Clustering

IE500 Data Mining

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Outline

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- What is Cluster Analysis?
- K-Means Clustering
- Density-based Clustering
  - DBSCAN
- Proximity Measures
- Anomaly Detection
  - Statistical Approaches
  - Distance-based Approaches

What is Cluster Analysis?

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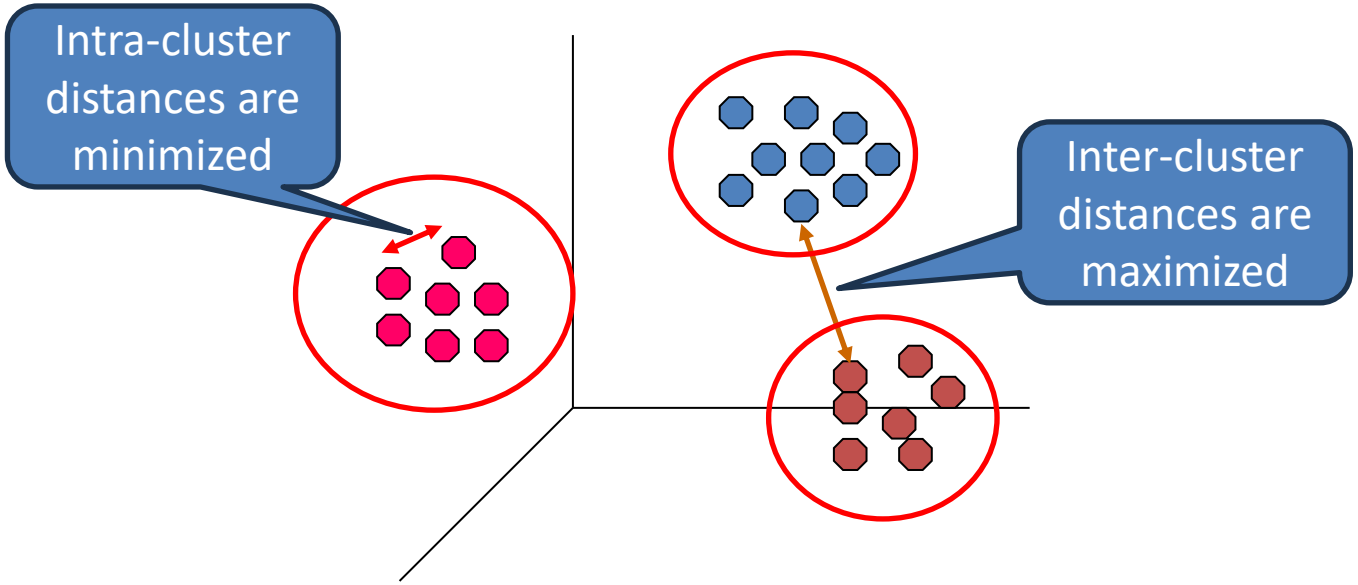
- Finding groups of objects such that the objects in a group
  - will be similar to one another
  - and different from the objects in other groups
- Goal: Get a better understanding of the data



Cluster Analysis as Unsupervised Learning

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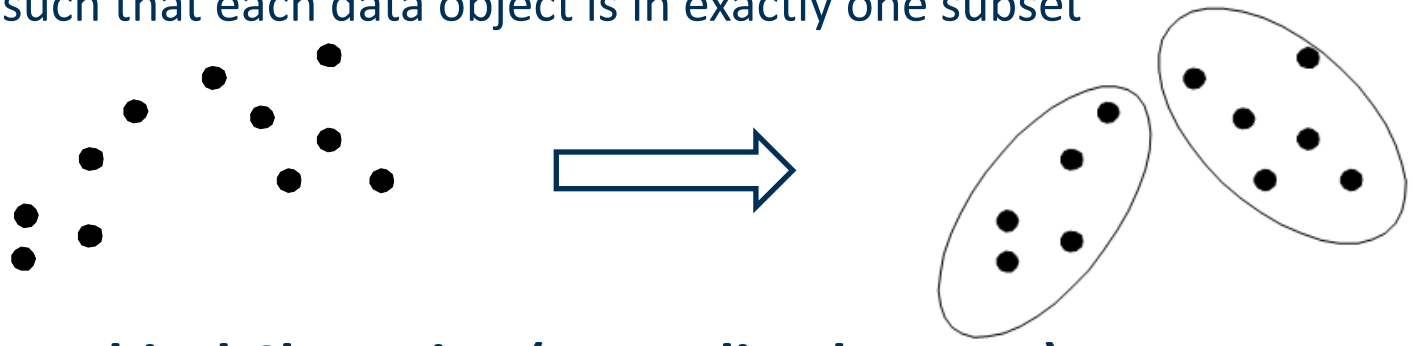
- **Supervised learning**: Discover patterns in the data that relate data attributes with a target (class) attribute
  - The set of classes is known before
  - Class attributes are usually provided by human annotators
  - Patterns are used for prediction of the target attribute for new data

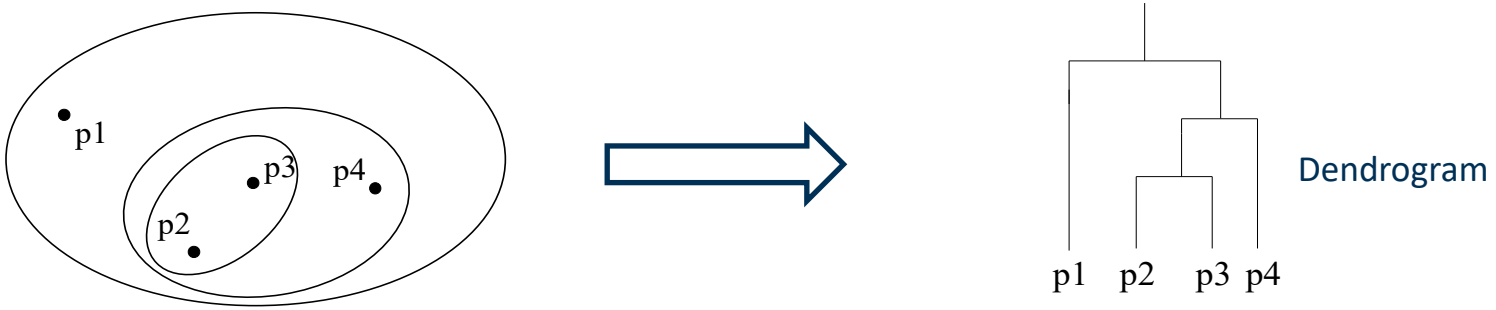
- **Unsupervised learning**: The data has no target attribute
  - We want to explore the data to find some intrinsic structures in it
  - The set of classes/clusters is not known before
  - Cluster Analysis and Association Rule Mining are unsupervised learning tasks

