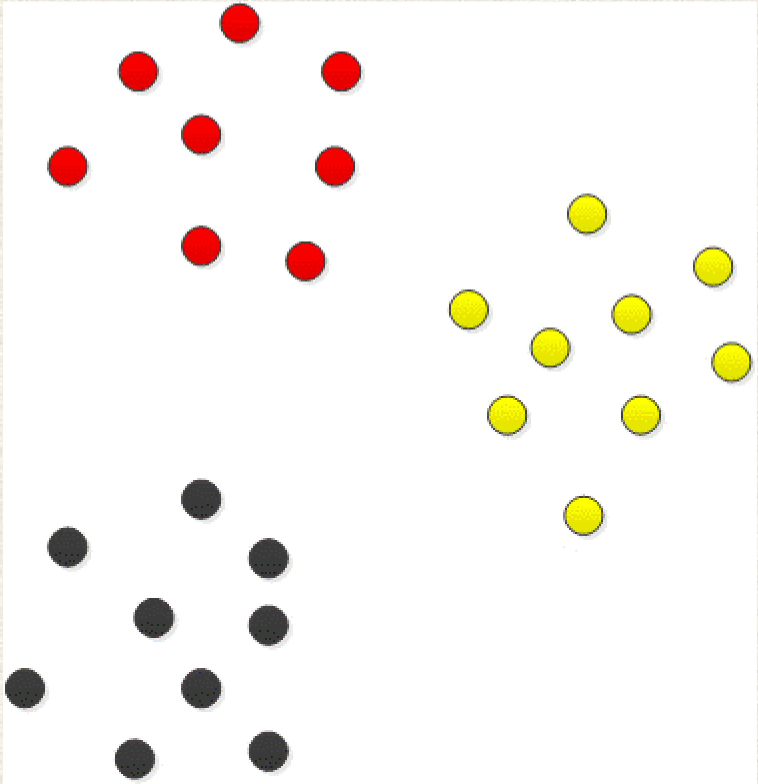
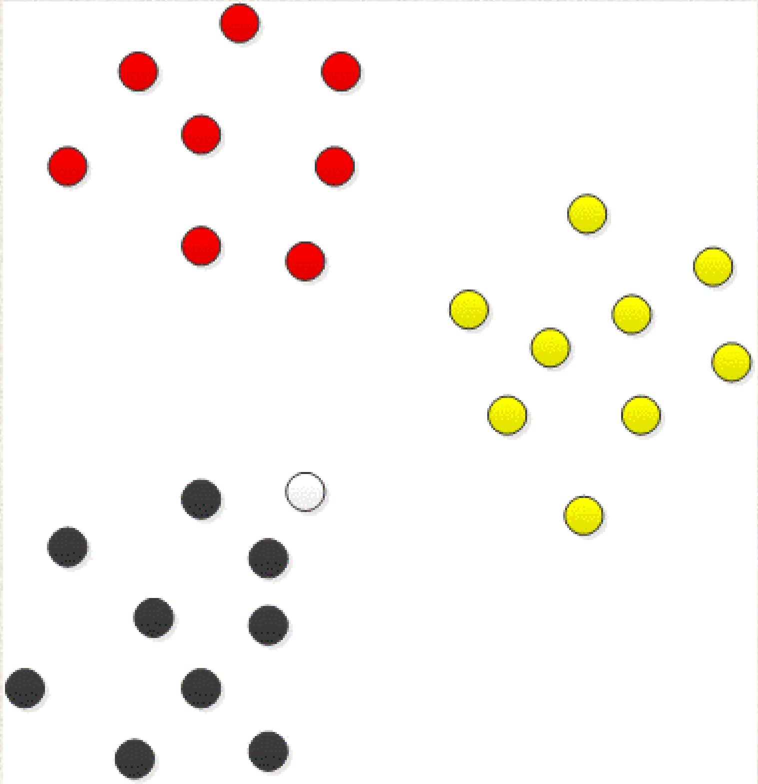
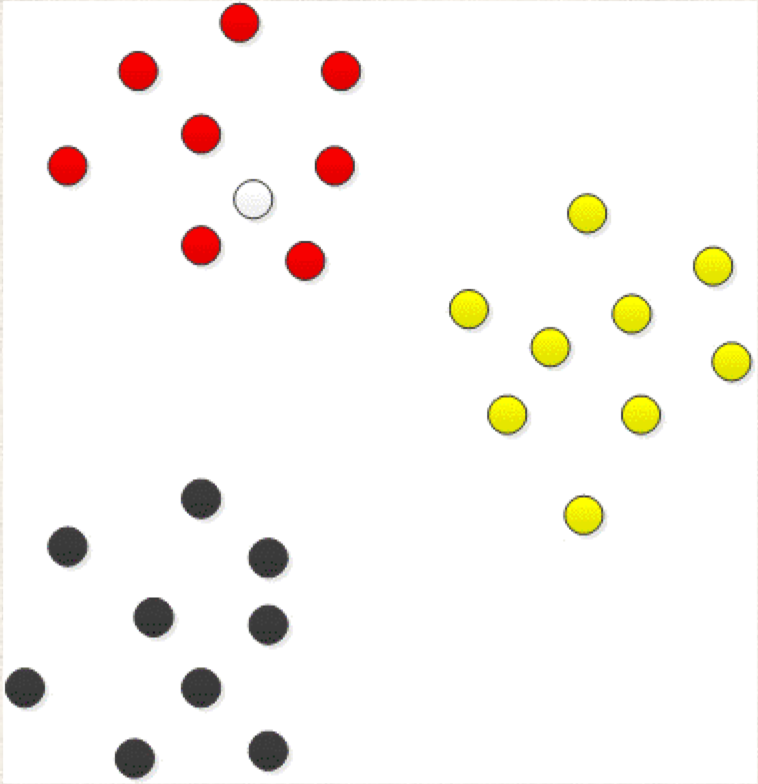
