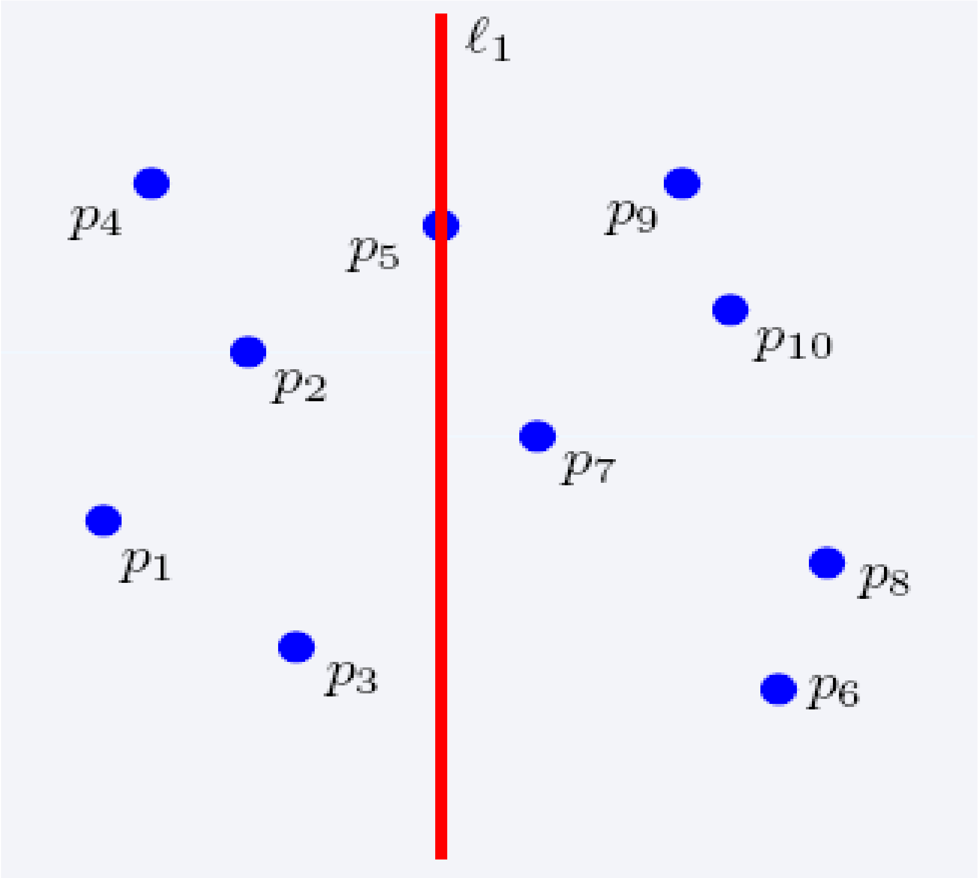
- kd-tree construction algorithm
  - Select the x or y dimension (alternating between the two)
  - Partition the space into two with a line passing from the median point
  - Repeat recursively in the two partitions as long as there are enough points