Types of Clusterings

- **Partitional Clustering**
  - A division of data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset



- **Hierarchical Clustering (see online lectures)**
  - A set of nested clusters organized as a hierarchical tree



Aspects of Cluster Analysis

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- **A clustering algorithm**
  - Partitional algorithms
  - Density-based algorithms
  - Hierarchical algorithms
  - …
- **A proximity (similarity, or dissimilarity) measure**
  - Euclidean distance
  - Cosine similarity
  - Data type-specific similarity measures
  - Domain-specific similarity measures
- **Clustering quality**
  - Intra-clusters distance $\Rightarrow$ minimized
  - Inter-clusters distance $\Rightarrow$ maximized
  - The clustering should be useful with regard to the goal of the analysis

The Notion of a Cluster is Ambiguous

How many clusters do you see?

Six Clusters

Two Clusters

Four Clusters

The usefulness of a clustering depends on the **goal of the analysis**

Example Applications

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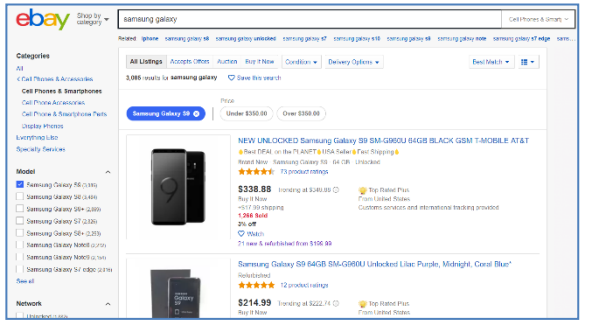
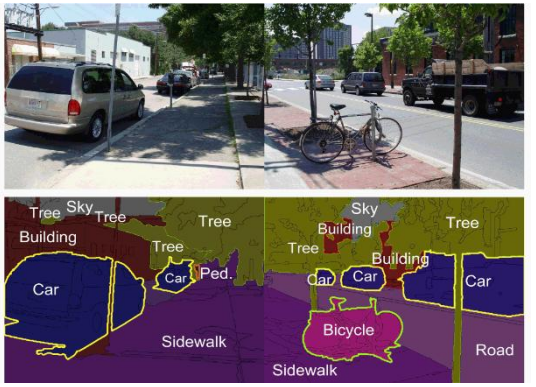
- Market Segmentation
  - Goal: Identify groups of similar customers
  - Level of granularity depends on the task at hand

- E-Commerce
  - Identify offers of the same product on electronic markets



- Image Recognition
  - Identify parts of an image that belong to the same object



K-Means Clustering

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- Partitional clustering algorithm
- Each cluster is associated with a **centroid** (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified beforehand

- Algorithm:

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

K-Means Example, Step 1

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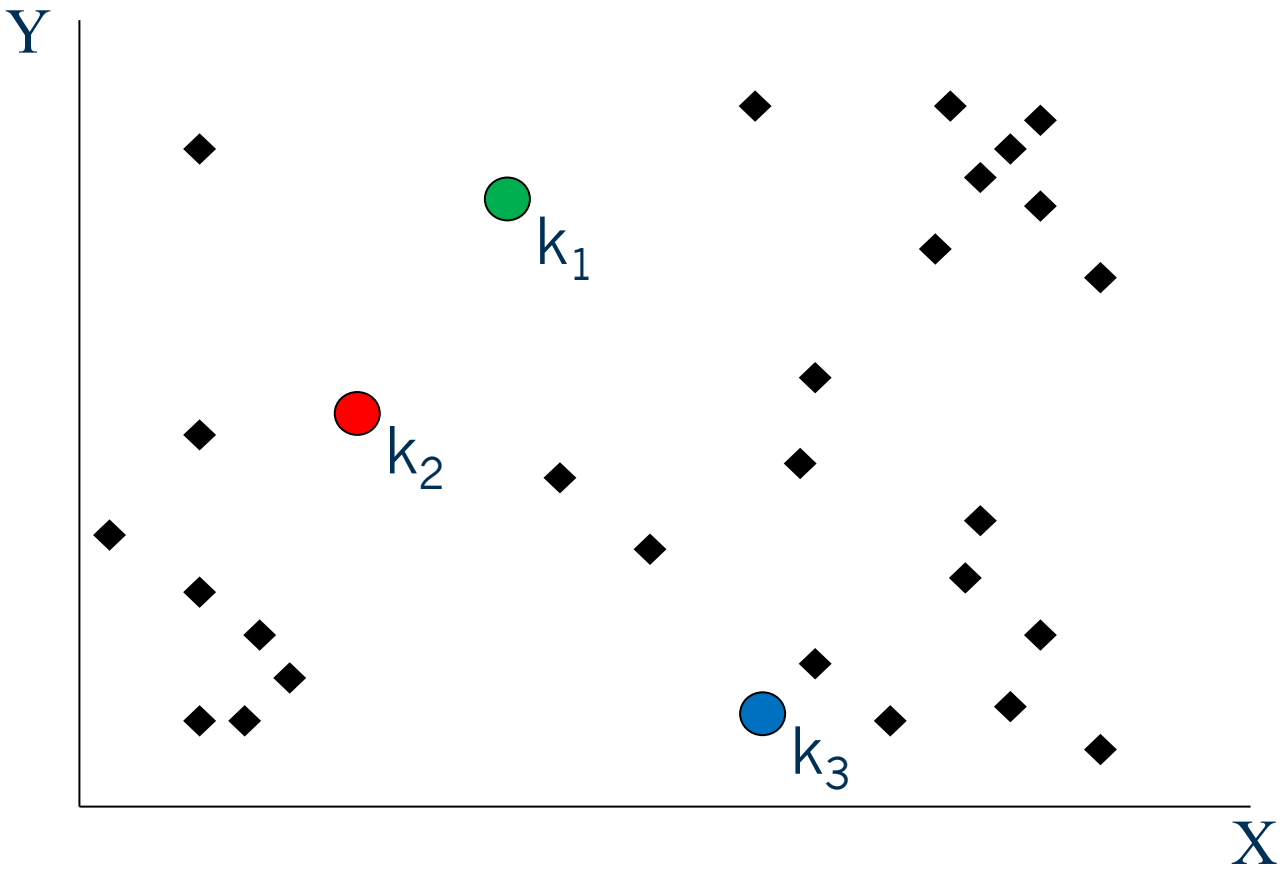
- Randomly pick 3 initial centroids