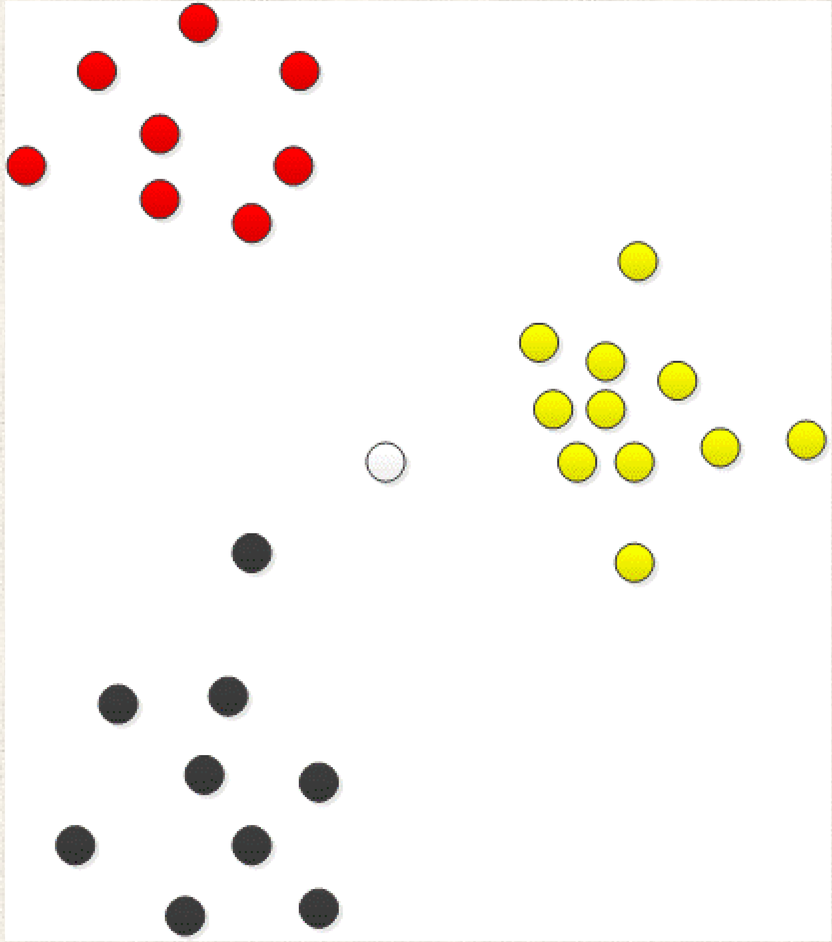
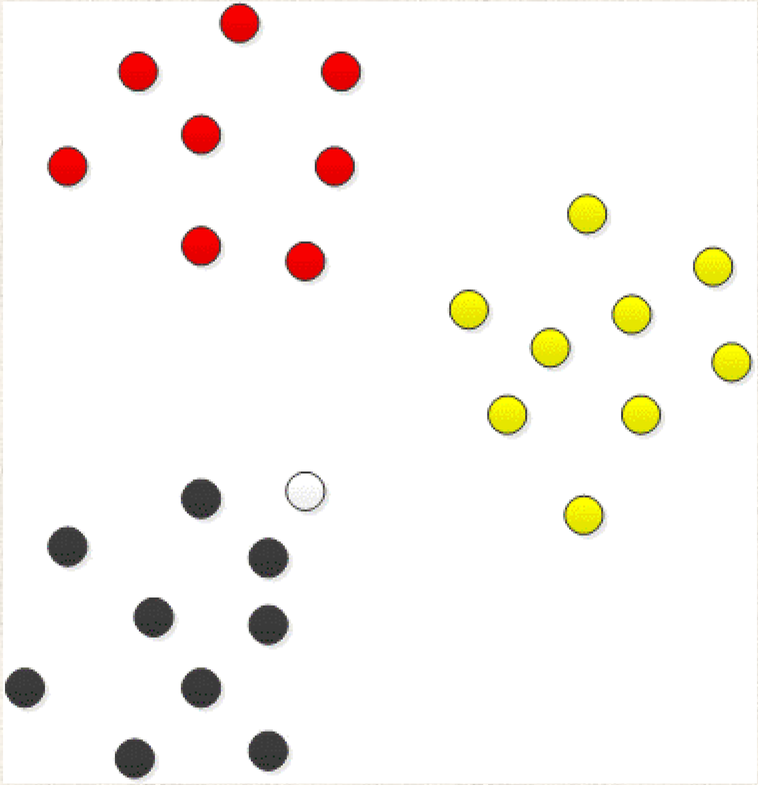
K - Nearest Neighbor Method – An Instance based method





