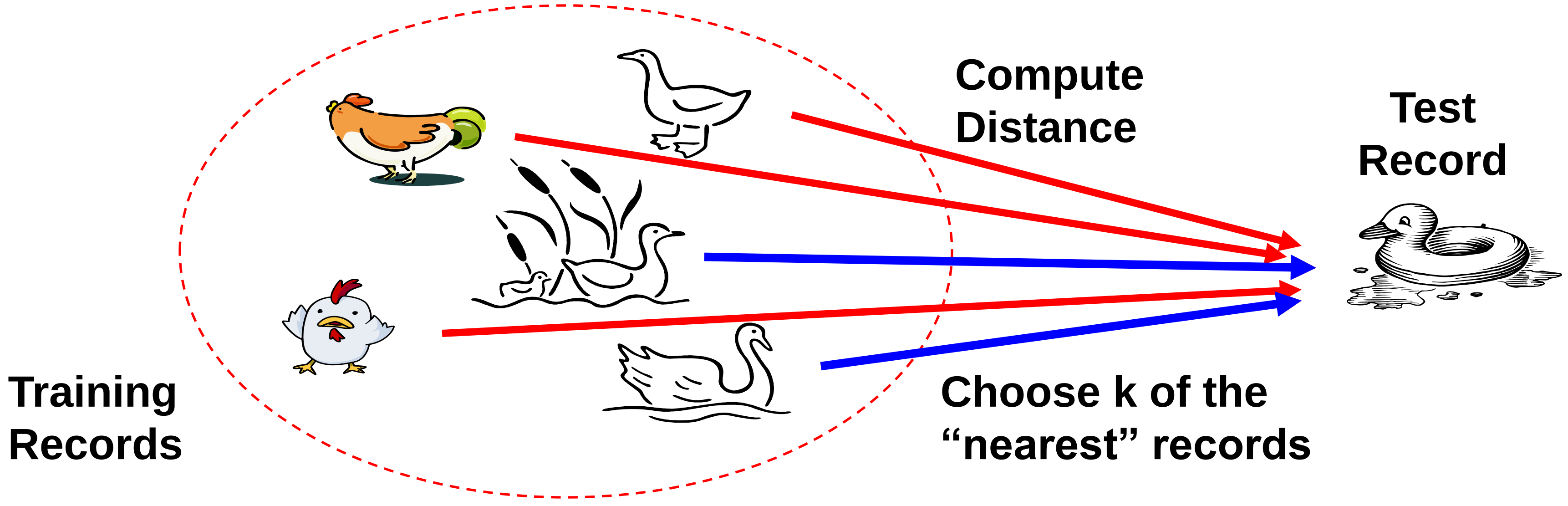
KNN

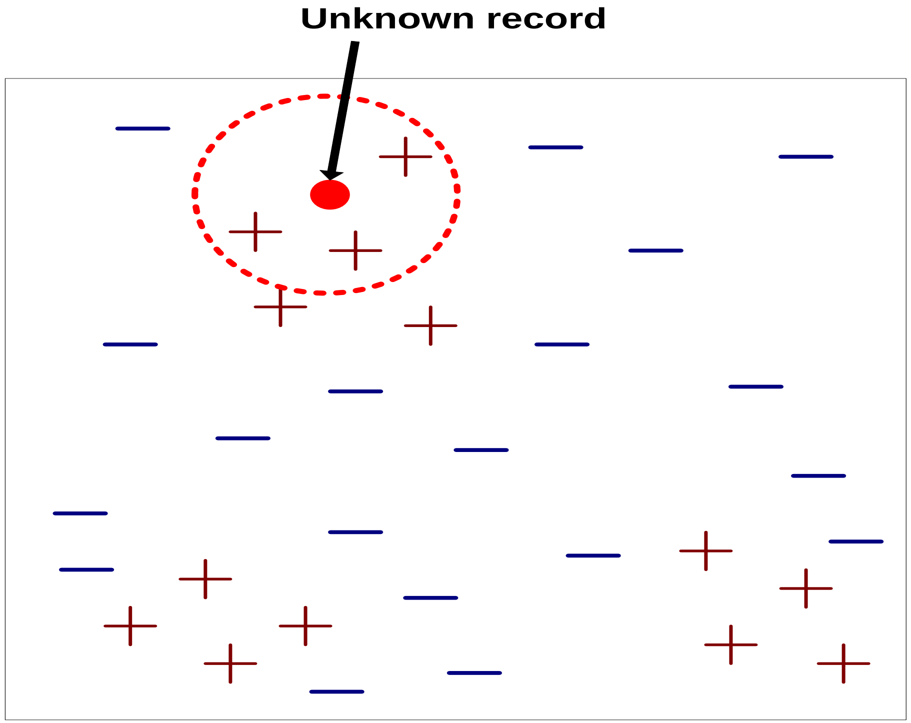
CS277

Nearest Neighbor Classifiers

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



Nearest-Neighbor Classifiers



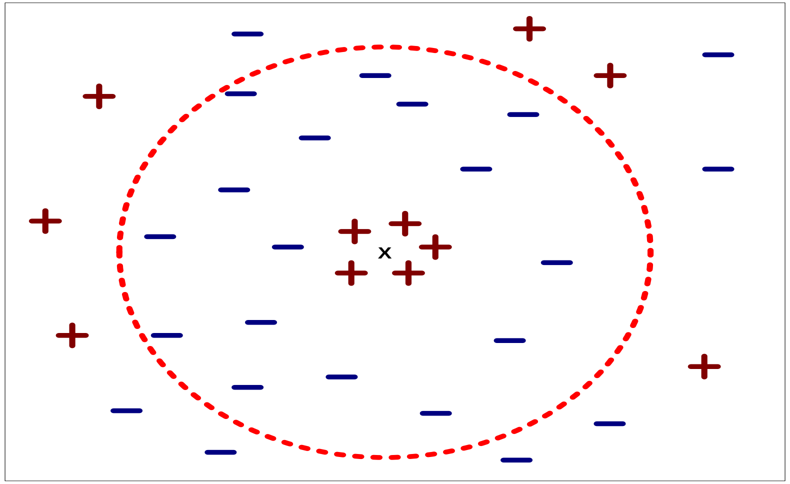
- Requires the following:
  - A set of labeled records
  - Proximity metric to compute distance/similarity between a pair of records
    - e.g., Euclidean distance
  - The value of *k*, the number of nearest neighbors to retrieve
  - A method for using class labels of K nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

How to Determine the class label of a Test Sample?