K-Means Example, Step 3

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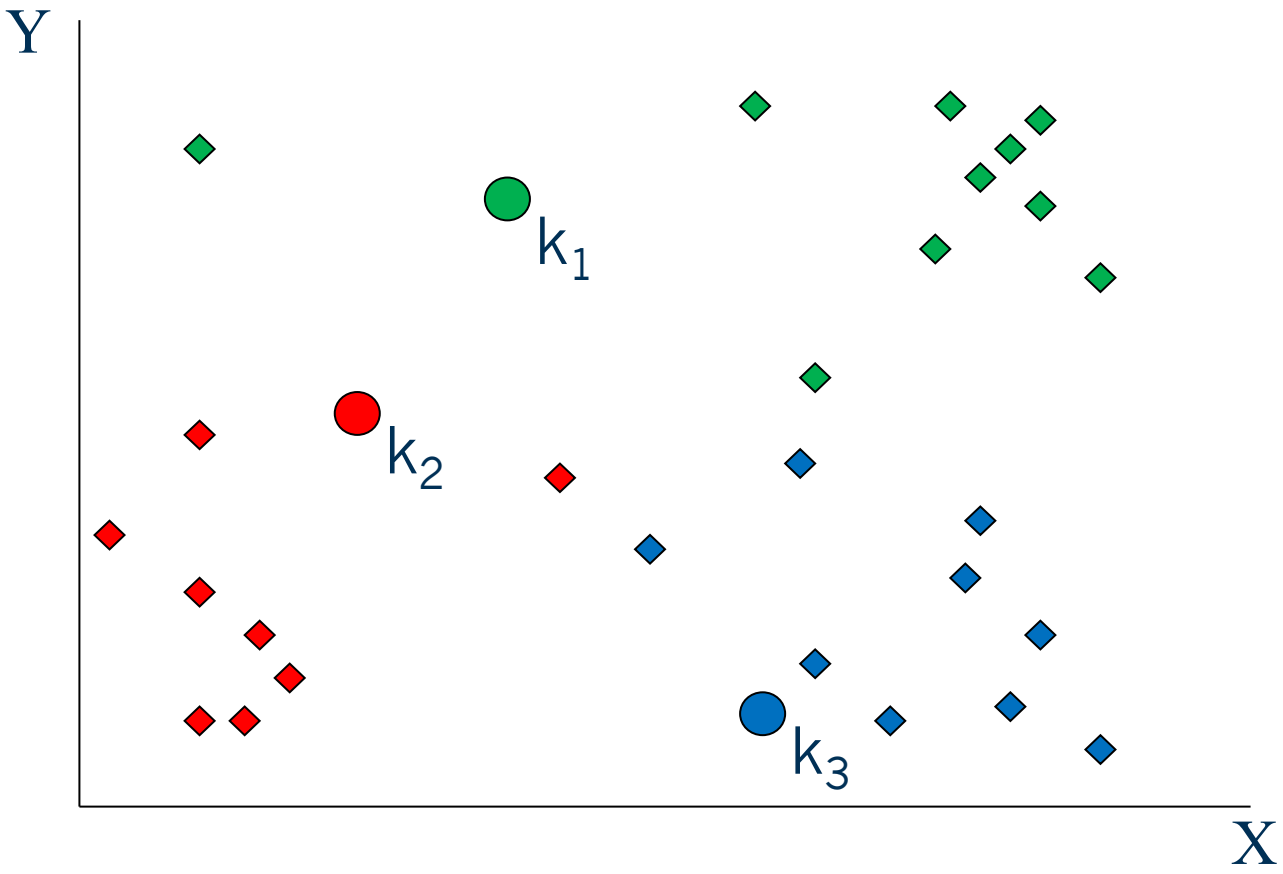
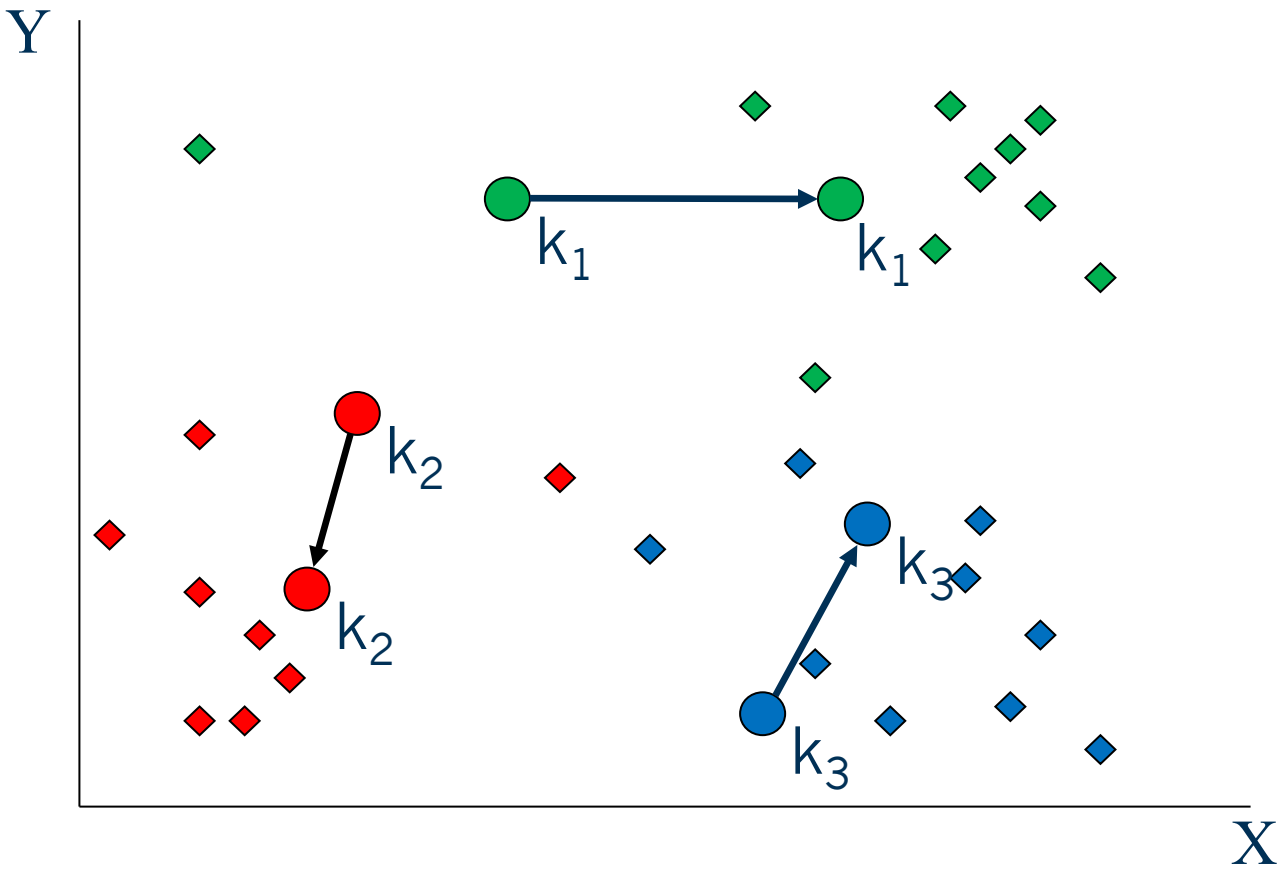
- Assign each point to the closest centroid