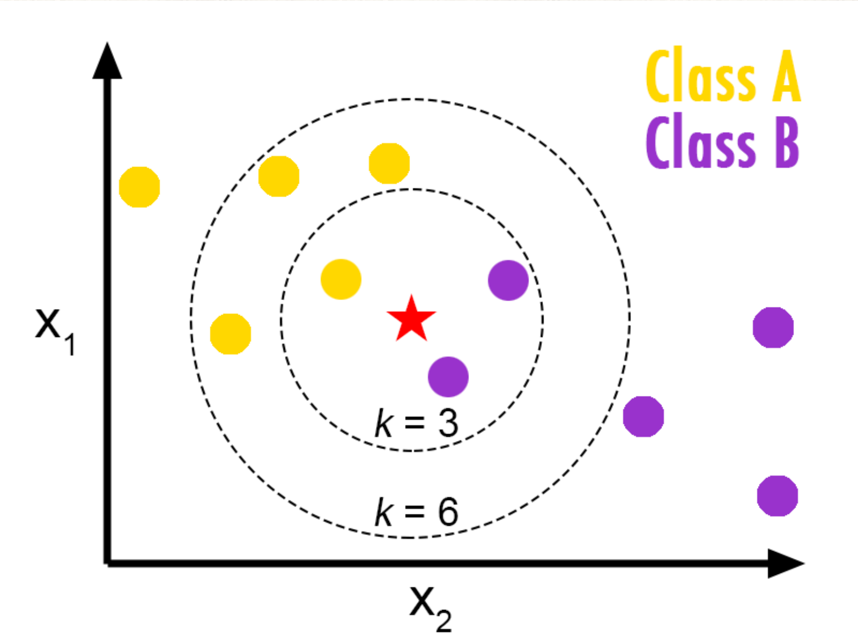



The Nearest Neighbor Method



- ***Observation:*** similar examples tend to belong to the same class.
- ***Idea:*** assign a test input with the class label from the example in the training data set that is the most similar to the test input.
- ***Implementation:*** calculate the distances between the test input and the examples in the data set and find the one with the shortest distance.

The K - Nearest Neighbor Method



- ***Observation:*** similar examples tend to belong to the same class.
- ***Idea:*** assign a test input with the dominating class label from the examples in the training data set that are within the neighborhood of the test input.
- ***Implementation:*** calculate the distances between the test input and the examples in the training data set and find the K ones that are the most closest to the test input and find the dominating class label within these K neighboring examples.

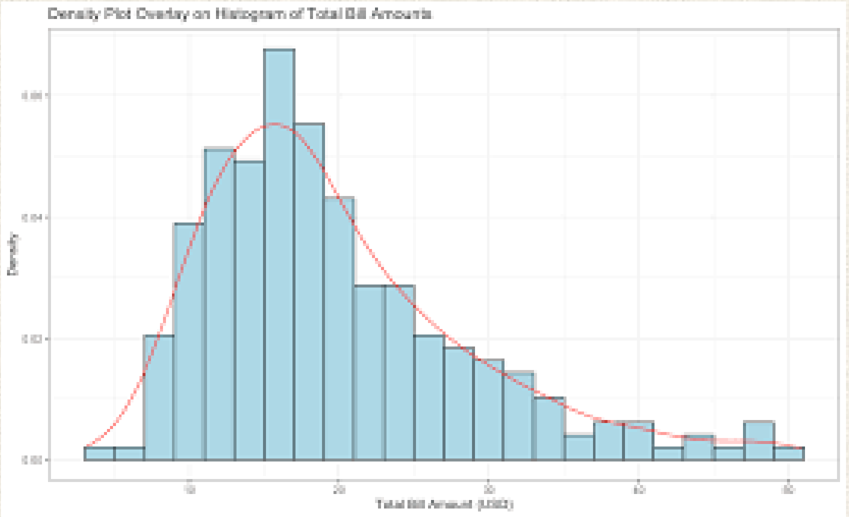
Histogram density model

In the case of a single continuous variable x. Given N sample values from x.

- Partition x into distinct bins of width Δ_i
- Count the number of observations of x falling in bin i as n_i
- Probability density value for bin i is given by

$$p_i = \frac{n_i}{N\Delta_i}$$

Hence, we have, $\sum_{i=1}^{m} p_i \Delta_i = 1$



- Let's suppose we have a data set comprising N_k points in class $\mathcal{C}_k$ with N points in total so that $\sum_{k=1}^{C} N_k = N$.

- If we wish to classify a new point $\boldsymbol{x}$, we draw a sphere centered on $\boldsymbol{x}$ containing precisely K points irrespective of their class. Suppose this sphere has volume V and contains K_k points from class $\mathcal{C}_k$.