- Take the majority vote of class labels among the k-nearest neighbors
- Weight the vote according to distance
  - weight factor, $w = 1/d^2$

Nearest Neighbor Classification…

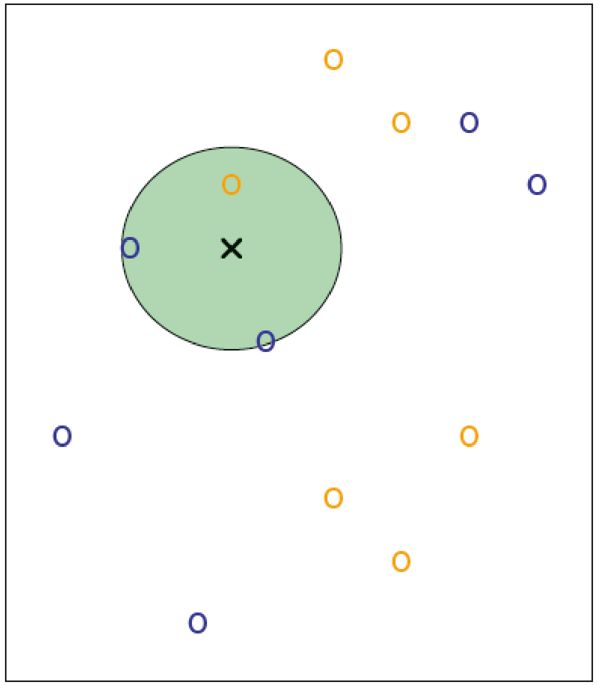
- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



Nearest Neighbor Classification…

- **How to handle missing values in training and test sets?**
  - Proximity computations normally require the presence of all attributes
  - Some approaches use the subset of attributes present in two instances
    - This may not produce good results since it effectively uses different proximity measures for each pair of instances
    - Thus, proximities are not comparable

K=3



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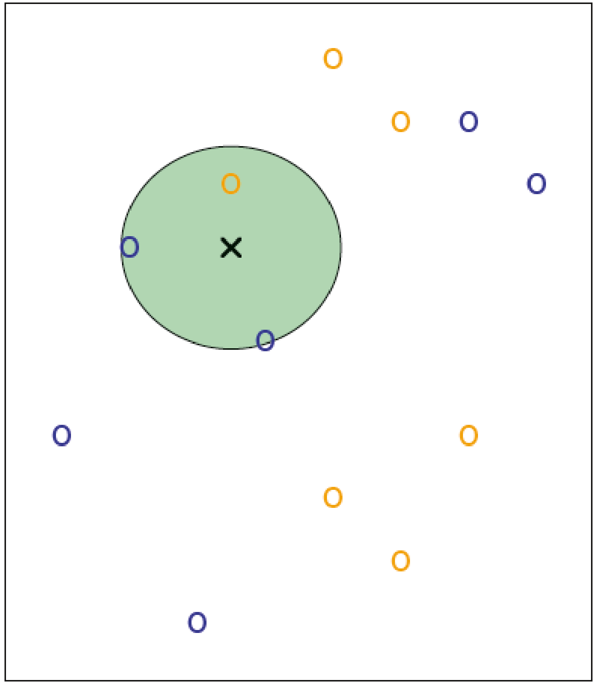
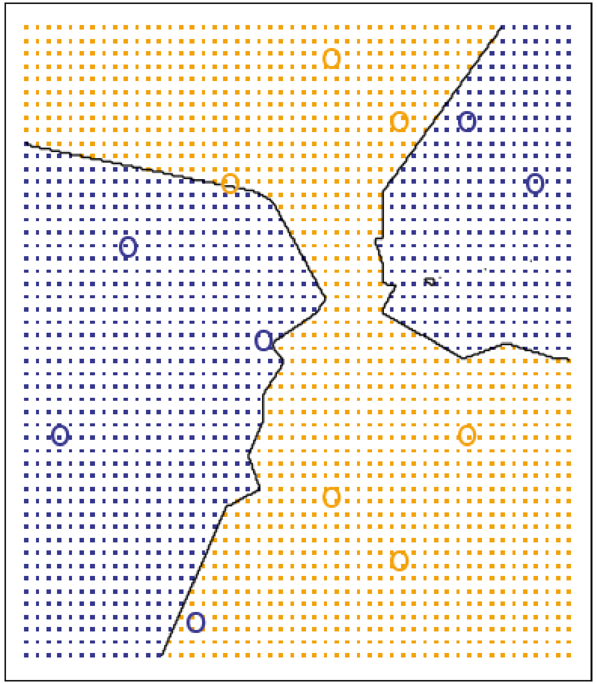
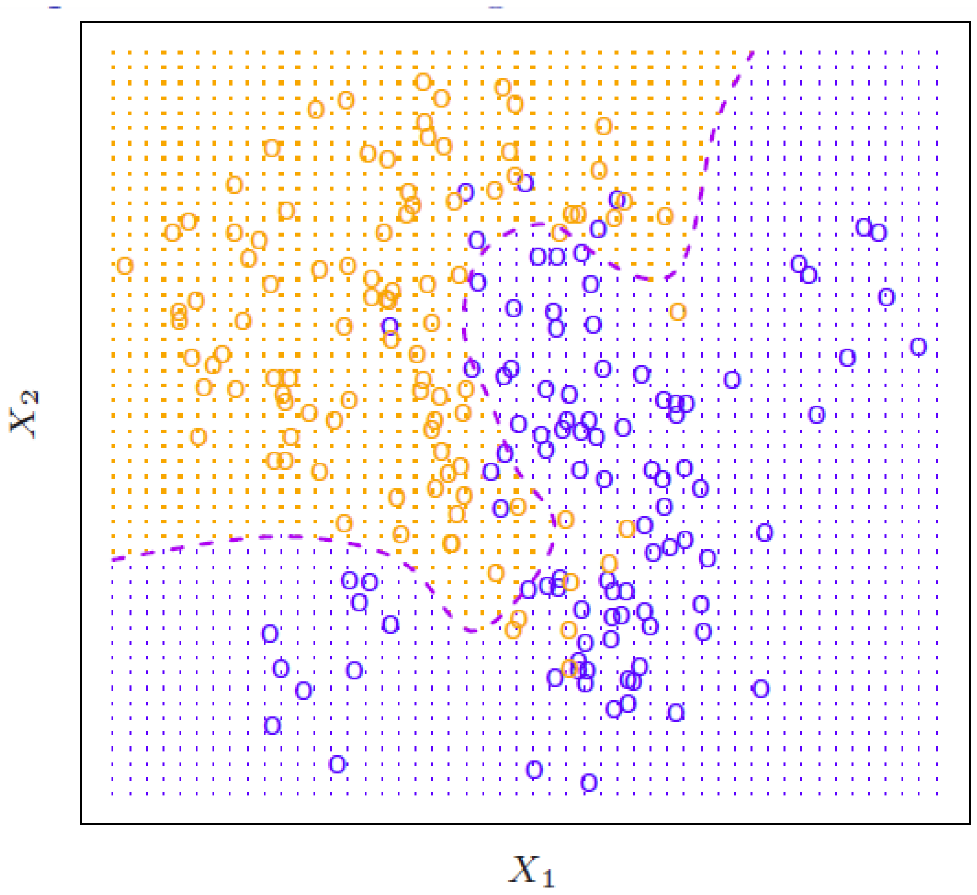
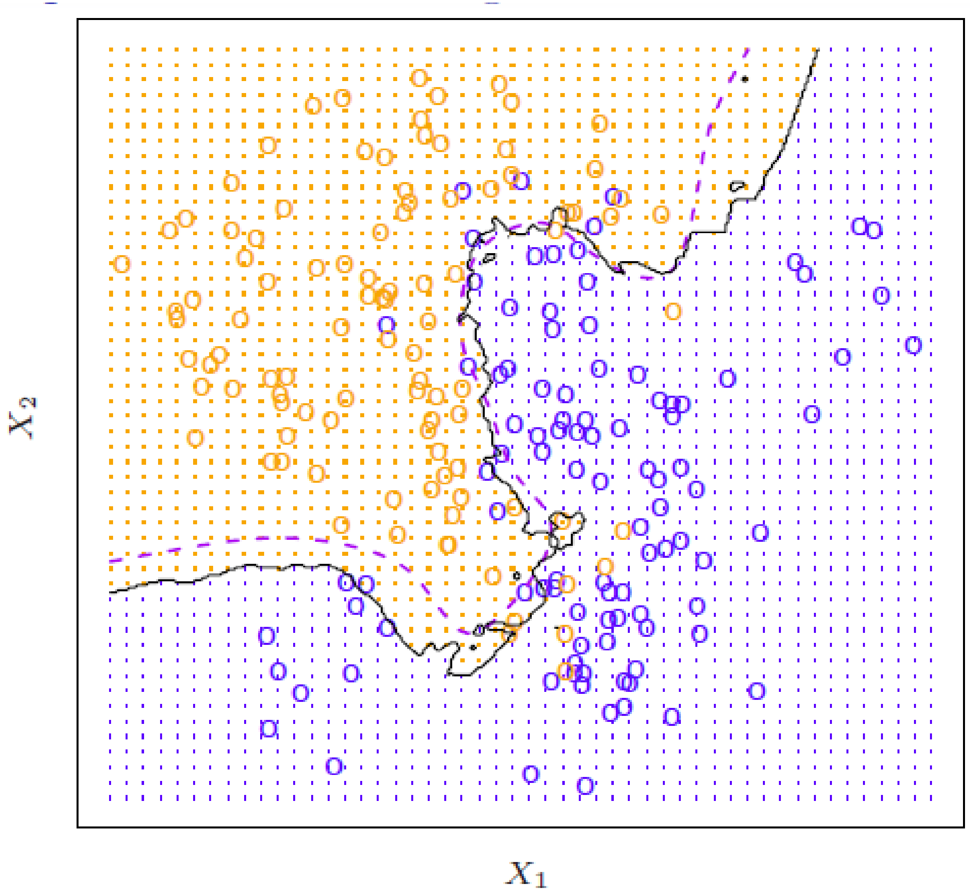