K-Means Example, Step 4

- Move each centroid to the mean of each cluster



K-Means Example, Step 5

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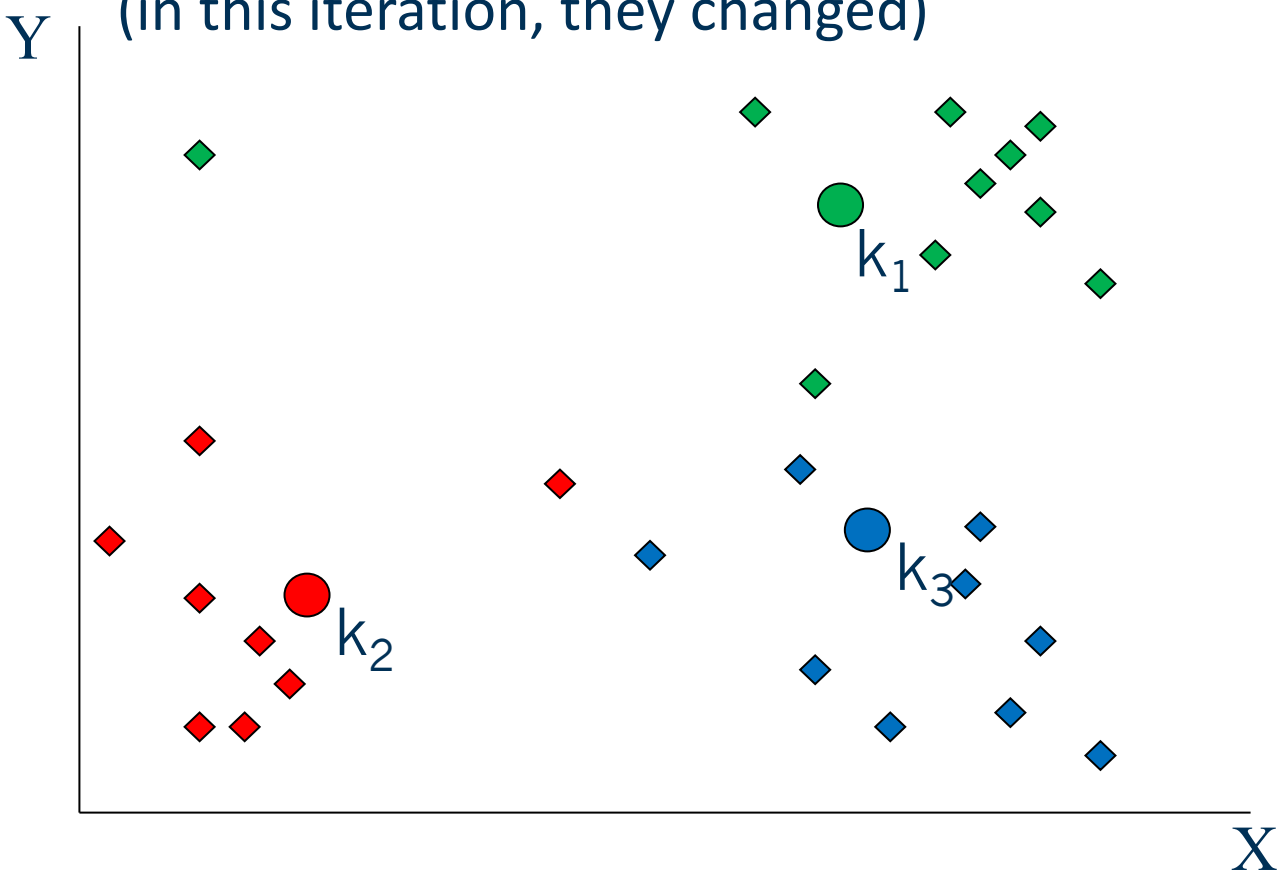
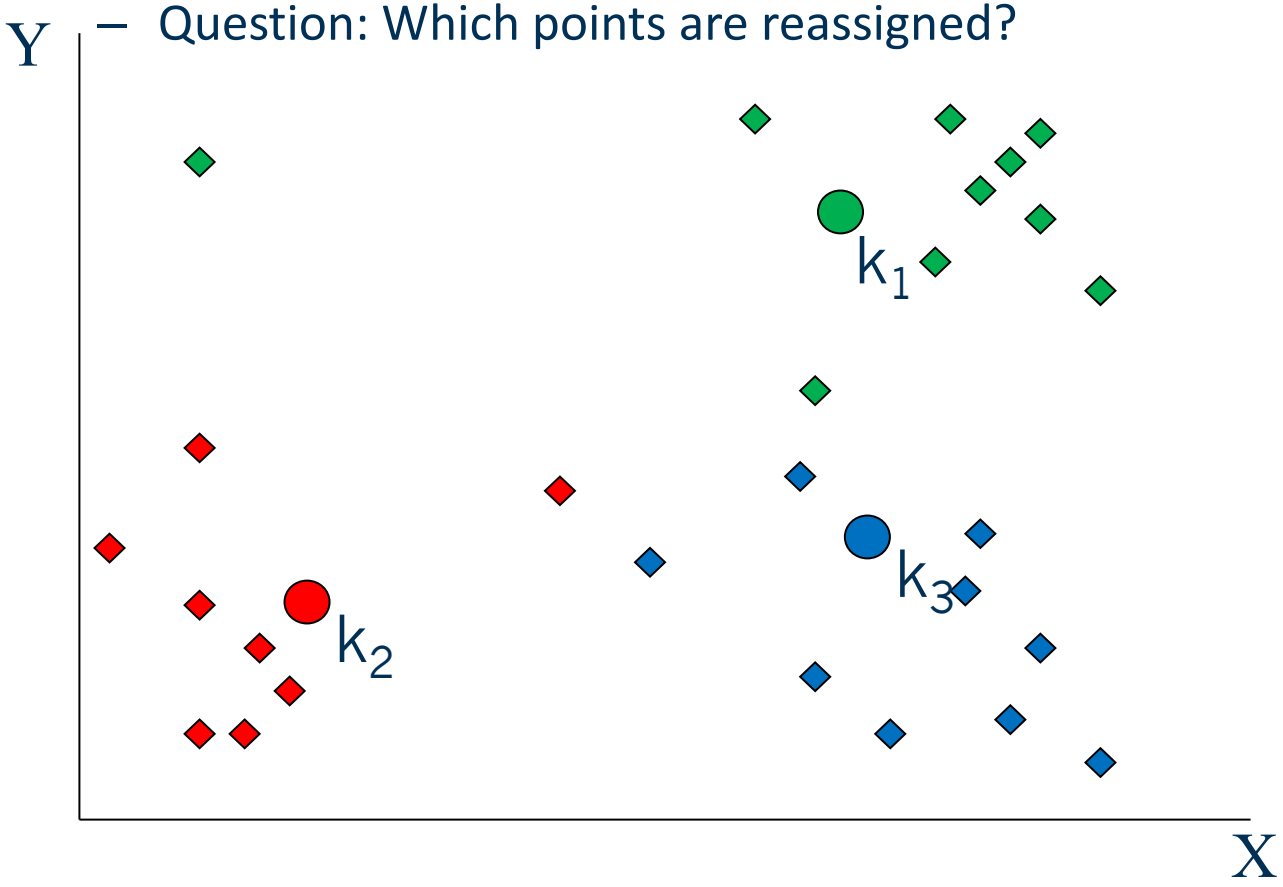
- Repeat until the centroids don't change (in this iteration, they changed)