- We want to classify the new point $\boldsymbol{x}$ to class $\mathcal{C}_k$ that has the highest ***posterior probability of class membership:***

$$p(\mathcal{C}_k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\boldsymbol{x})}$$

- Then the likelihood can be estimated as:

$$p(\boldsymbol{x}|\mathcal{C}_k) = \frac{K_k}{N_k V}$$

- The unconditional density can be estimated as:

$$p(\boldsymbol{x}) = \frac{K}{NV}$$

- The class prior can be calculated as:

$$p(\mathcal{C}_k) = \frac{N_k}{N}$$

- Applying ***Bayes' theorem*** gives the ***posterior probability of class membership***:

$$p(\mathcal{C}_k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\boldsymbol{x})} = \frac{K_k}{K}$$

- To minimize the probability of misclassification, we assign the test point $\boldsymbol{x}$ to the class having the largest posterior probability, i.e., the largest value of K_k/K

- ***To classify a new point, we identify the K nearest points from the training data set and then assign the new point to the class having the greatest number of representatives amongst the K nearest neighbor set.***

The KNN Classification Algorithm

Begin

load the training data set $\{\boldsymbol{x}_i, y_i\}$, and the test data point $\boldsymbol{x}$

Choose the value of K, set $\mathcal{D} = \{\}$

For $i = 1$ to N

calculate $d_i = \|\boldsymbol{x} - \boldsymbol{x}_i\|$

append $\{y_i, d_i\}$ to $\mathcal{D}$

End

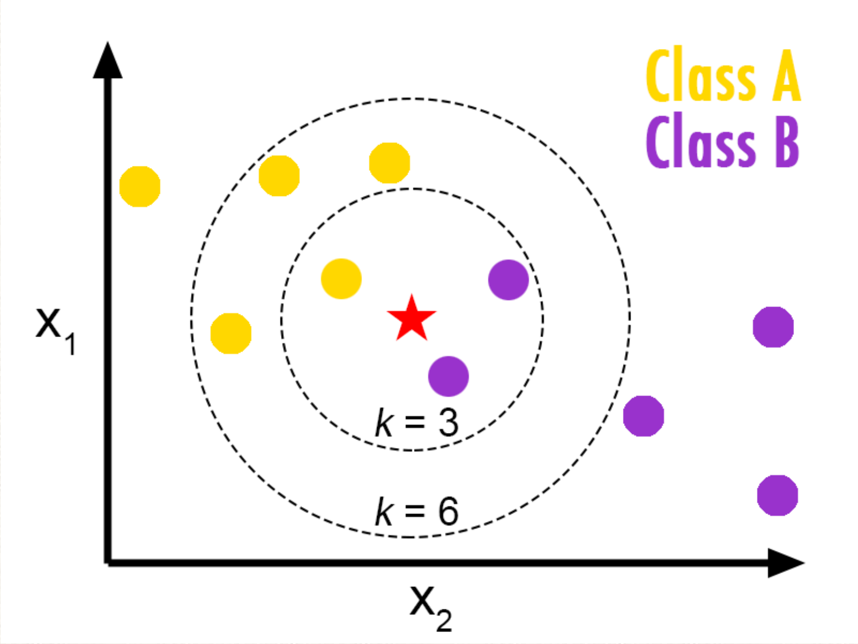
sort $\mathcal{D}$ in the ascend order with respect to d value

pick the first K entries $\{y_n, d_n\}, n = 1, \ldots, K$ from $\mathcal{D}$

$y = mode(\{y_n, d_n\}, n = 1, \ldots, K)$

Return y

End



Metrics used in the KNN method

- ***Distance functions*** are used in KNN method as measure of similarity of instances

- Commonly used distance functions in machine learning include the following:

Let $\boldsymbol{x} = [x_1 \quad \cdots \quad x_m]^T \; and \; \boldsymbol{y} = [y_1 \quad \cdots \quad y_m]^T$ be two vectors, then the distances between $\boldsymbol{x} \; and \; \boldsymbol{y}$ are:

- *Euclidean* distance

$$d(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{m} (x_i - y_i)^2 \right)^{\frac{1}{2}}$$

- *Minkowsky* distance

$$d(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{m} |x_i - y_i|^p \right)^{\frac{1}{p}}$$

- *Manhantan* distance

$$d(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} |x_i - y_i|$$

- *Chebyshev* distance

$$d(\boldsymbol{x},\boldsymbol{y}) = \max_{i} |x_i - y_i|$$

- *Hamming* distance:

$$d_i = \begin{cases} 1, & if\ x_i \neq y_i \\ 0, & otherwise \end{cases};\ \ d(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{m} d_i$$

Let $\boldsymbol{x} = [x_1 \quad \cdots \quad x_m]^T$ *and* $\boldsymbol{y} = [y_1 \quad \cdots \quad y_m]^T$ be two vectors, we have,

- Cosine similarity measure:

$$sim(\boldsymbol{x}, \boldsymbol{y}) = \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|} = \frac{\sum_{i=1}^{m} x_i y_i}{\sqrt{\sum_{i=1}^{m} x_i^2} \sqrt{\sum_{i=1}^{m} y_i^2}}$$

- Correlation:

$$corr(\boldsymbol{x}, \boldsymbol{y}) = \frac{\sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2} \sqrt{\sum (y_i - \bar{y})^2}} = \frac{\langle \boldsymbol{x} - \overline{\boldsymbol{x}}, \boldsymbol{y} - \overline{\boldsymbol{y}} \rangle}{\|\boldsymbol{x} - \overline{\boldsymbol{x}}\| \|\boldsymbol{y} - \overline{\boldsymbol{y}}\|} = sim(\boldsymbol{x} - \overline{\boldsymbol{x}}, \boldsymbol{y} - \overline{\boldsymbol{y}})$$

Questions about the KNN method

Q1: How do we train a KNN algorithm?