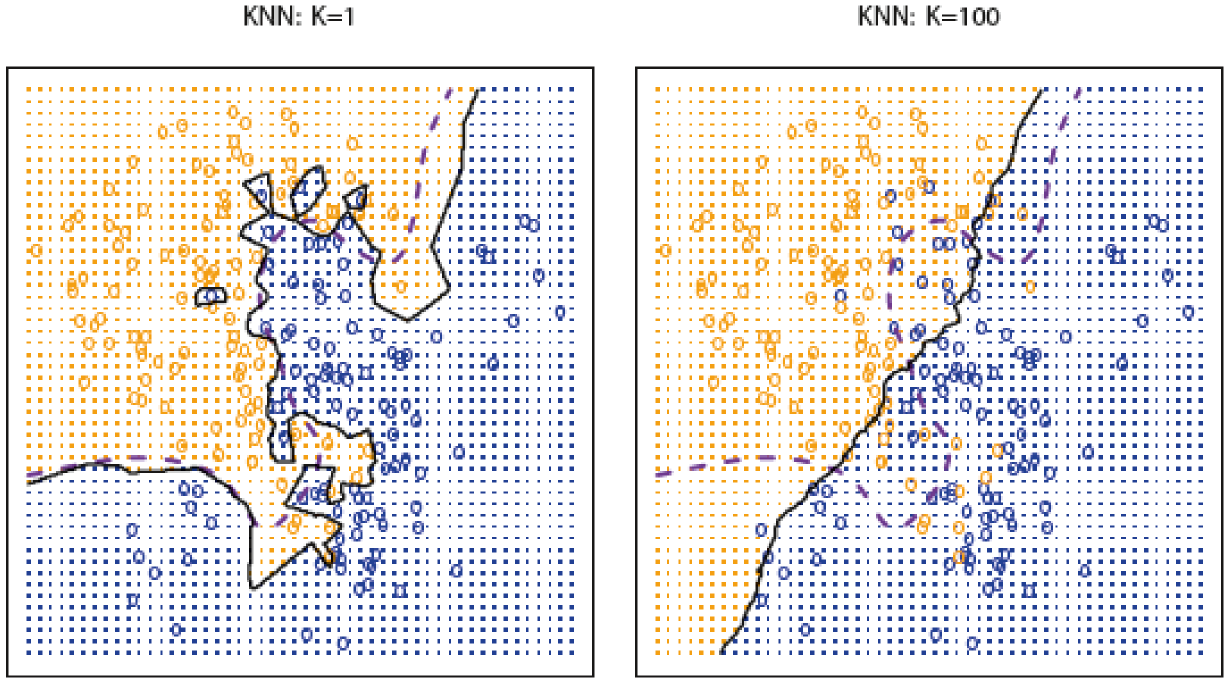
KNN



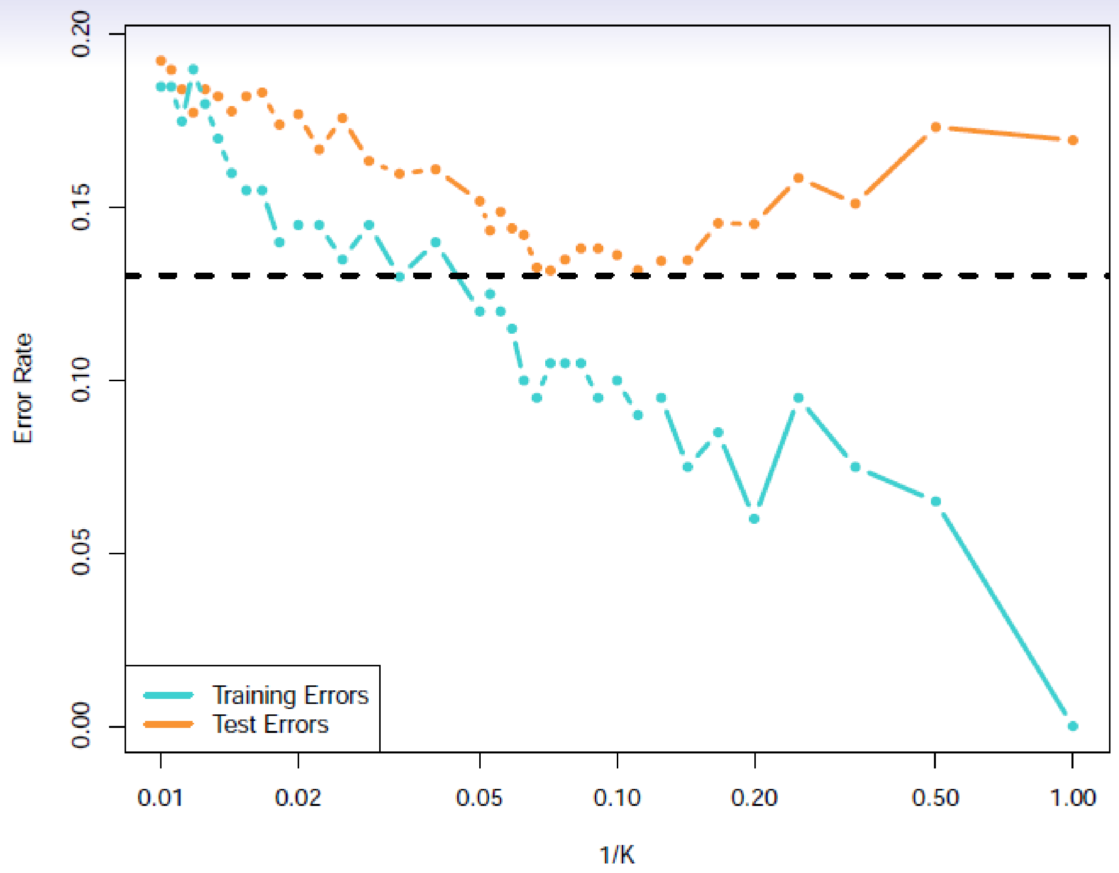
K=10



A Comparisons of K=1 vs K=100



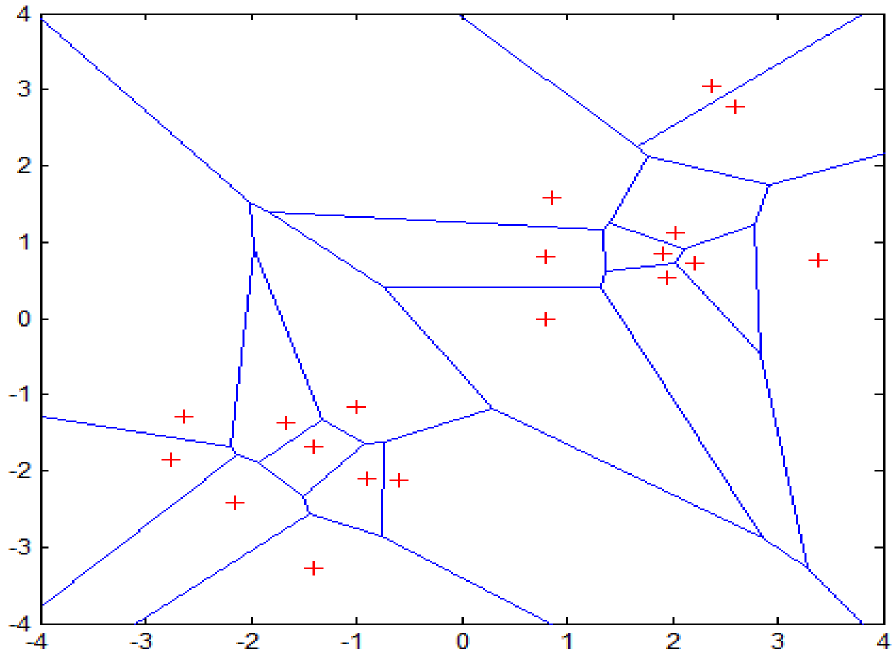
Error rate vs 1/k



Nearest-neighbor classifiers

- Nearest neighbor classifiers are local classifiers

- They can produce decision boundaries of arbitrary shapes.



1-NN decision boundary is a Voronoi Diagram

Distance Metrics

Minkowsky:

$$D(x,y) = \left(\sum_{i=1}^{m} |x_i - y_i|^r \right)^{1/r}$$

Euclidean:

$$D(x,y) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

Manhattan / city-block:

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

Nearest Neighbor Classification…

- **Data preprocessing is often required**
  - 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

  - Time series are often standardized to have 0 means a standard deviation of 1

Standardization

- Transform raw feature values into z-scores $z_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j}$
  - x_{ij} is the value for the *i*th sample and *j*th feature
  - $\mu_j$is the average of all x_{ij} for feature *j*
  - σ_i is the standard deviation of all x_{ij} over all input samples
- Range and scale of z-scores should be similar (providing distributions of raw feature values are alike)
- Z-scores allow you to take data points drawn from populations with different means and standard deviations and place them on a common scale.

Choice of proximity measure matters

Mathematical technique to calculation similarity and dissimilarity of data points

- For documents, cosine is better than correlation or Euclidean

Cosine similarity is not a popular proximity measure but it is more important for comparing documents.

1 1 1 1 1 1 1 1 1 1 1 0	vs	0 0 0 0 0 0 0 0 0 0 0 1
0 1 1 1 1 1 1 1 1 1 1 1		1 0 0 0 0 0 0 0 0 0 0 0

Euclidean distance = 1.4142 for both pairs, but the cosine similarity measure has different values for these pairs.

Cosine Similarity

•If **A** and **B** are two vectors, then

cos(**A**, **B**) = <**A**,**B**> / ||**A**|| ||**B**|| ,

where <**A**,**B**> indicates inner product or vector dot product of vectors, **A** and **B**, and **||A||** and ||B|| are the L2 norms

- The result of the cosine similarity ranges from -1 to 1.
  - Value 1: indicates that the vectors are identical
  - Value 0: means that the vectors are orthogonal (not similar at all)
  - Value -1: implies opposite vectors
- The cosine similarity is often used in text analysis to determine the similarity between documents represented as vectors in a high-dimensional space, where each dimension corresponds to a specific term or word.

KNN: Advantages vs Disadvantages

Advantages