K-Means Example, Repeated Step 3

- Reassign points if they are now closer to a different centroid
  - Question: Which points are reassigned?



K-Means Example, Repeated Step 3

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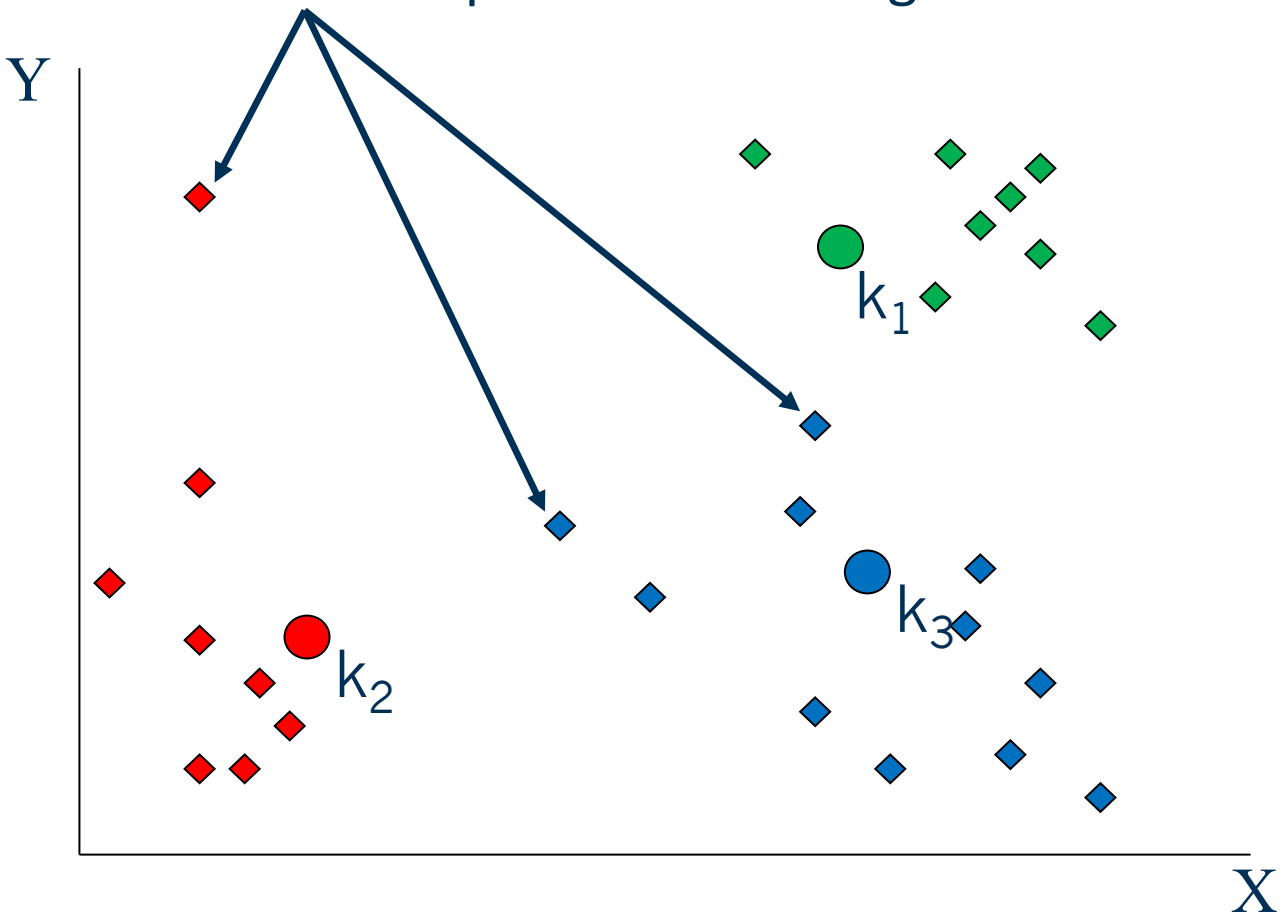
- Answer: Three points are reassigned