Nearest Neighbor Search



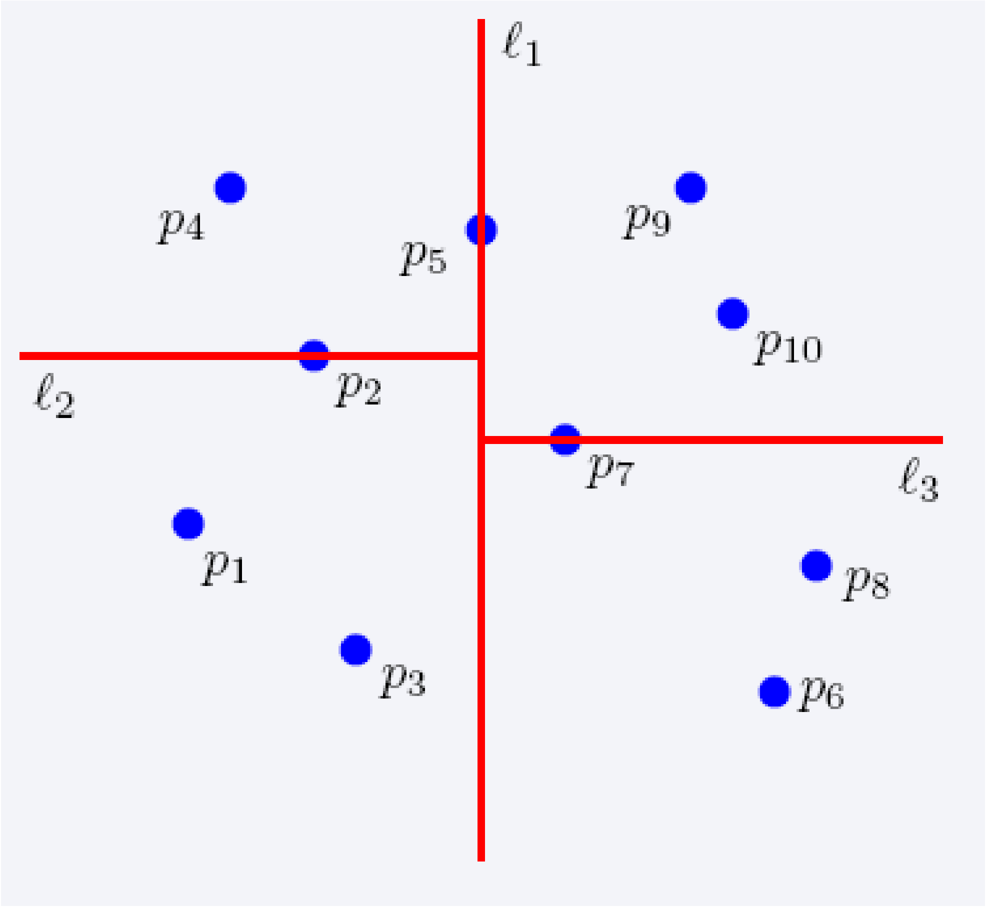
2-dimensional kd-trees

Nearest Neighbor Search



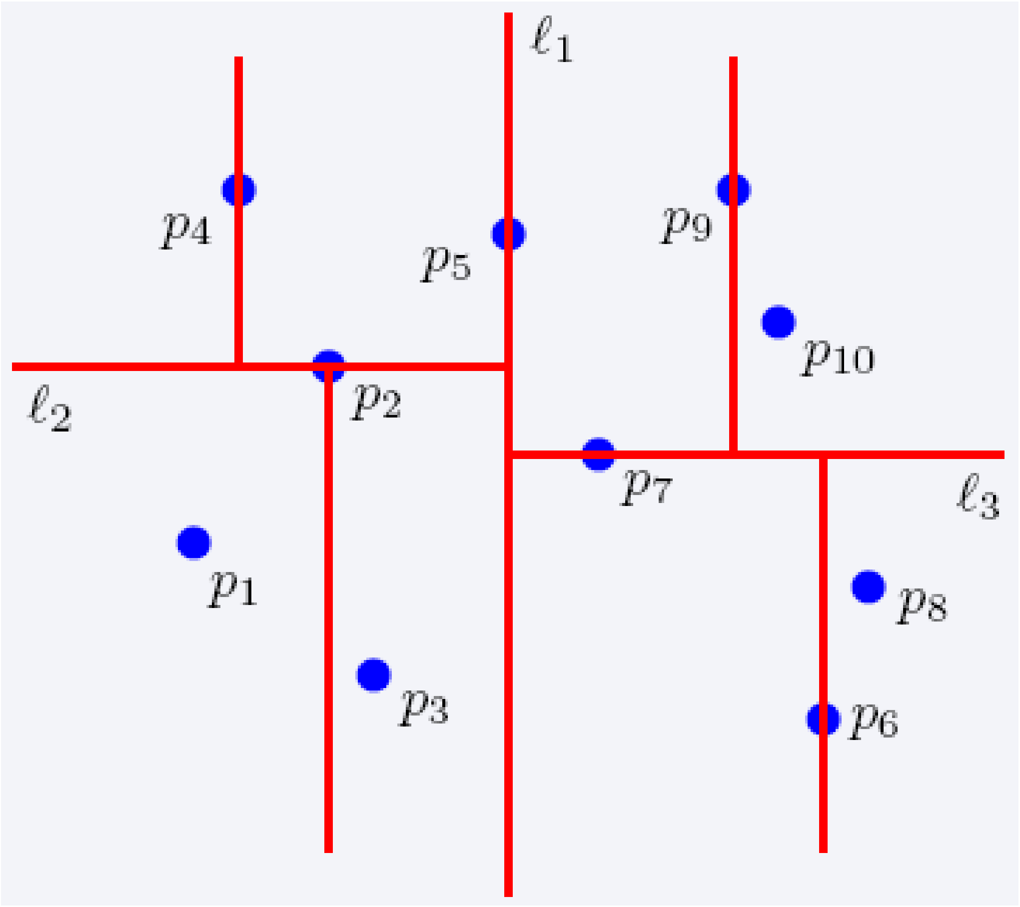
2-dimensional kd-trees

Nearest Neighbor Search



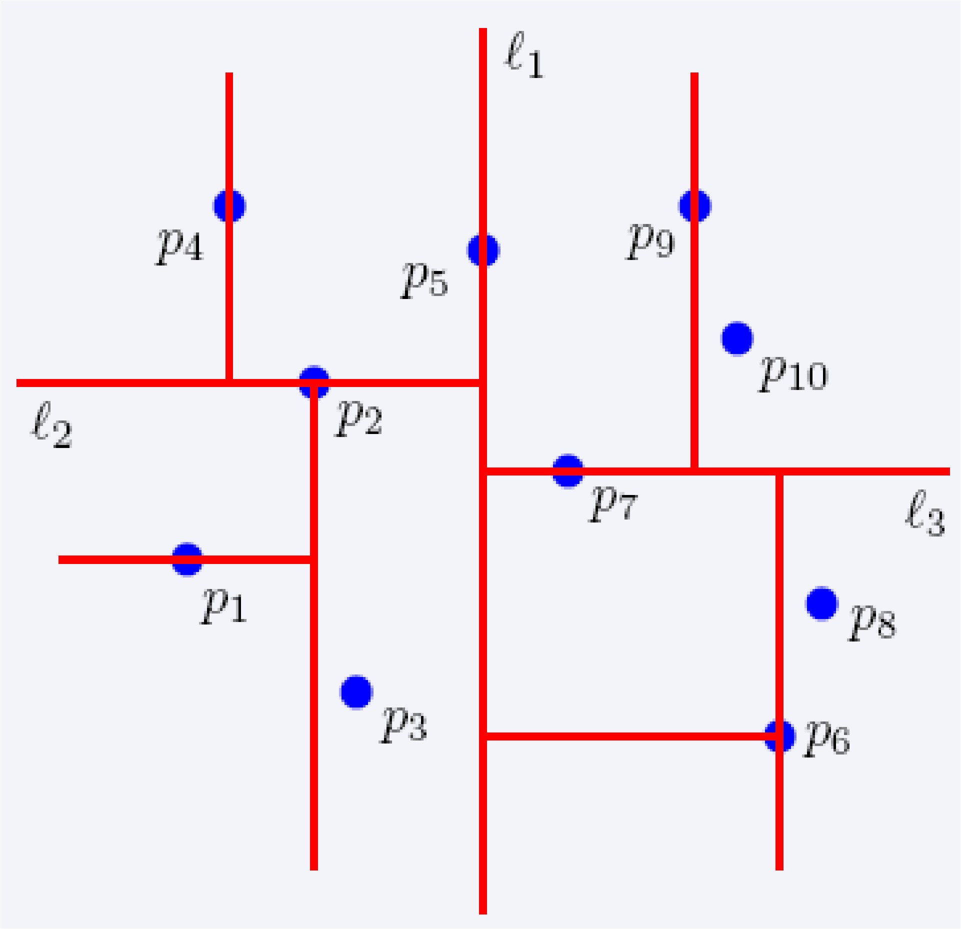
2-dimensional kd-trees

Nearest Neighbor Search



2-dimensional kd-trees

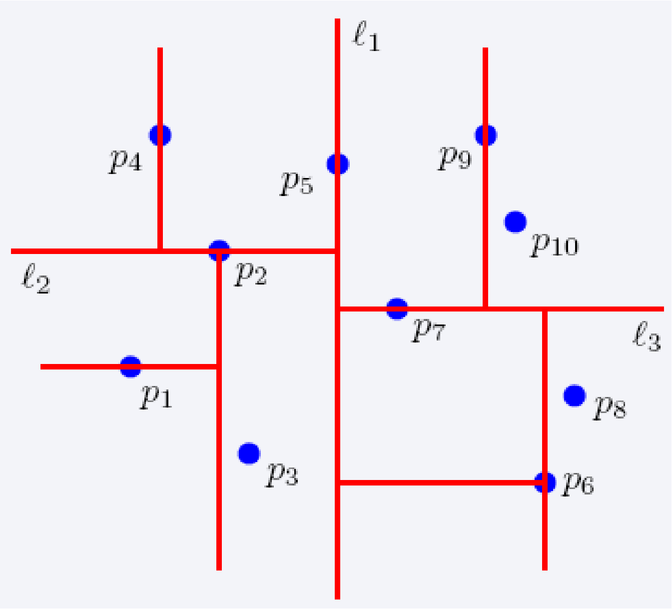
Nearest Neighbor Search

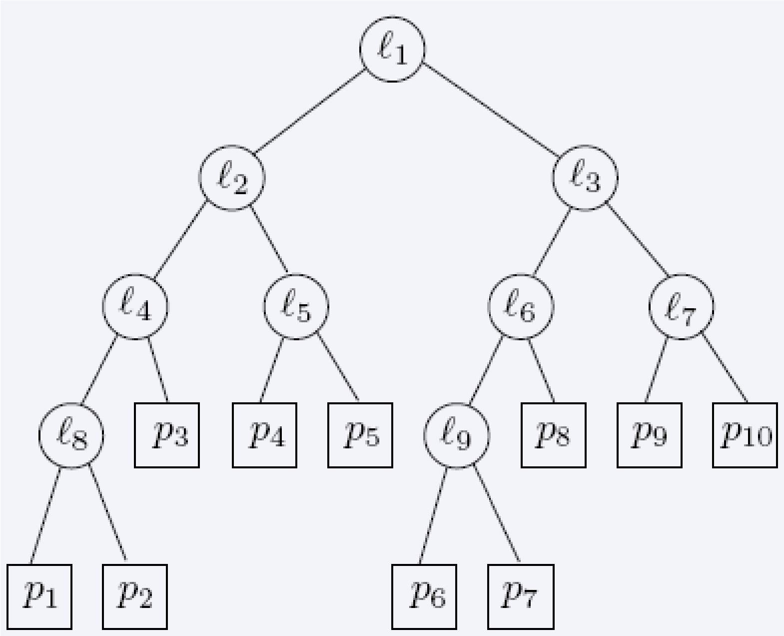


2-dimensional kd-trees