- No training phase
- It can learn complex models easily
- It is robust to noisy training data

Disadvantages

- Determining the value of parameter K can be difficult as different K values can give different results.
- It is hard to apply on High Dimensional data
- Computation cost is high as each query has to go through all the records, which takes O(N) time, where N is the number of records.

Nearest Neighbour : Computational Complexity

- Expensive

  To determine the k - nearest neighbours it calculates the distances from all other N trianing points

  - To determine the nearest neighbour of a query point *q*, must compute the distance to all *N* training examples
    - + Pre-sort training examples into fast data structures (kd-trees)
    - + Compute only an approximate distance (LSH)
    - + Remove redundant data (condensing)
- Storage Requirements

  It is required to store all the trianing points to predict the class of new data point

  - Must store all training data **P**
    - + Remove redundant data (condensing)
    - - Pre-sorting often increases the storage requirements
- High Dimensional Data

  With the increase in the dimension the computational cost increases dramatically

  - "Curse of Dimensionality"
    - Required amount of training data increases exponentially with dimension
    - Computational cost also increases dramatically
    - Partitioning techniques degrade to linear search in high dimension

Reduction in Computational Complexity

- Reduce size of training set
  - Condensation, editing

Reducing the size of training data set can decrease the computational complexity

- Use geometric data structure for high dimensional search

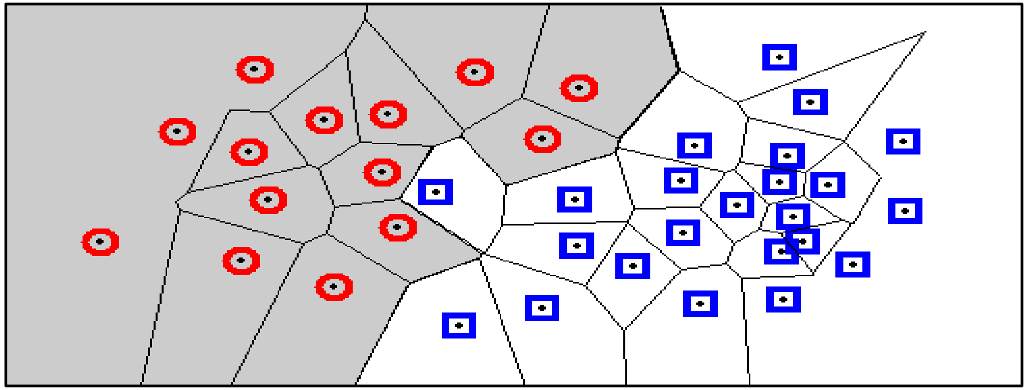
Geometric data structure ??

What is an Imbalanced dataset?

A dataset is said to be imbalanced if the instances of a class are either very less or very high in number as compared to the instances of other class.

CNN basically removes the majority class instances in such a manner that there is no information loss and the dataset becomes balanced.

Condensation: Decision Regions



Each cell contains one sample, and every location within the cell is closer to that sample than to any other sample.

A Voronoi diagram divides the space into such cells.

Every query point will be assigned the classification of the sample within that cell. The *decision boundary* separates the class regions based on the 1-NN decision rule.

Knowledge of this boundary is sufficient to classify new points.

The boundary itself is rarely computed; many algorithms seek to retain only those points necessary to generate an identical boundary.