Q2: Does a KNN algorithm need a training set/test set?

Q3: Can the KNN method be applied to the regression problem?

Q4: Is KNN a good candidate for online (real-time) classification?

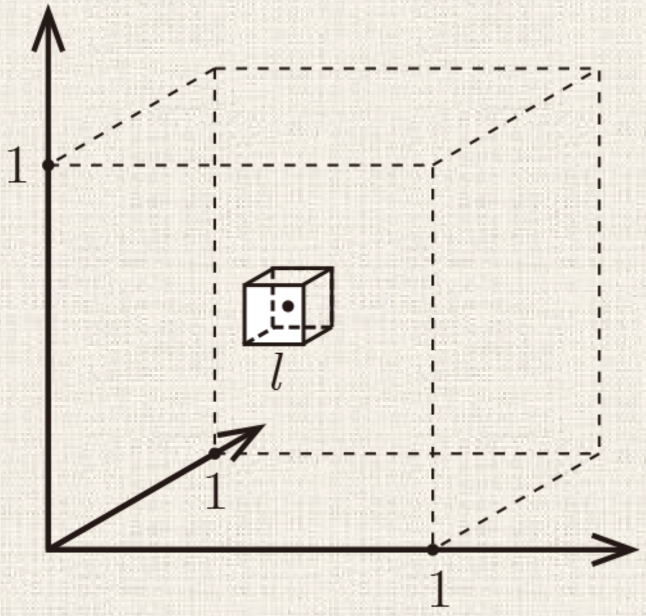
The curse of dimensionality

- The loss of locality in ***higher dimensions***
  - Consider N data points uniformly distributed in a d dimensional unit hypercube.
  - Let's find out a hypercube of edge l that contains K nearest neighbors of a test point. That is, we want to find a cube of edge l to contain a fraction $r = \frac{K}{N}$ of the entire data set.
  - Since the data points are uniformly distributed, this means the volume of the cube is fraction r of the unit cube, i.e.,

$$l^d = r \Rightarrow l = r^{\frac{1}{d}}$$

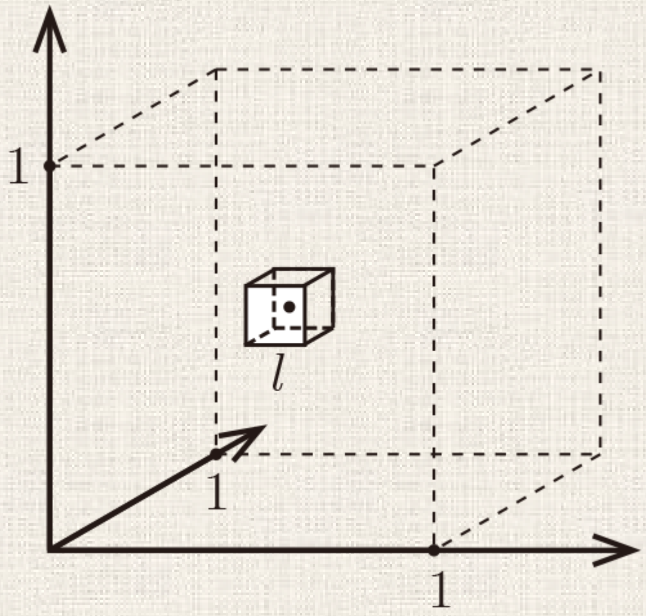
  - When $d \to \infty$, we have $l \to 1$. i.e., the hypercube is close to the entire unit hypercube where the data is uniformly distributed!!! This is true even for very small r value.

$$0 < l < 1$$



For example, let $N = 1000, K = 10$, we have, $r = 0.01$

$$l^d = r \Rightarrow l = r^{\frac{1}{d}}$$



d	l
1	0.01
2	0.1
3	0.21
10	0.63
100	0.96
1000	0.995

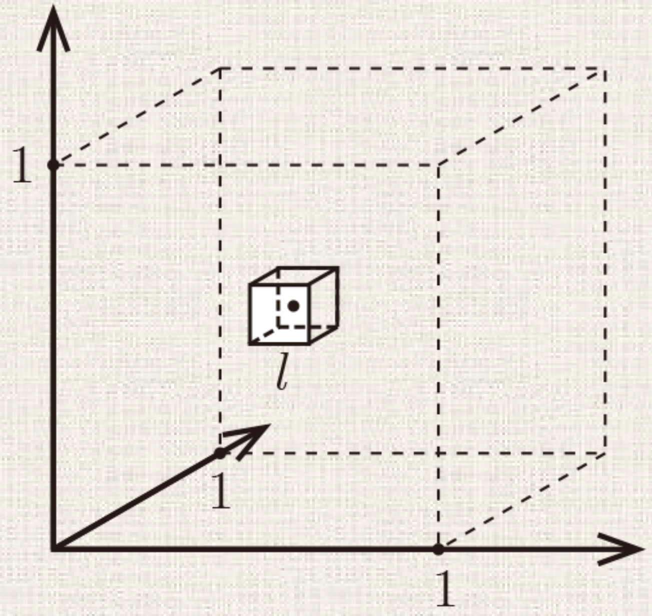
To find the 10 – nearest neighbor, we need almost the entire input space in high dimensions!!!