Nearest Neighbor Search

2-dimensional kd-trees

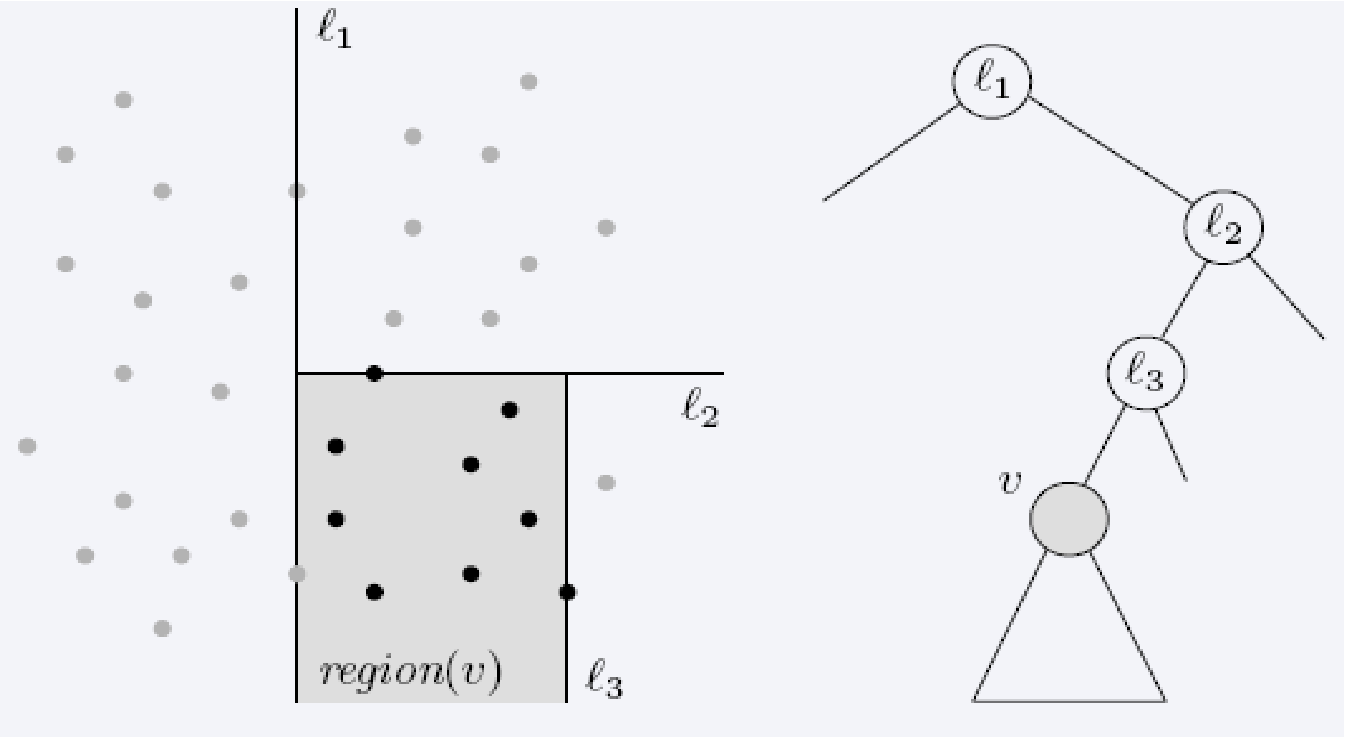




Nearest Neighbor Search

2-dimensional kd-trees

region(u) – all the black points in the subtree of u



Nearest Neighbor Search

2-dimensional kd-trees

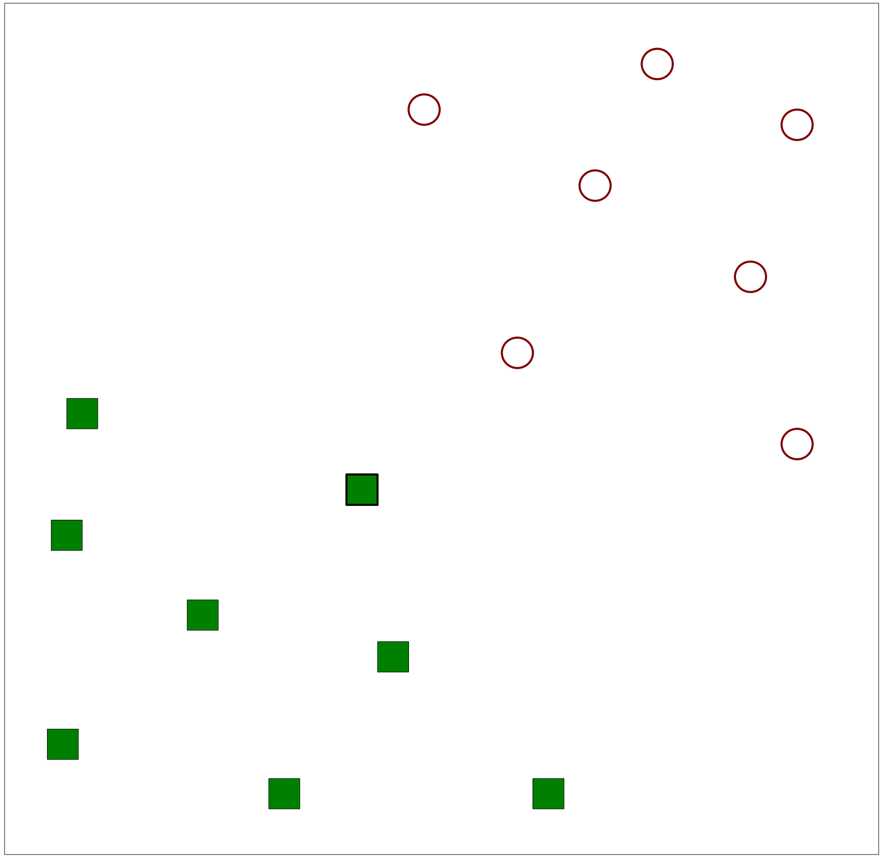
- A binary tree:
  - Size **O(n)**
  - Depth **O(logn)**
  - Construction time **O(nlogn)**
  - Query time: worst case **O(n),** but for many cases **O(logn)**