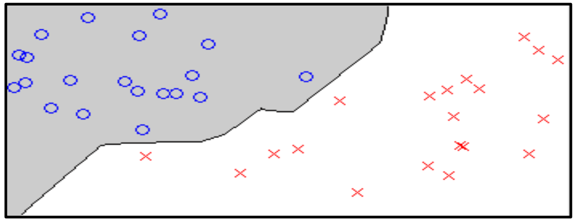
Condensing

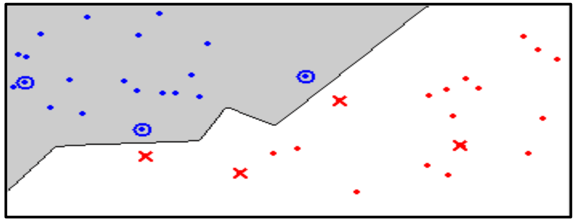
- Aim is to reduce the number of training samples
- Retain only the samples that are needed to define the decision boundary

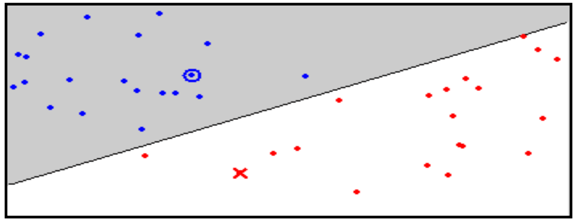
  Condensing targets to retains only those samples that are needed to define the decision boundaries

- Decision Boundary Consistent – a subset whose nearest neighbour decision boundary is identical to the boundary of the entire training set

- Minimum Consistent Set – the smallest subset of the training data that correctly classifies all of the original training data


Original data

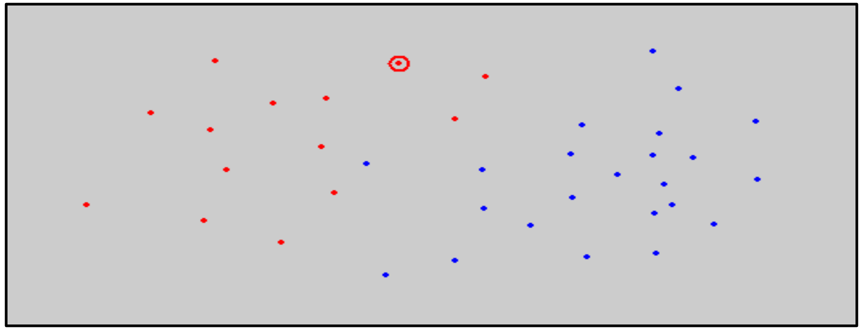

Condensed data


Minimum Consistent Set

Condensing

- Condensed Nearest Neighbour (CNN)

1. Initialize subset with a single (or K) training example
2. Classify all remaining samples using the subset, and transfer any incorrectly classified samples to the subset
3. Return to 2 until no transfers occurred or the subset is full



- Incremental
- Order dependent
- Neither minimal nor decision boundary consistent
- $O(n^3)$ for brute-force method

Condensing

- Condensed Nearest Neighbour (CNN)

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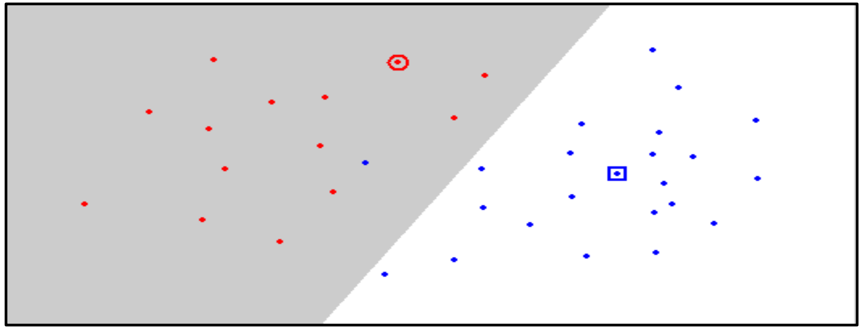

See there is one point in the classification that is falsely classified.

Condensing

- Condensed Nearest Neighbour (CNN)

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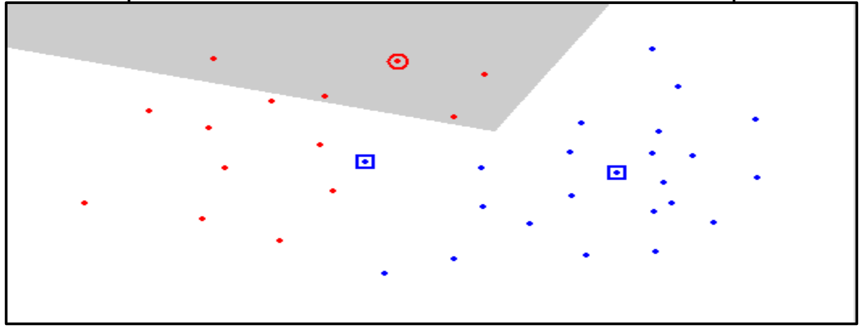

After transferring the incorrectly classified sample point, we got a number of points that became falsely classified.

Condensing

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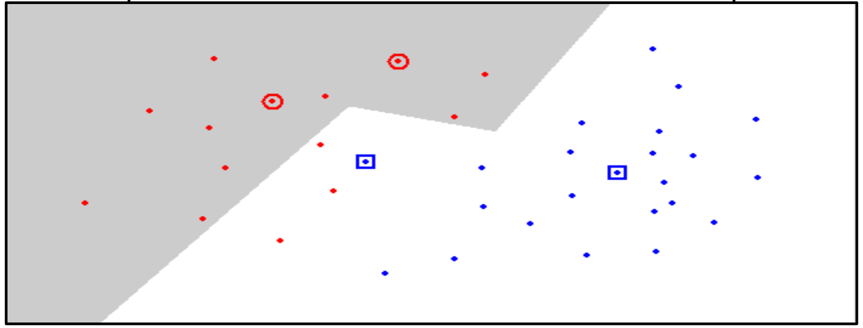

Condensing

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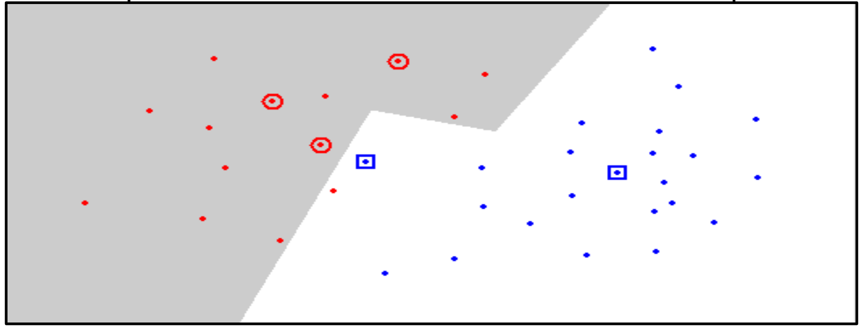
Repeat till the classification becomes correct
ie, all data points are correctly classified



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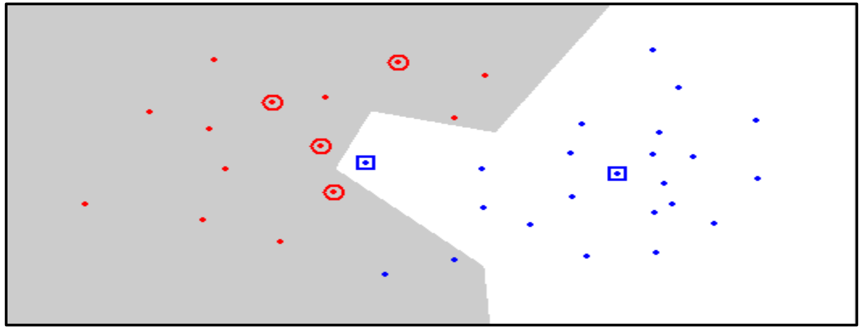