K-Means Example, Repeated Step 4

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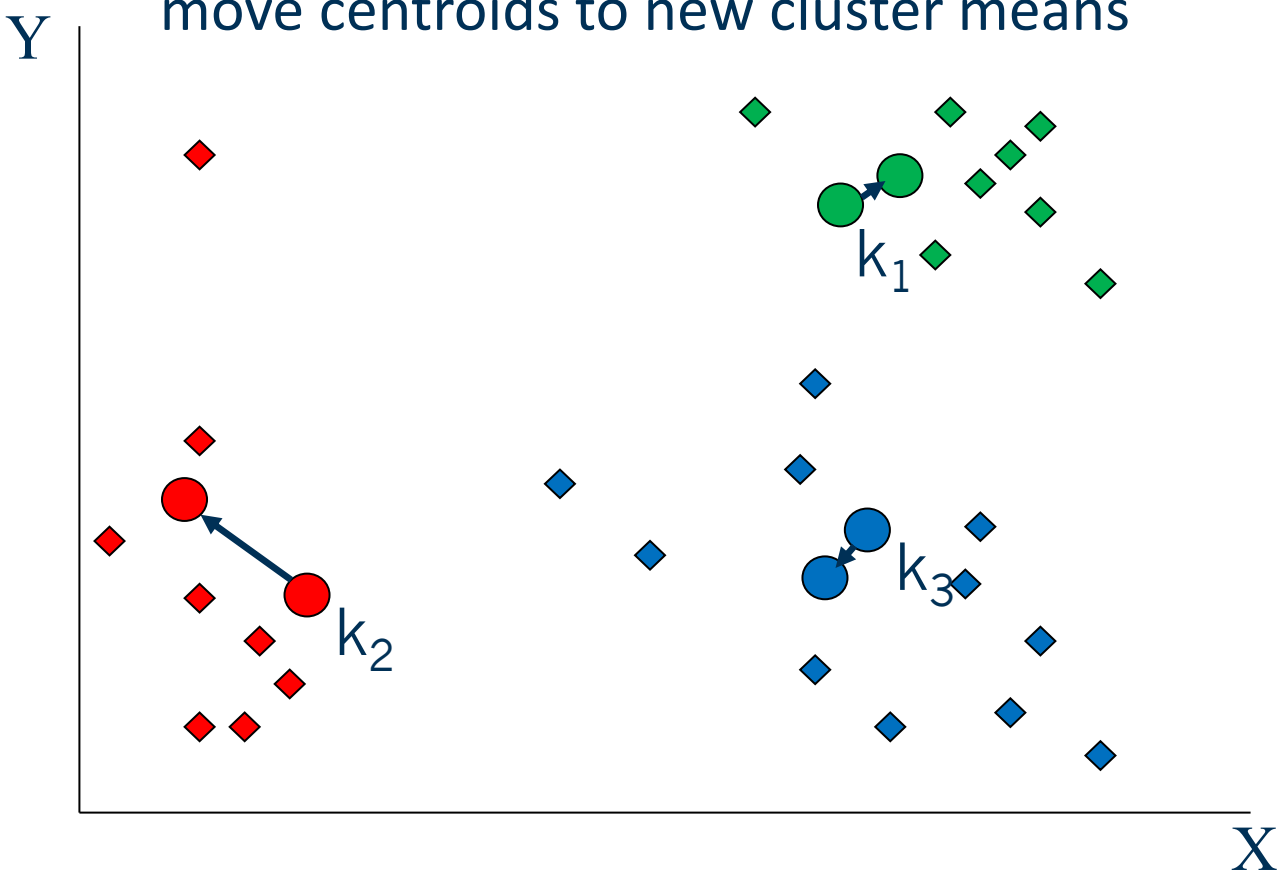
- Re-compute cluster means and move centroids to new cluster means