Generalizes to d dimensions

- Example of Binary Space Partitioning

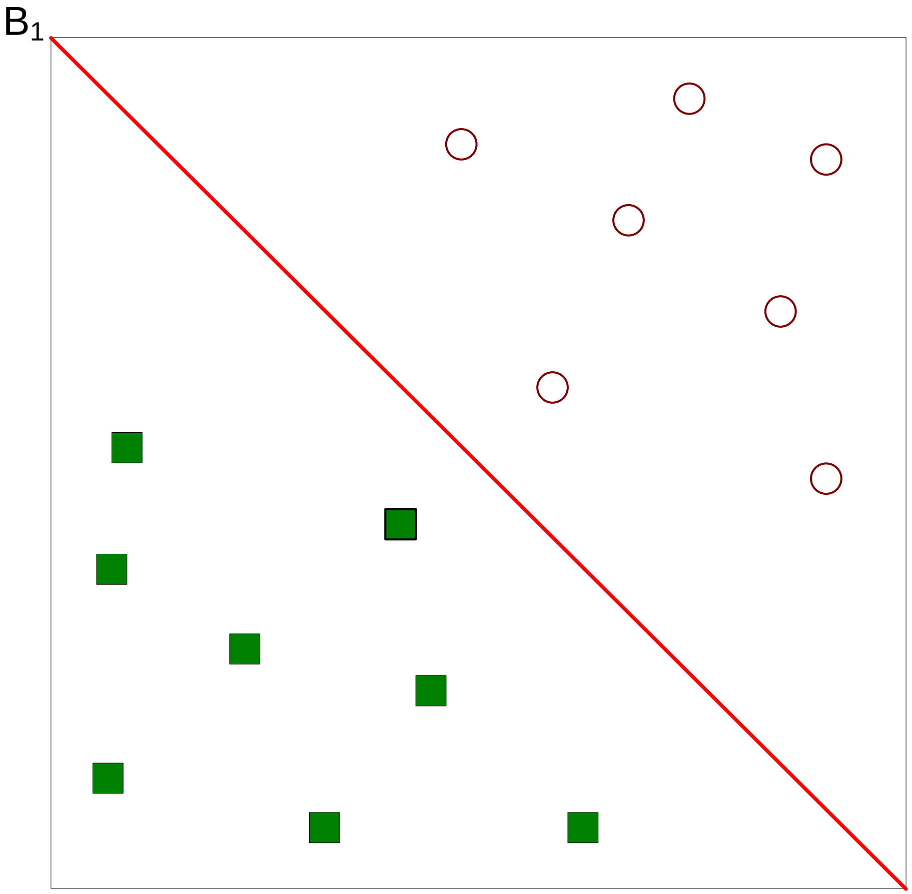
SUPPORT VECTOR MACHINES

Support Vector Machines



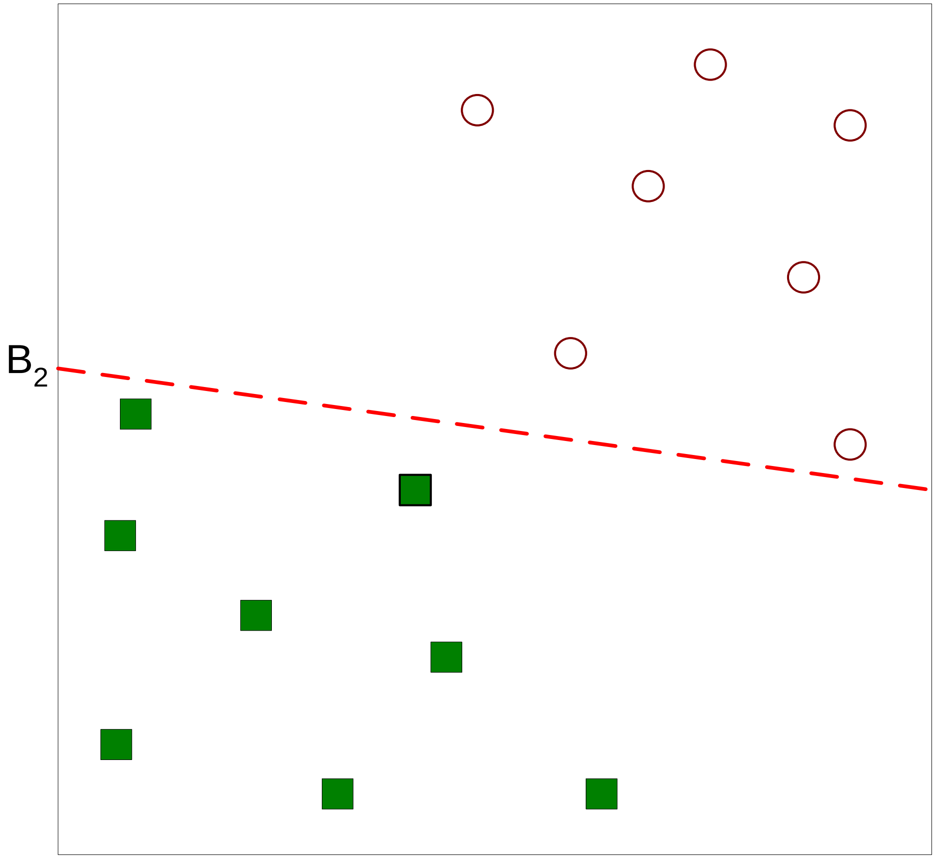
- Find a linear hyperplane (decision boundary) that will separate the data