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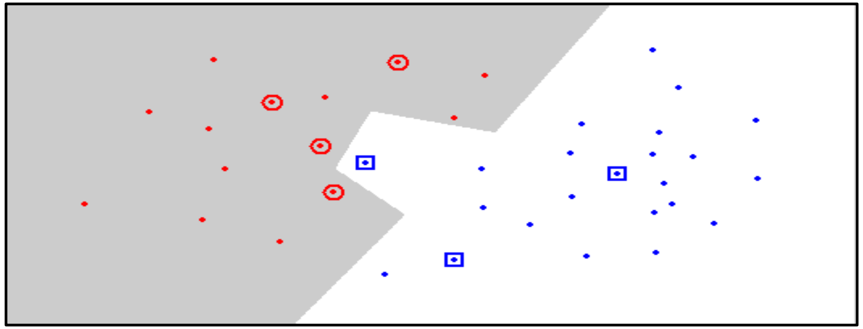


KD TREE axis selection

There are different strategies for choosing an axis when dividing, but the most common one would be to cycle through each of the K dimensions repeatedly and select a midpoint along it to divide the space. For instance, in the case of 2-dimensional points with x and y axes, we first split along the x-axis, then the y-axis, and then the x-axis again, continuing in this manner until all points are accounted for

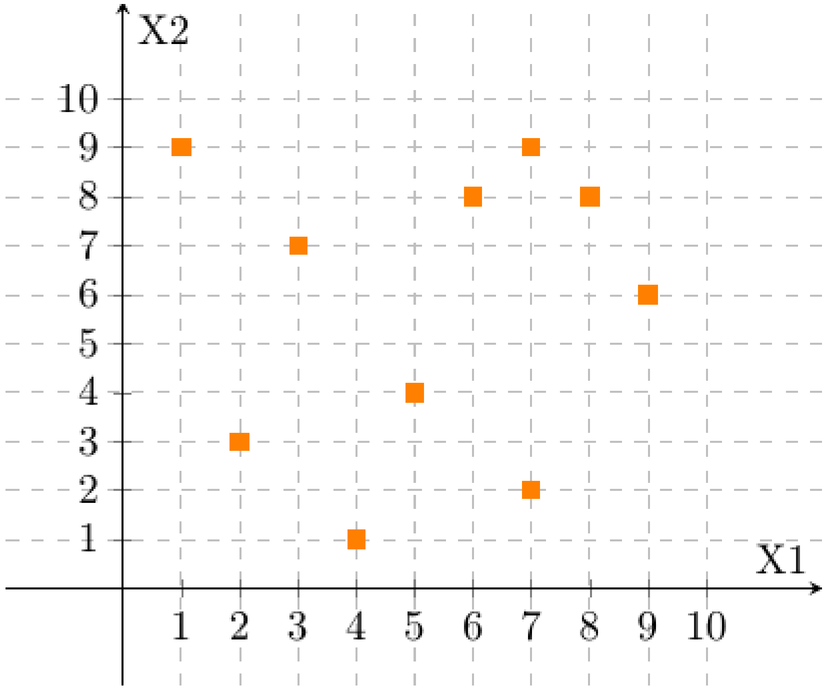
KD Tree

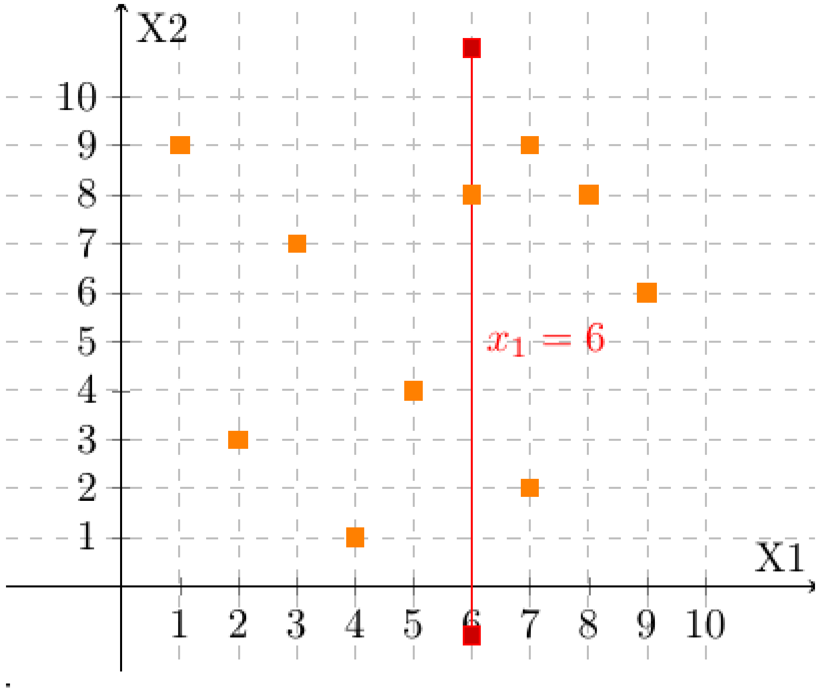
A data structure that organizes points in a k-dimensional space. It is also known as a K-Dimensional Tree.

- KD Tree is a space partitioning data structure for organizing points in K-Dimensional space.
- It is useful for representing data efficiently.
- In KD Tree the data points are organized and partitioned on the basis of some specific conditions.
- Some axis-aligned **cuts** are used to create different regions, keeping track of points that lie in these regions
  - Split the regions at the **median** of the observations.
- Each region is represented by a node in the tree

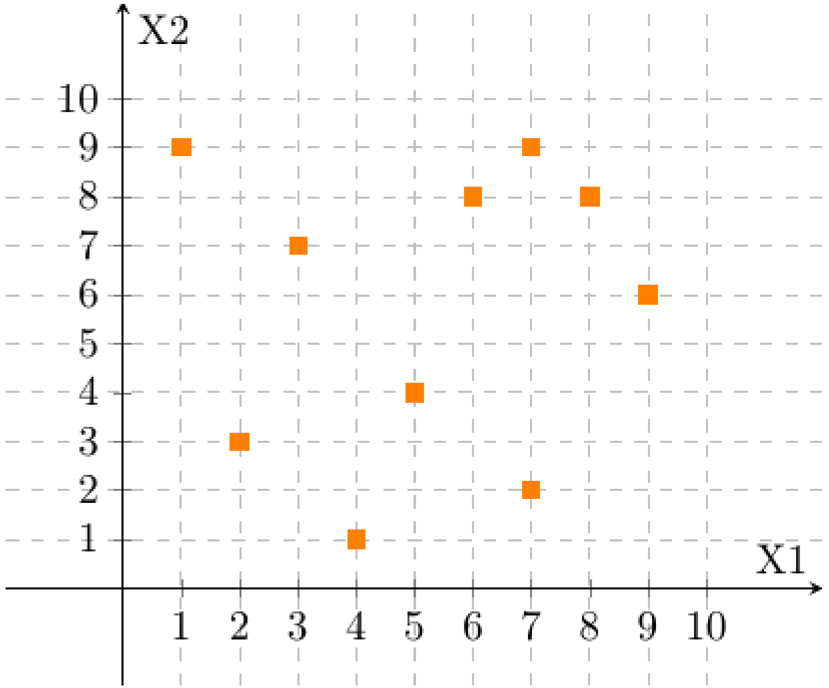
Every non-leaf node in the tree acts as a hyperplane, dividing the space into two partitions. This hyperplane is perpendicular to the chosen axis, which is associated with one of the K dimensions.