- To find the 10 – nearest neighbor, we need almost the entire input space in high dimensions!!!
- This breaks down the KNN assumptions because in high dimensions, the points in K nearest neighbor are not particularly closer (similar) than any other data points in the training set.
- Can we increase the number of training data points until the K nearest neighbors are truly closer to the test point?
- How many data points do we need such that l, the size of the neighborhood become truly small?

For example,

let $l = 0.1$. then, $r = \frac{K}{N} = l^d \Rightarrow N = \frac{K}{l^d} = K \times 10^d$

When $d = 10$, N becomes a huge number!!!



Dimension reduction (PCA) may provide a solution to alleviate the problem!

The Naïve Bayes Classifier – A generative approach

- The training data set is given as $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{N}$, where, an instance $\boldsymbol{x}_i$ belongs to class $\mathcal{C}_k$ if $y_i = k, k = 1, \dots, K$.

- Given a new instance, $\boldsymbol{x} = [x_1 \quad x_2 \quad \cdots \quad x_d]^T$, we wish to predict the class of this instance.

- The ***Bayesian approach*** to classify the new instance is to assign the most probable target value, y_{MAP}, given the attribute values $x_1, \dots, x_d$. That is,

$$y_{MAP} = \underset{k}{argmax}\, P(\mathcal{C}_k | x_1, \dots, x_d)$$

- Using ***Bayes' theorem***, this probability can be written as:

$$y_{MAP} = \underset{k}{argmax} \frac{P(x_1, \dots, x_d | \mathcal{C}_k) P(\mathcal{C}_k)}{P(x_1, \dots, x_d)}$$

$$= \underset{k}{argmax} \, P(x_1, \dots, x_d | \mathcal{C}_k) P(\mathcal{C}_k)$$

- ***Assume the attributes are conditionally independent given the target value***, we have

$$P(x_1, \dots, x_d | \mathcal{C}_k) = P(x_1 | \mathcal{C}_k) P(x_2 | \mathcal{C}_k) \cdots P(x_d | \mathcal{C}_k) = \prod_{j=1}^{d} P(x_j | \mathcal{C}_k)$$

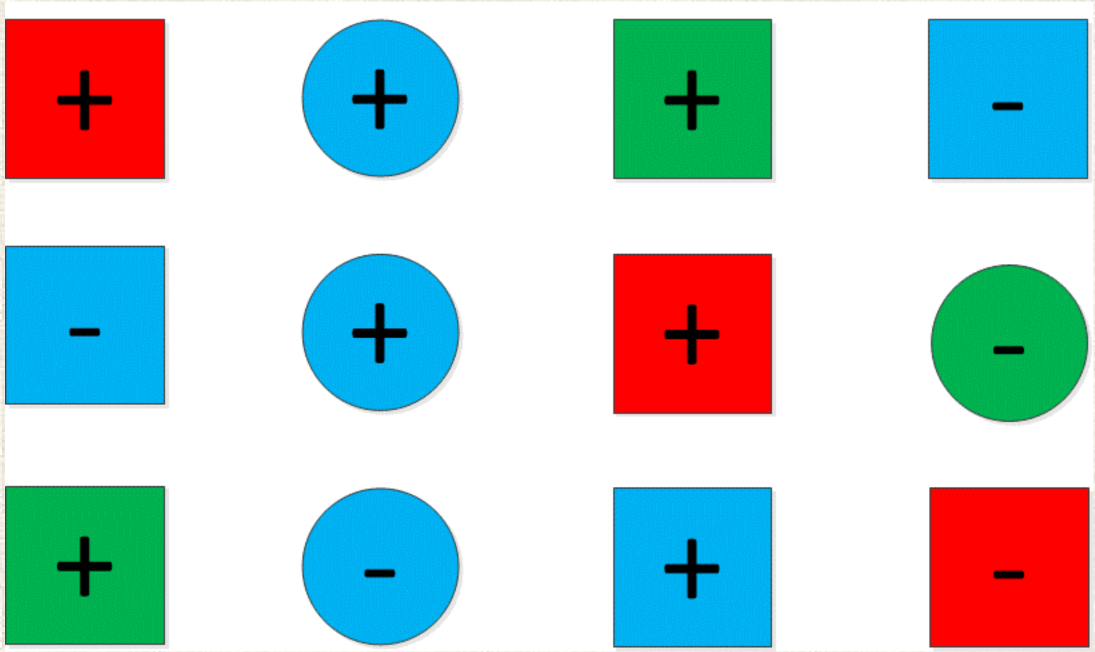
- Then we have,

$$y_{MAP} = \underset{k}{argmax} \, P(\mathcal{C}_k) \prod_{j=1}^{d} P(x_j | \mathcal{C}_k)$$