Support Vector Machines



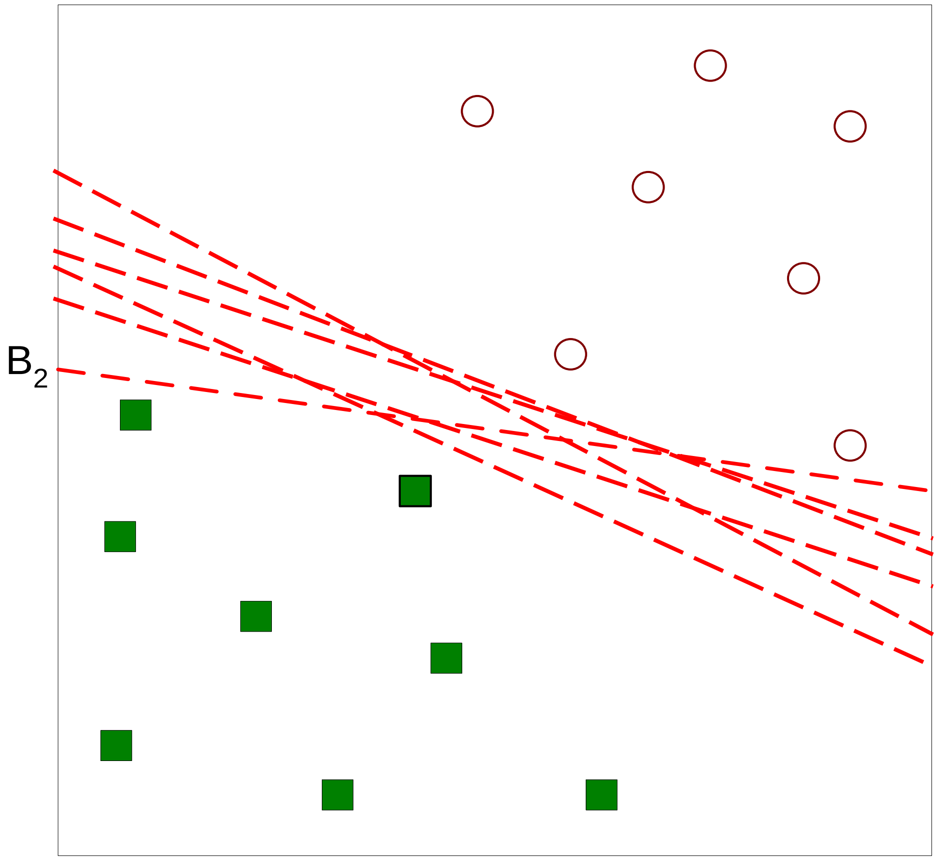
- One Possible Solution

Support Vector Machines



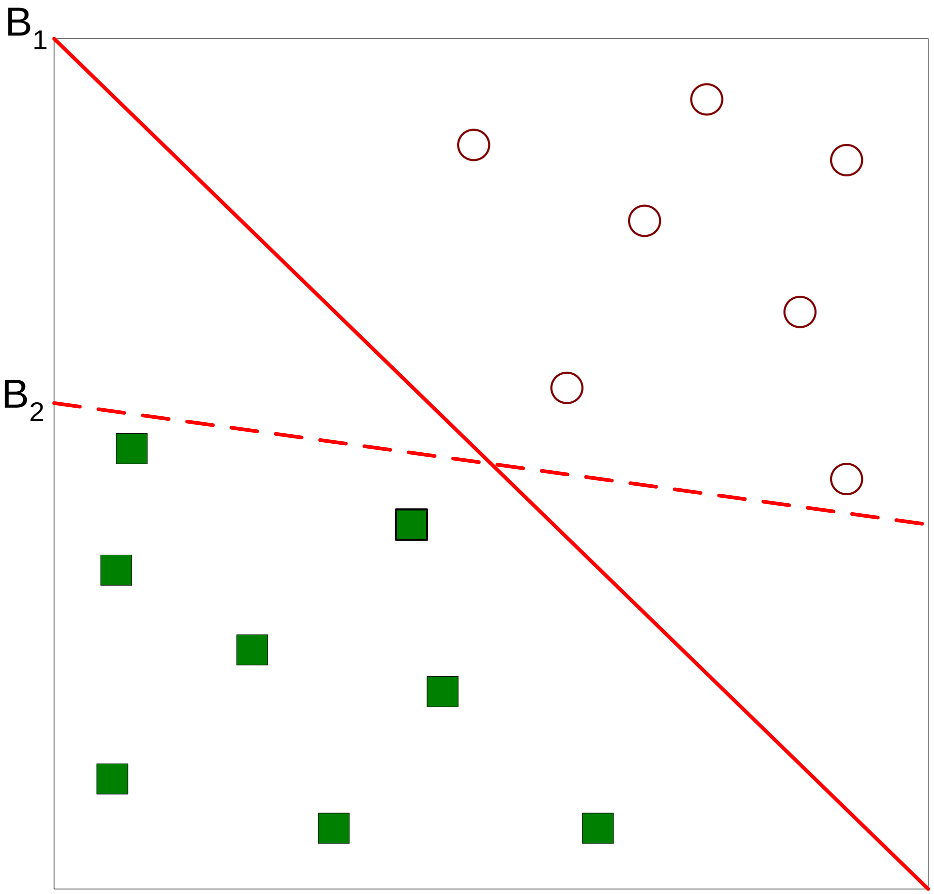
- Another possible solution

Support Vector Machines



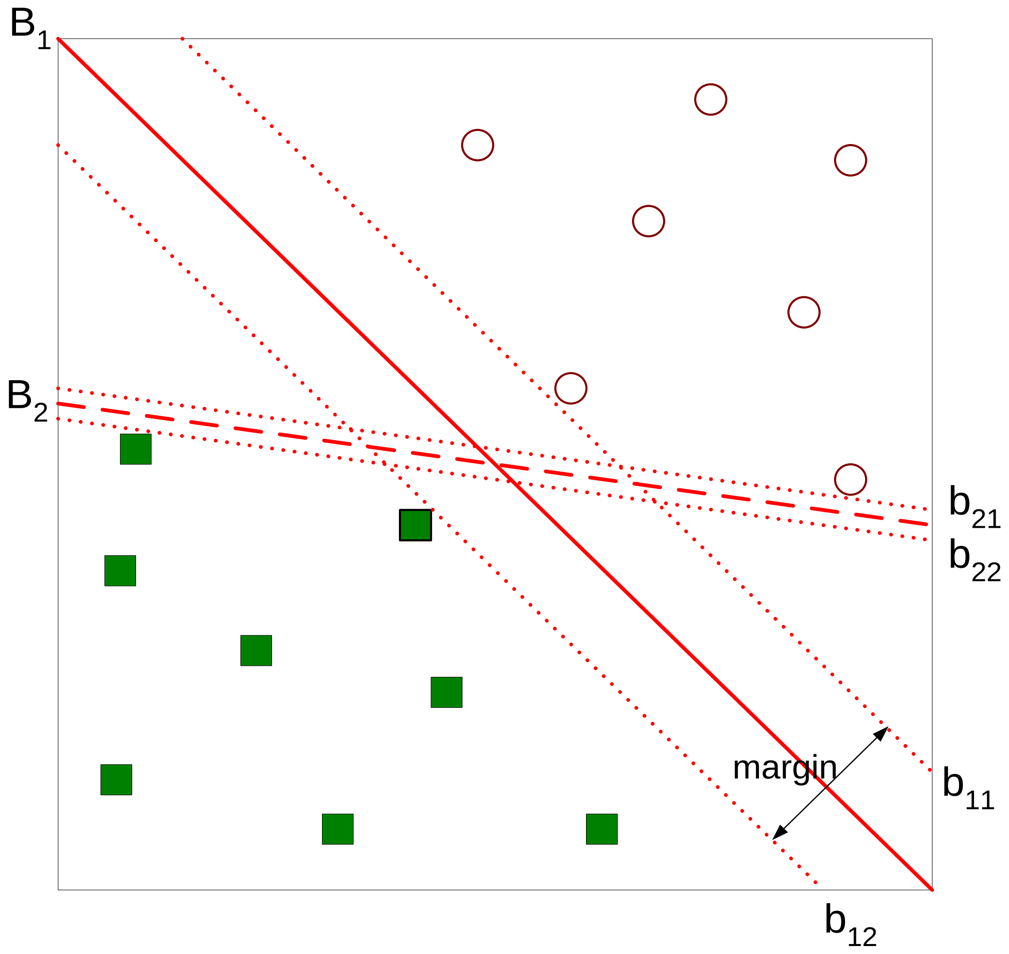
- Other possible solutions

Support Vector Machines



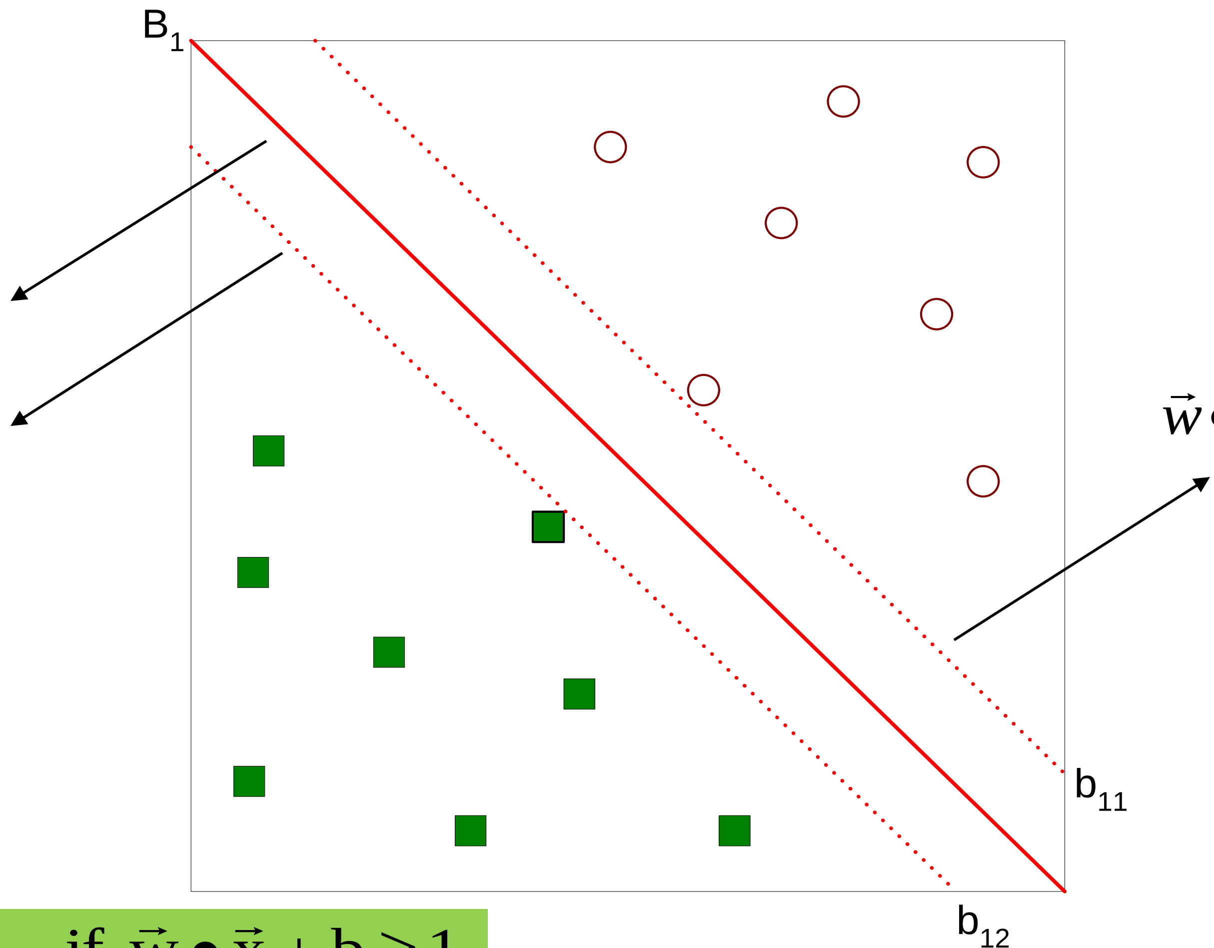
- Which one is better? B1 or B2?
- How do you define better?

Support Vector Machines



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

Support Vector Machines



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

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

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

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

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

Support Vector Machines

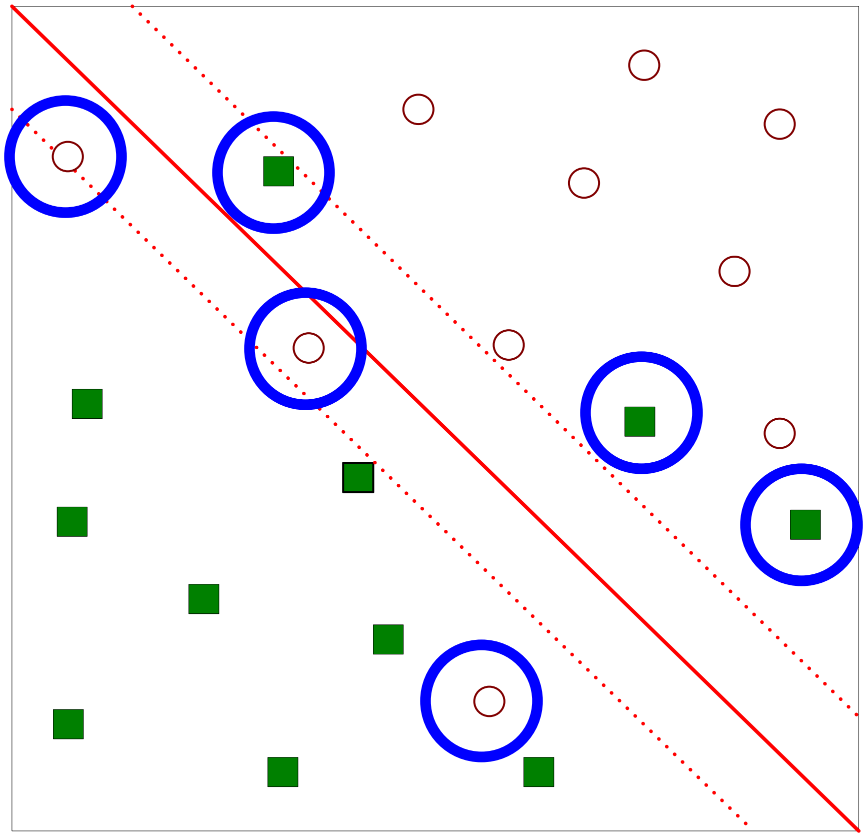
- We want to maximize: $\text{Margin} = \dfrac{2}{\|\vec{w}\|^2}$
  - Which is equivalent to minimizing: $L(w) = \dfrac{\|\vec{w}\|^2}{2}$
  - But subjected to the following constraints:

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

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

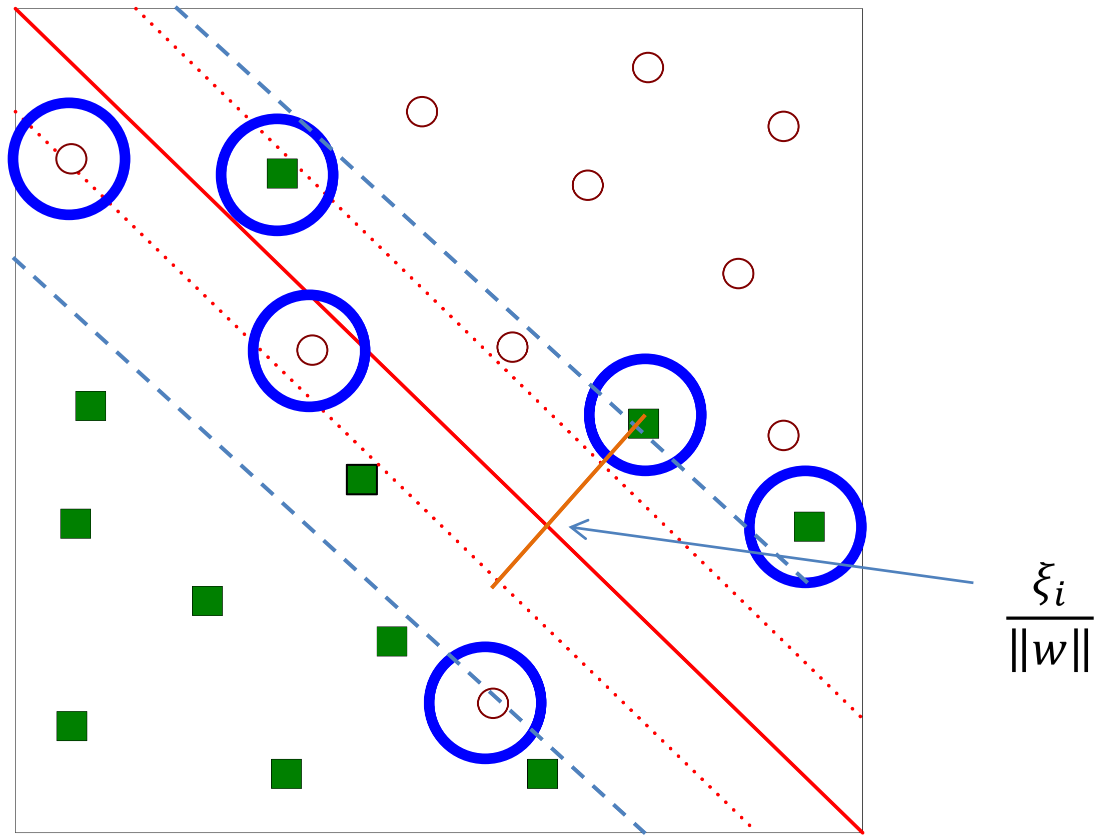
Support Vector Machines

- What if the problem is not linearly separable?



Support Vector Machines

- What if the problem is not linearly separable?



Support Vector Machines

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

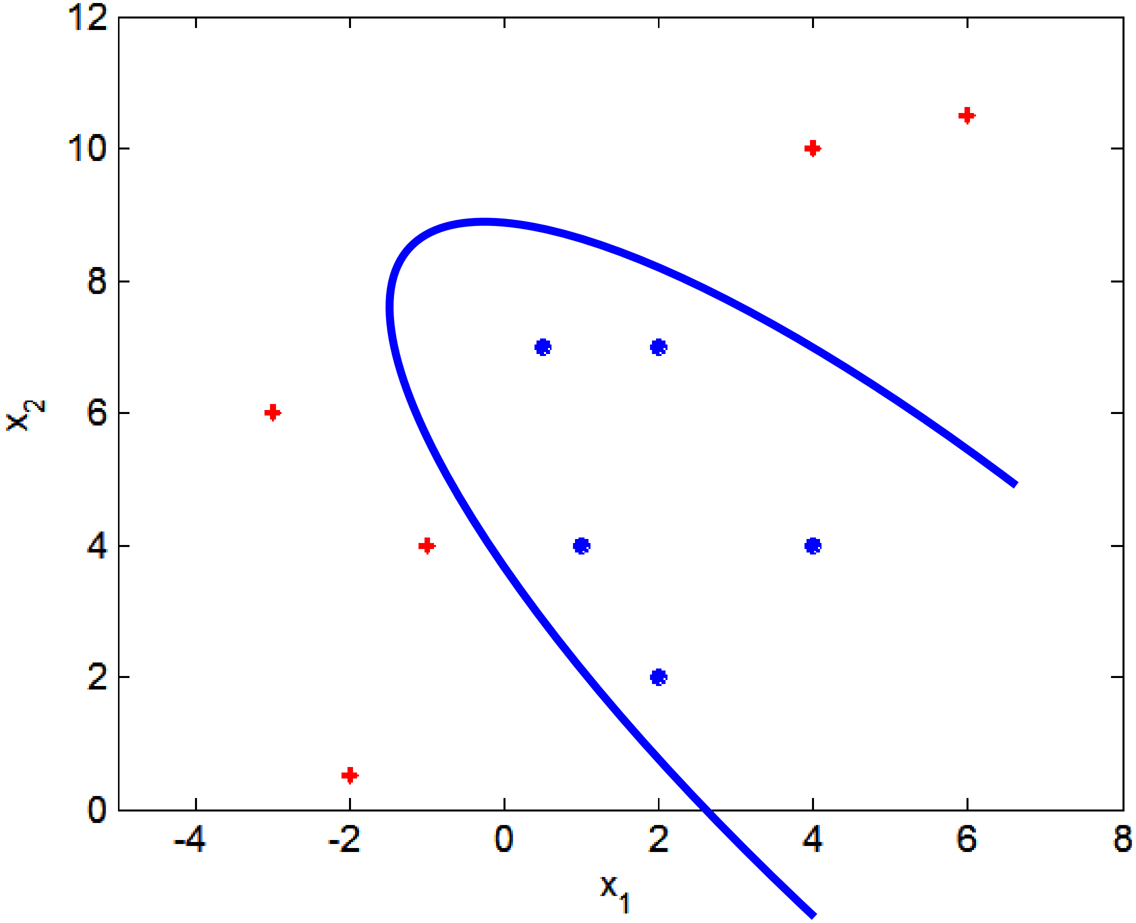
$$L(w) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k \right)$$

    - Subject to:

$$\vec{w} \cdot \overrightarrow{x_i} + b \geq 1 - \xi_i \text{ if } y_i = 1$$
$$\vec{w} \cdot \overrightarrow{x_i} + b \leq -1 + \xi_i \text{ if } y_i = -1$$