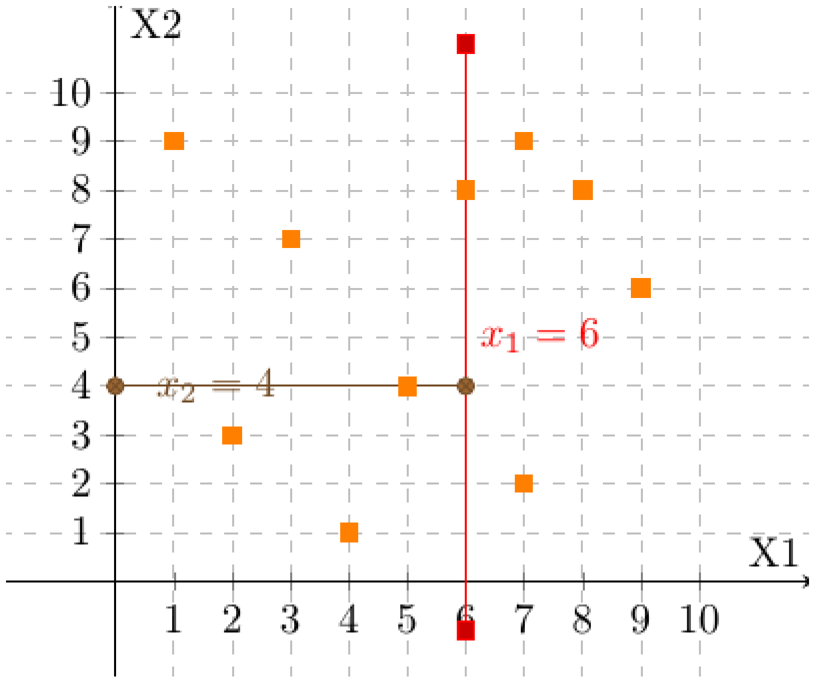
Example





Example





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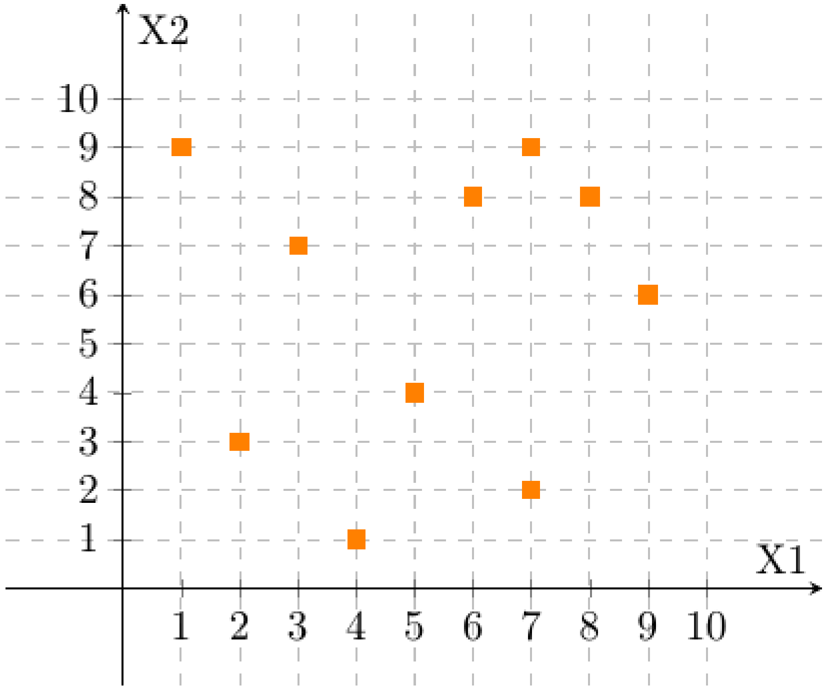