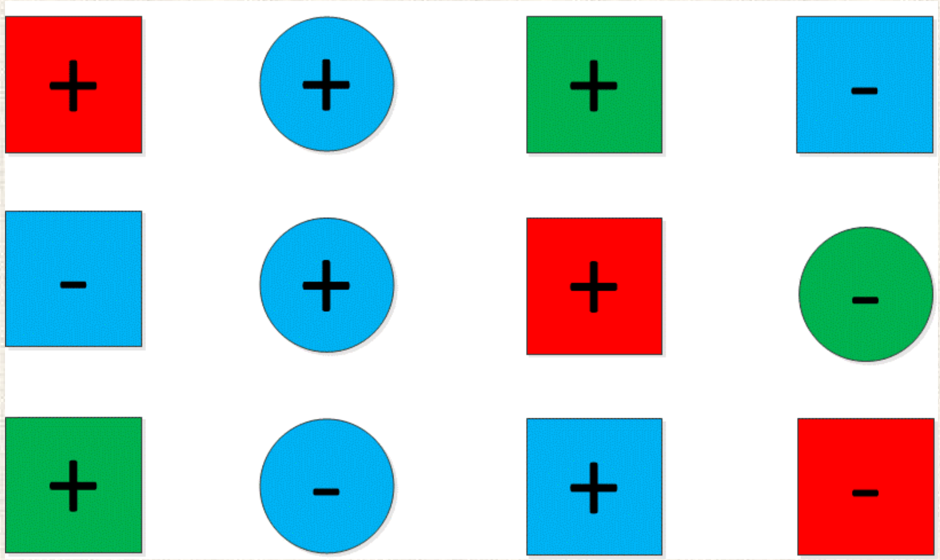
- This is why the method is called "***naïve***" Baye's method

The Naïve Bayes Classifier – A Toy Example

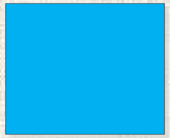
- The training data set is given as:



- $y_i \in \{+, -\}, i = 1,2, \ldots, 12$ are the class labels.
- $\boldsymbol{x}_i = [x_{i1} \quad x_{i2}]^T, x_{i1} \in \{blue, green, red, yellow\}, x_{i2} \in \{square, circle\}, i = 1, \ldots, 12$ are the feature vectors.



- Given the following new input, let's use ***naïve Bayes method*** to predict its class:



- The feature vector is $\boldsymbol{x} = [x_1, x_2]^T = [blue, square]^T$

- Under the assumption that the training samples are $i.i.d$, we have the class priors as:

$$P(+) = \frac{7}{12} = 0.58; \quad P(-) = \frac{5}{12} = 0.42$$

- ***Assuming features are conditionally independent for given class***, the class conditional probabilities can be calculated as:

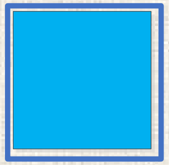
$$P(\boldsymbol{x}|+) = P(x_1 = blue, x_2 = square|+) = P(blue|+)P(square|+) = \frac{3}{7} \times \frac{5}{7} = 0.31$$

$$P(\boldsymbol{x}|-) = P(x_1 = blue, x_2 = square|-) = P(blue|-)P(square|-) = \frac{3}{5} \times \frac{3}{5} = 0.36$$

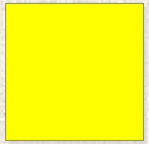
- Then the posterior can be calculated as:

$$P(+|\boldsymbol{x}) = P(\boldsymbol{x}|+)P(+) = 0.58 \times 0.31 = 0.18$$

$$P(-|\boldsymbol{x}) = P(\boldsymbol{x}|-)P(-) = 0.42 \times 0.36 = 0.15$$

- Since $P(+|\boldsymbol{x}) = 0.18 > P(-|\boldsymbol{x}) = 0.15$, the sample point $\boldsymbol{x}$ =  is classified as $+$.

- Suppose a new sample as the following is given:



- The feature vector is $\boldsymbol{x} = [x_1, x_2]^T = [yellow, square]^T$, the color attribute value “yellow” is not present in the training data set. This causes the class conditional probability to become:

$$P(\boldsymbol{x}|+) = P(x_1 = yellow, x_2 = square|+) = P(yellow|+)P(square|+) = 0 \times \frac{5}{7} = 0$$

$$P(\boldsymbol{x}|-) = P(x_1 = yellow, x_2 = square|-) = P(yellow|-)P(square|-) = 0 \times \frac{3}{5} = 0$$

And the posteriors will hence be all calculated as 0s.

- This problem can be solved by using the ***Laplace smoothing*** (***additive smoothing***) technique to calculate the class conditional probability:

$$P(x_i|\mathcal{C}_k) = \frac{N_{x_i,\mathcal{C}_k} + 1}{N_{\mathcal{C}_k} + d}$$

where, $N_{x_i,\mathcal{C}_k}$ is the number of time feature x_i appears in training data set from class $\mathcal{C}_k$;

$N_{\mathcal{C}_k}$ is the total count of all features appears in training data set from class $\mathcal{C}_k$; d is the dimensionality of the feature vector