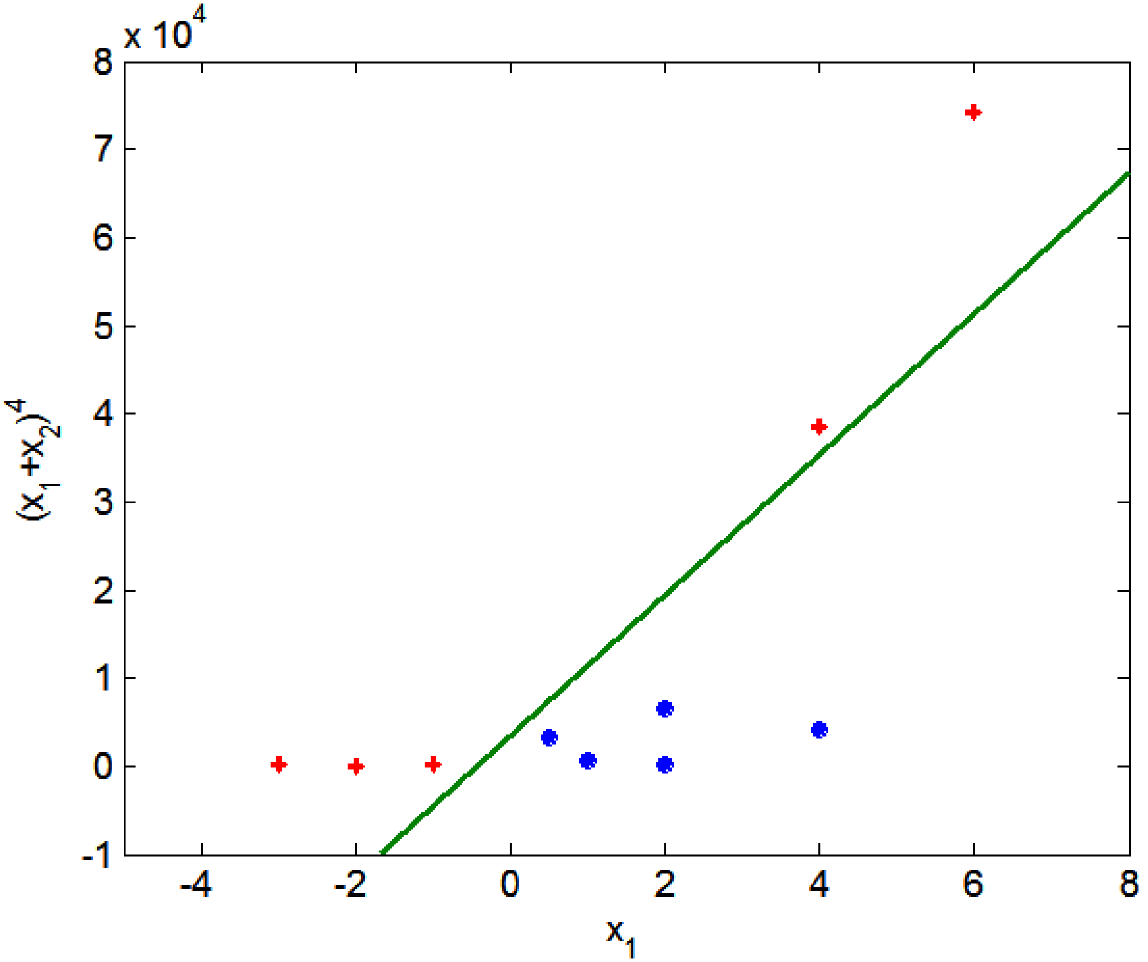
Nonlinear Support Vector Machines

- What if decision boundary is not linear?



Nonlinear Support Vector Machines

- Transform data into higher dimensional space



LOGISTIC REGRESSION

Classification via regression

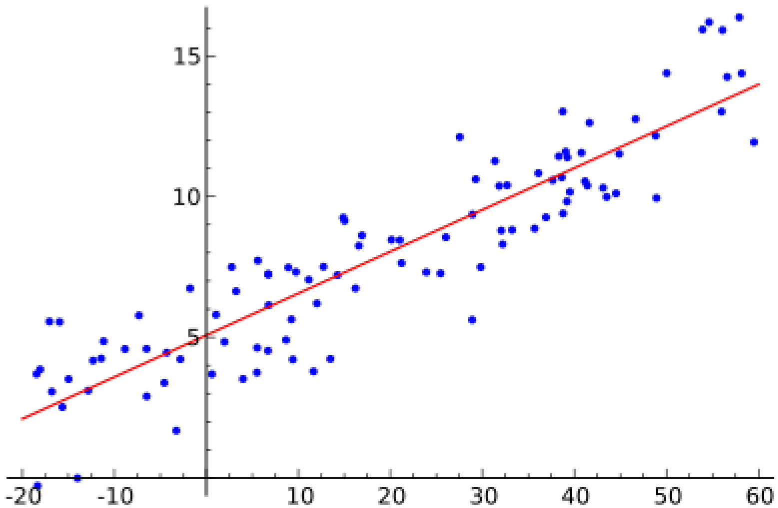
- Instead of predicting the class of an record we want to predict the probability of the class given the record
- The problem of predicting continuous values is called regression problem
- General approach: find a continuous function that models the continuous points.

Example: Linear regression

- Given a dataset of the form $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ find a linear function that given the vector x_i predicts the y_i value as $y_i' = w^T x_i$
  - Find a vector of weights w that minimizes the sum of square errors

$$\sum_i (y_i' - y_i)^2$$

  - Several techniques for solving the problem.



Classification via regression

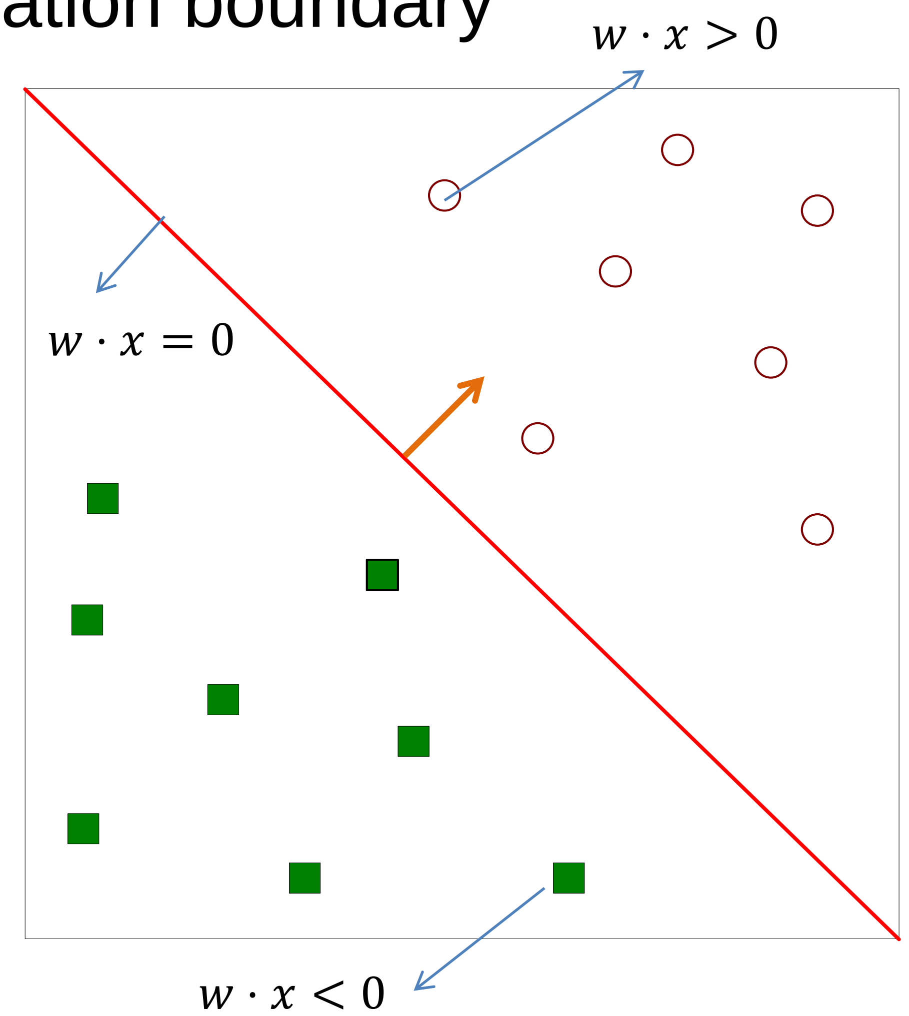
- Assume a linear classification boundary