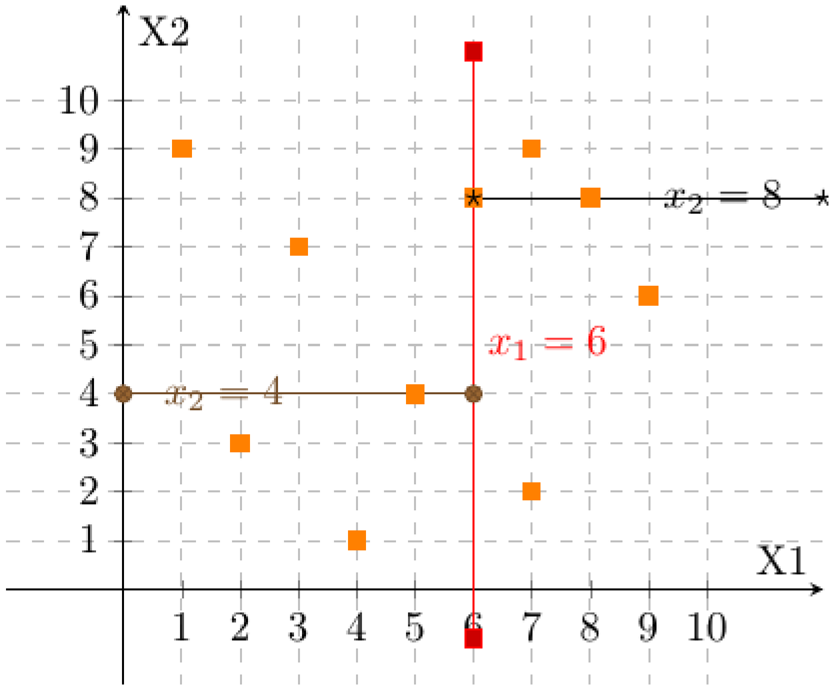

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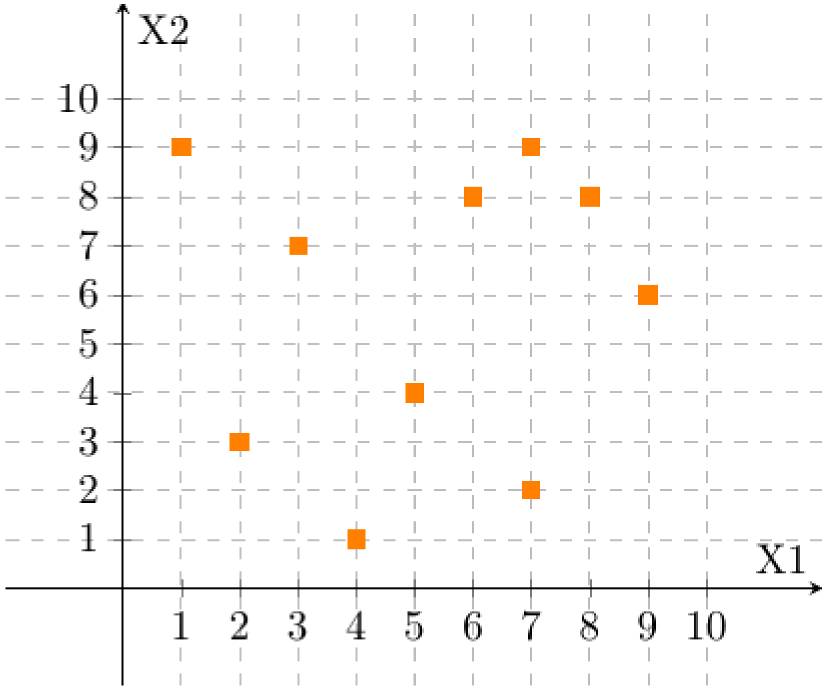
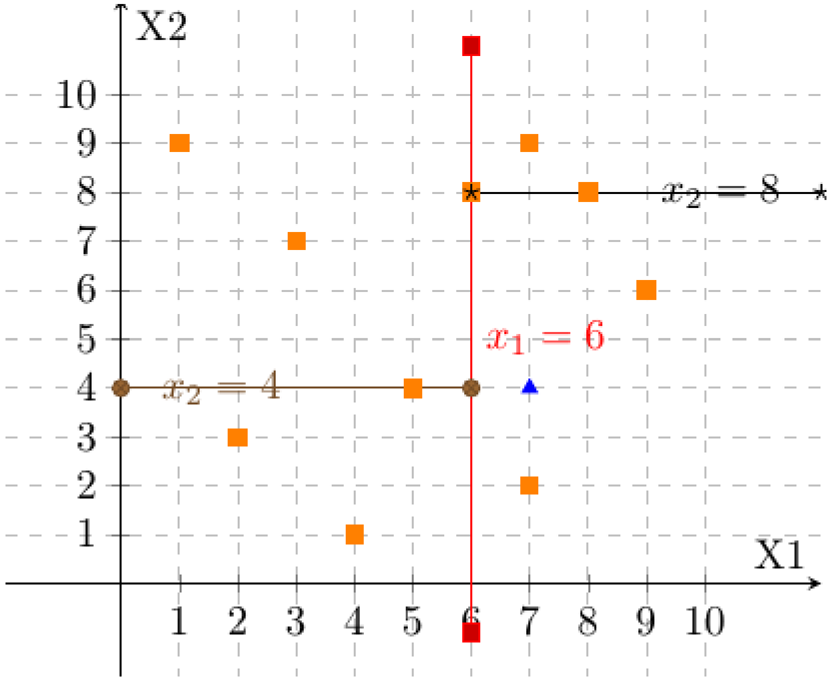




Advantages of KD Tree

- At each level of the tree, KDTree divides the range of the domain in half. Hence they are useful for performing range searches.
- The complexity lies in between O(log N) to O(N) where N is the number of nodes in the tree.

Disadvantages of KD Tree

- Degradation of performance when high dimensional data is used. The algorithm will need to visit many more branches. If the dimensionality of a dataset is K then the number of nodes $N \gg 2^k$.
- If the query point is far from all the points in the dataset then we might have to traverse the whole tree to find the nearest neighbors.

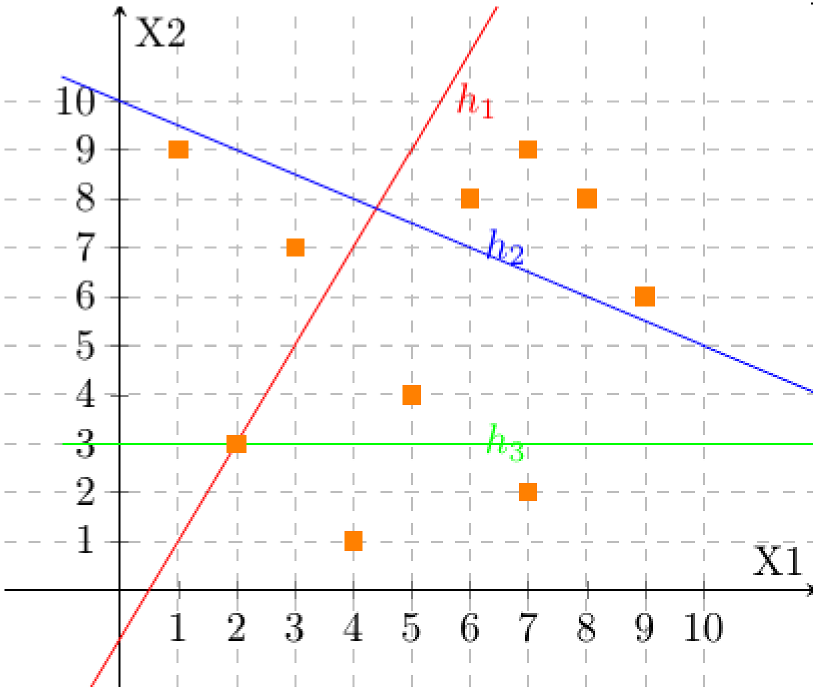
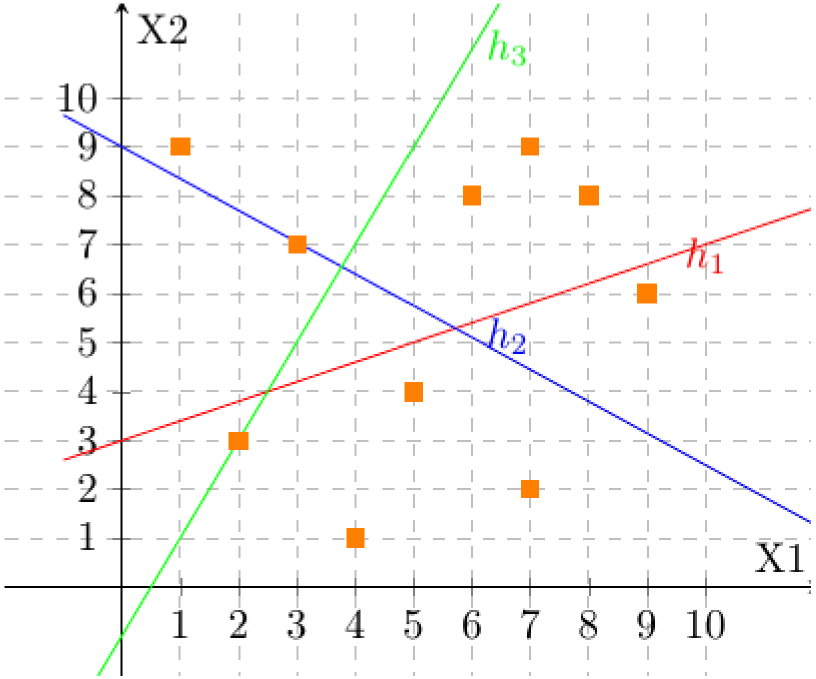
LSH: Locality Sensitive Hashing

- Locality Sensitive Hashing is a technique to enable creating a hash or putting items in buckets such that
  - Similar items go to the same bucket with high probability
  - Dissimilar items go into the same bucket with low probability

Underlying Idea

- Generate a series of *hyperplanes* that partition the space.
- Items lying in the same partition have the same hash value.
- Consider a dataset with N points, each with d dimensions.
- Generate a random set of K hyperplanes: $h_1, h_2, \ldots, h_K$
- For every point in the dataset ($1 \leq i \leq N$), generate a hash as follows:
- For $k \in 1 \ldots K$
  - kth bit of hash = 1 if $x_i . h_k < 0$
  - kth bit of hash = 0 if $x_i . h_k \geq 0$

- To maximize the probability of finding similar items in the same bucket/ same hash, repeat the process L times generating L different sets of K hyperplanes and corresponding hashes for each item
  - Effectively L independent hash tables are constructed for the dataset
- Given a point , in order to retrieve a similar item:
- For each repetition (each hash table constructed) $1 \leq l \leq L$
  - generate the corresponding hash
  - Compare with all other elements in the same bucket of the hash table – add items which are close in value to the output set.


X2
X1
h_1
h_2
h_3

X2
X1
h_1
h_2
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