K-Means Example, Repeated Step 5

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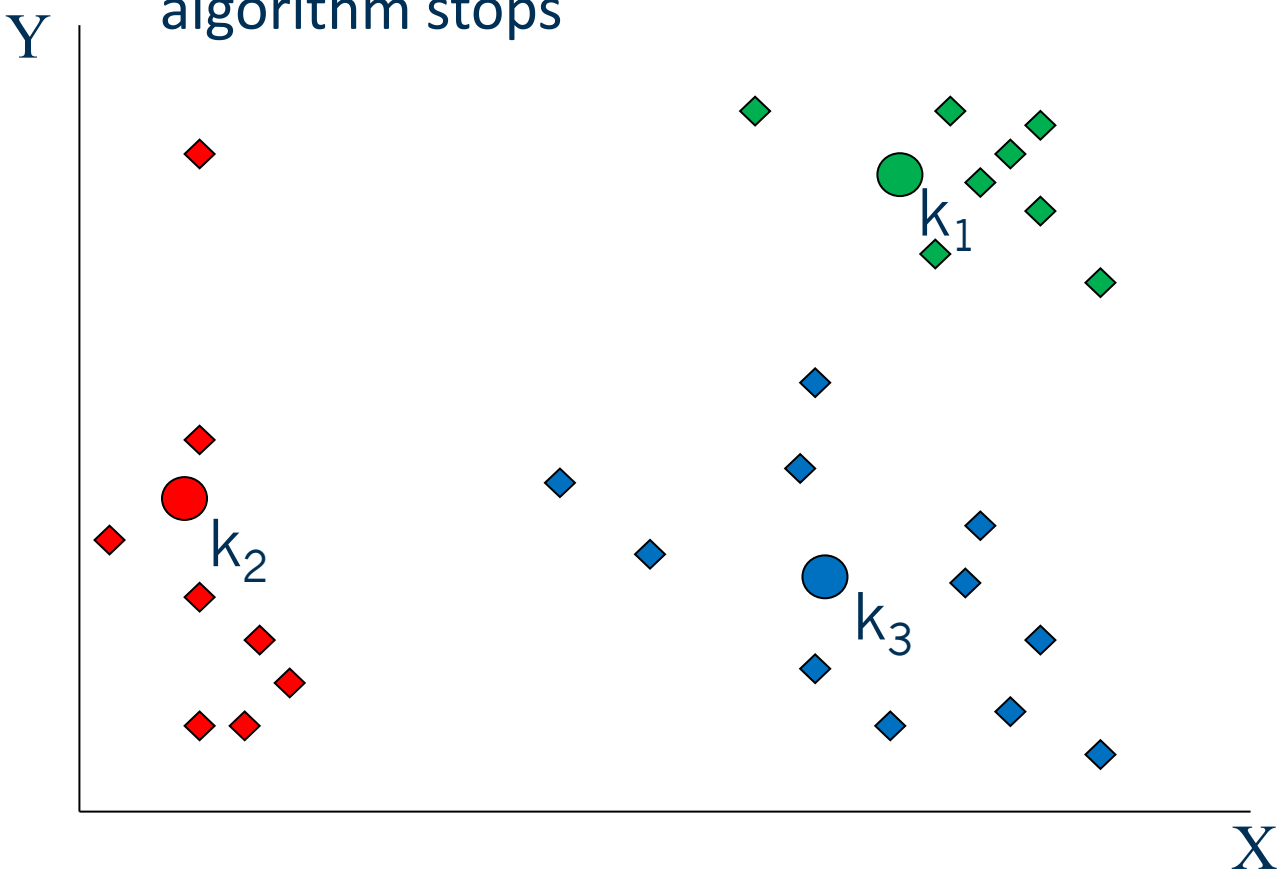
- No points are reassigned, thus centroids don't change and algorithm stops



Convergence Criteria

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- Default convergence criterion
  - No (or minimum) change of centroids
- Alternative convergence criteria
  - No (or minimum) re-assignments of data points to different clusters
  - Stop after x iterations
  - Minimum decrease in the sum of squared error (SSE)
    - See next slide

Evaluating K-Means Clusterings

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- Widely used cohesion measure: **Sum of Squared Error (SSE)**
  - For each point, the error is the distance to the nearest centroid
  - To get SSE, we square these errors and sum them

$$SSE = \sum_{j=1}^{k} \sum_{x \in C_j} dist(x, m_j)^2$$

    - C_j is the j-th cluster
    - m_j is the centroid of cluster C_j
      (the **m**ean vector of all the data points in C_j)
    - $dist(x, m_j)$ is the distance between data point x and centroid m_j
- Given several clusterings (= groupings),
  we should prefer the one with the smallest SSE

Illustration: Sum of Squared Error

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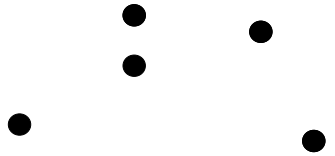
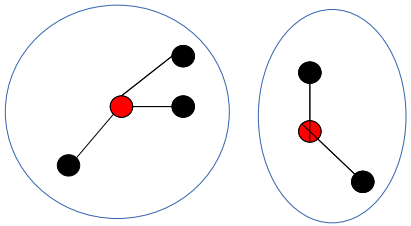
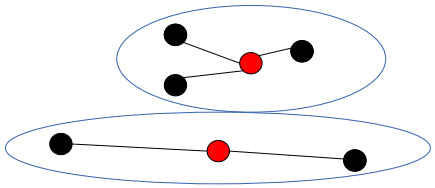
- Clustering problem given:



- Good clustering
  - small distances to centroids



- Not so good clustering
  - larger distances to centroids



Weaknesses of K-Means: Initial Seeds

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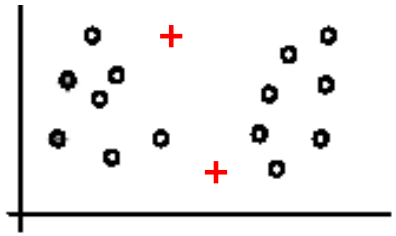
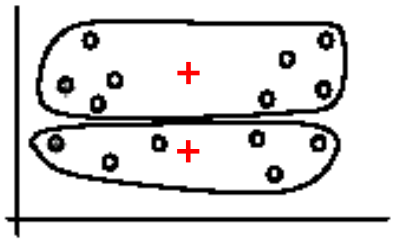
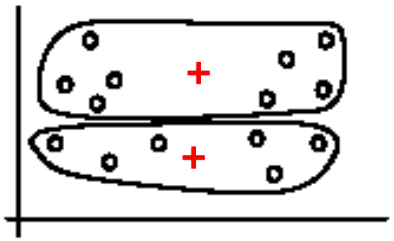
- Clustering results may vary significantly depending on initial choice of seeds (**number** and **position** of seeds)



(A). Random selection of seeds (centroids)



(B). Iteration 1



(C). Iteration 2

Weaknesses of K-Means: Initial Seeds

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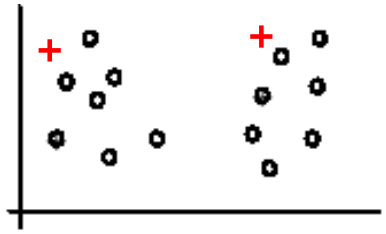
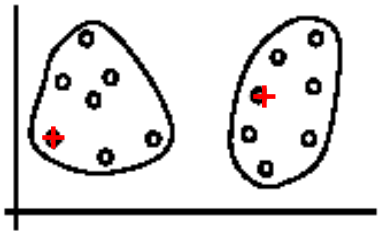
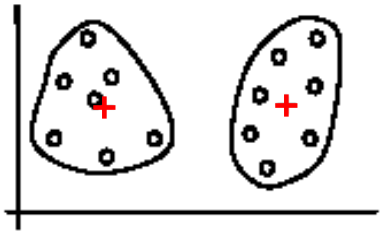
- If we use **different seeds**, we get good results