For the positive class the bigger the value of $w \cdot x$, the further the point is from the classification boundary, the higher our certainty for the membership to the positive class

- Define $P(C_+|x)$ as an increasing function of $w \cdot x$

For the negative class the smaller the value of $w \cdot x$, the further the point is from the classification boundary, the higher our certainty for the membership to the negative class

- Define $P(C_-|x)$ as a decreasing function of $w \cdot x$



Logistic Regression

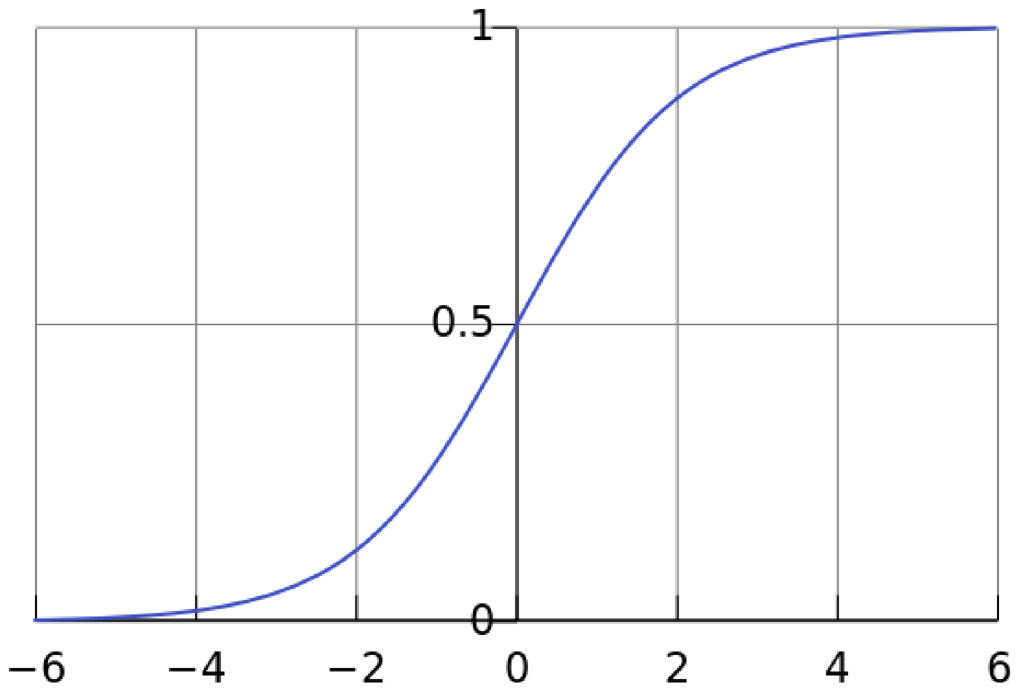
The logistic function

$$f(t) = \frac{1}{1 - e^{-t}}$$

$$P(C_+|x) = \frac{1}{1 - e^{-w \cdot x}}$$

$$P(C_-|x) = \frac{e^{-w \cdot x}}{1 - e^{-w \cdot x}}$$

$$\log \frac{P(C_+|x)}{P(C_-|x)} = w \cdot x$$



Logistic Regression: Find the vector w that maximizes the probability of the observed data

Logistic Regression

- Produces a probability estimate for the class membership which is often very useful.
- The weights can be useful for understanding the feature importance.
- Works for relatively large datasets
- Fast to apply.

NAÏVE BAYES CLASSIFIER

Bayes Classifier

- A probabilistic framework for solving classification problems
- **A, C** random variables
- Joint probability: **Pr(A=a,C=c)**
- Conditional probability: **Pr(C=c | A=a)**
- Relationship between joint and conditional probability distributions

$$\Pr(C, A) = \Pr(C \mid A) \times \Pr(A) = \Pr(A \mid C) \times \Pr(C)$$

- **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?

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

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 $P(C| A_1, A_2,\ldots,A_n)$

- Can we estimate $P(C| A_1, A_2,\ldots,A_n)$ 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
    $P(A_1, A_2, \ldots, A_n|C)\ P(C)$
- 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:
  - $P(A_1, A_2, \ldots, A_n | C_j) = P(A_1|C_j)\, P(A_2|C_j) \cdots P(A_n|C_j)$
  - We can estimate $P(A_i| C_j)$ for all A_i and C_j.
  - New point X is classified to C_j if

$$P(C_j|X) = P(C_j) \prod_i P(A_i|C_j)$$

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

How to Estimate Probabilities from Data?

- For continuous attributes:
  - Discretize the range into bins
    - one ordinal attribute per bin
    - 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 $P(A_i|c)$

How to Estimate Probabilities from Data?

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Evade**
1	Yes	Single	125K	No
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7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Normal distribution:

$$P(A_i \mid c_j) = \frac{1}{\sqrt{2\pi\sigma_{ij}^2}} e^{-\frac{(A_i - \mu_{ij})^2}{2\sigma_{ij}^2}}$$

  - One for each (A_i, c_i) pair
- For (Income, Class=No):
  - If Class=No
    - sample mean = 110
    - sample variance = 2975

$$P(Income = 120 \mid No) = \frac{1}{\sqrt{2\pi}(54.54)} e^{-\frac{(120-110)^2}{2(2975)}} = 0.0072$$

Example of Naïve Bayes Classifier

Given a Test Record:

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

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

- P(X|Class=No) = P(Refund=No|Class=No) $\times$ P(Married| Class=No) $\times$ P(Income=120K| Class=No) = 4/7 $\times$ 4/7 $\times$ 0.0072 = 0.0024
- P(X|Class=Yes) = P(Refund=No| Class=Yes) $\times$ P(Married| Class=Yes) $\times$ P(Income=120K| Class=Yes) = 1 $\times$ 0 $\times$ 1.2 $\times$ 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:

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

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

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

N_i: number of attribute values for attribute A_i

p: prior probability

m: parameter

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

A: attributes

M: mammals

N: non-mammals

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

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

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

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

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

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

=> Mammals

Implementation details

- Computing the conditional probabilities involves multiplication of many very small numbers
  - Numbers get very close to zero, and there is a danger of numeric instability
- We can deal with this by computing the logarithm of the conditional probability

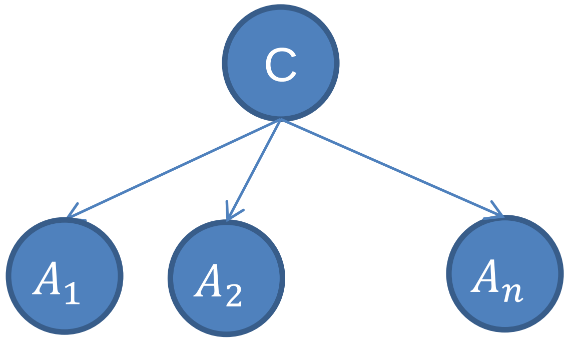
$$\log P(C|A) \sim \log P(A|C) + \log P(A)$$
$$= \sum_i \log P(A_i|C) + \log P(A)$$

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)
- Naïve Bayes can produce a probability estimate, but it is usually a very biased one
  - Logistic Regression is better for obtaining probabilities.

Generative vs Discriminative models

- Naïve Bayes is a type of a generative model
  - Generative process:
    - First pick the category of the record
    - Then given the category, generate the attribute values from the distribution of the category
    - Conditional independence given C



- We use the training data to learn the distribution of the values in a class

Generative vs Discriminative models

- Logistic Regression and SVM are discriminative models
  - The goal is to find the boundary that discriminates between the two classes from the training data
- In order to classify the language of a document, you can
  - Either learn the two languages and find which is more likely to have generated the words you see
  - Or learn what differentiates the two languages.