- Then, using this new technique, the class conditional probability of the new sample $\boldsymbol{x}$ can be calculated as:

$$P(\boldsymbol{x}|+) = P(x_1 = yellow, x_2 = square|+) = P(yellow|+)P(square|+)$$

$$= \frac{1}{7+2} \times \frac{5}{7} = 0.08$$

$$P(\boldsymbol{x}|-) = P(x_1 = yellow, x_2 = square|-) = P(yellow|-)P(square|-)$$

$$= \frac{1}{5+2} \times \frac{3}{5} = 0.09$$

- *Note that the Laplace smoothing formula is used to calculate the likelihood of the features that do not present in the training data set.*

- The posterior probability of the classes can be calculated as:

$$P(+|\boldsymbol{x}) = P(\boldsymbol{x}|+)P(+) = 0.08 \times 0.58 = 0.0464$$

$$P(-|\boldsymbol{x}) = P(\boldsymbol{x}|-)P(-) = 0.09 \times 0.42 = 0.0378$$

Therefore, the new sample should be classified as $+$

The Naïve Bayes Classifier – Text Documents Classification

- ***Inputs:***
  - a document $\boldsymbol{x}$
  - A fixed set of classes $\{\mathcal{C}_1, \dots, \mathcal{C}_K\}$ e.g., {“spam”, ”ham”}, {“computer science”, ”biology”, ”statistics”, ”economics”, ”politics”}
  - A training set of N hand-labeled documents $\{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_N, y_N)\}$ (training corpus)
- ***Output:***
  - The class of the document $\boldsymbol{x}$

Preprocessing of text documents

- ***Tokenization***: *breaks down a text corpus into individual words and removes punctuations*

A swimmer likes swimming; thus, he swims.

↓

a	swimmer	likes	swimming	thus	he	swims

Preprocessing of text documents

- ***Remove stop words***: stop words are particularly common in a text corpus and thus considered as rather uninformative (e.g., words such as ***so, and, or, the***, etc.) a stop list can be created and used for stop words removal.

A swimmer likes swimming; thus, he swims.

↓

swimmer	likes	swimming	he	swims

The Bag of Words Model

- ***Creation of the vocabulary***: after preprocessing, we can create the collection of all different words that occur in the training data set and each word is associated with a count of how it occurs. ***This is a set of non-redundant items where the order does not matter (bag of words)***.

Let D_1 and D_2 be two documents in a training dataset (corpus):

- D_1: "Each state has its own laws."
- D_2: "Every country has its own culture."

Based on these two documents, after proper preprocessing, the vocabulary can be created as:

$$V = \{each: 1, state: 1, has: 2, its: 2, own: 2, laws: 1, every: 1, country: 1, culture: 1\}$$

- ***Vectorization:*** The vocabulary can then be used to construct the *d*-dimensional feature vector for the individual documents. $d = |V|$ is the number of different words in the vocabulary.

- The following are the ***bag of words*** representation of two sample documents $D_1 \ and \ D_2$: (word position information does not matter)

V	**each**	**state**	**has**	**its**	**own**	**laws**	**every**	**country**	**culture**
$\boldsymbol{x}_{D_1}$	1	1	1	1	1	1	0	0	0
$\boldsymbol{x}_{D_2}$	0	0	1	1	1	0	1	1	1
Σ	1	1	2	2	2	1	1	1	1

- After transforming documents into numbers, popular supervised learning methods can be applied to do document classification.

Text Documents Classification using The Naïve Bayes Classifier

- Given a test document $\boldsymbol{x} = [x_1, x_2, \dots, x_d]^T$
- ***Prior probability estimate:***

$$P(\mathcal{C}_k) = \frac{\#\ of\ documents\ with\ \mathcal{C}_k}{Total\ \#\ of\ documents\ in\ the\ training\ data\ set}, \qquad k = 1,2,\dots,K$$

- ***Class conditional probability estimate: (Laplace smoothing if necessary)***

$$P(x_i|\mathcal{C}_k) = \frac{N(x_i, \mathcal{C}_k) + 1}{N(\mathcal{C}_k) + |V|}$$

Where, $N(x_i, \mathcal{C}_k)$ is the total number of occurrences of term x_i in all documents in the training data set with class $\mathcal{C}_k$; $N(\mathcal{C}_k)$ is the number of occurrences of all the terms in all documents in the training data set with class $\mathcal{C}_k$.

- ***Class conditional probability estimate:***

$$P(x_i|\mathcal{C}_k) = \frac{N(x_i, \mathcal{C}_k) + 1}{N(\mathcal{C}_k) + |V|}$$

Where, $N(x_i, \mathcal{C}_k)$ is the total number of occurrences of term x_i in all documents in the training data set with class $\mathcal{C}_k$; $N(\mathcal{C}_k)$ is the number of occurrences of all the terms in all documents in the training data set with class $\mathcal{C}_k$.

- Then, assuming features are conditionally independent given class, we have, ("naïve")

$$P(\boldsymbol{x}|\mathcal{C}_k) = P(x_1, x_2, \dots, x_d|\mathcal{C}_k) = \prod_{i=1}^{d} P(x_i|\mathcal{C}_k), k = 1, \dots, K$$

The chance of occurrence of value x_i is not affected by the values of other attributes.

- ***Calculation of the posterior probability:***

$$P(\mathcal{C}_k|x) \propto P(\boldsymbol{x}|\mathcal{C}_k)P(\mathcal{C}_k)$$