(A). Random selection of k seeds (centroids)



(B). Iteration 1



(C). Iteration 2

Improving the Clustering Results

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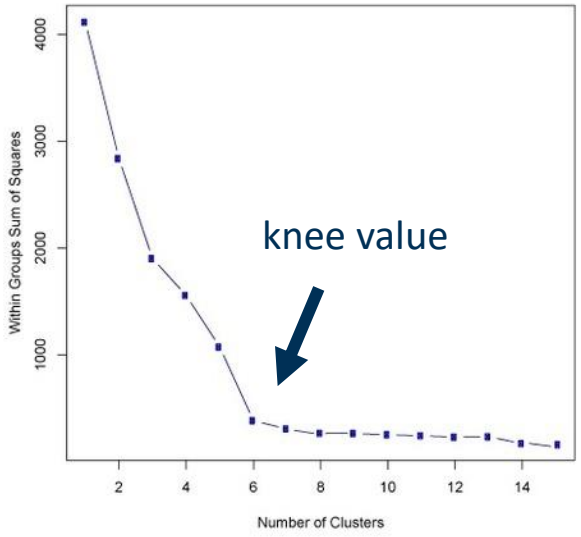
- Restart a number of times with different random seeds
  - chose the resulting clustering with the smallest sum of squared error (SSE)
- Run k-means with different values of k
  - The SSE for different values of k cannot directly be compared
    - Think: what happens for k → number of examples?
  - Workarounds
    - Choose k where SSE improvement decreases (knee value of k)
    - Employ X-Means
      - Variation of K-Means algorithm that automatically determines k
      - Starts with small k, then splits large clusters until improvement decreases



Choosing k – Cluster Evaluation

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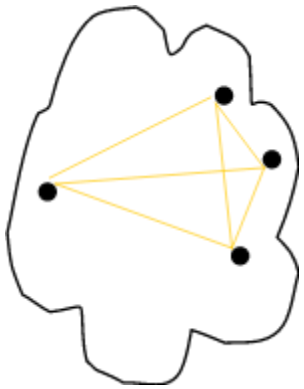
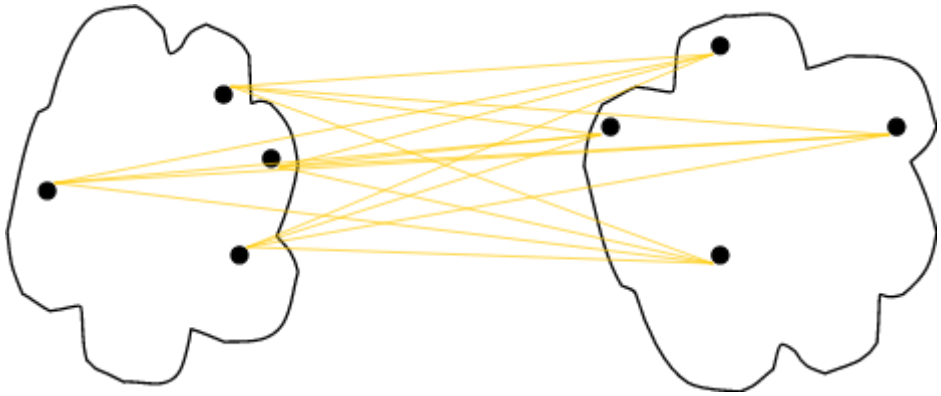
- Recap: we want to maximize
  - Cohesion: measures how closely related are objects in a cluster
  - Separation: measure how distinct or well-separated a cluster is from other clusters



Cohesion



Separation

Silhouette Coefficient

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- Cohesion $a(x)$: Average distance of x to **all other vectors in the same cluster**
- Separation $b(x)$: Average distance of x to **the vectors in other clusters.** Find the minimum among the clusters.
- Silhouette $s(x)$:

$$s(x) = \frac{b(x) - a(x)}{\max\{a(x), b(x)\}}$$

$s(x) \in [-1,1]$

-1 = bad
0 = indifferent
1 = good

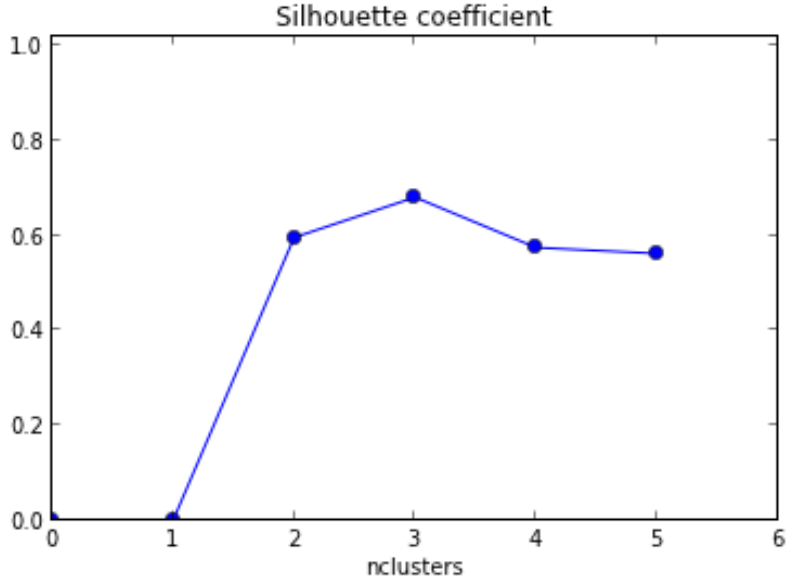
- Silhouette coefficient (SC):

$$SC = \frac{1}{N}\sum_{i=1}^{N} s(x_i)$$

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.silhouette_score.html

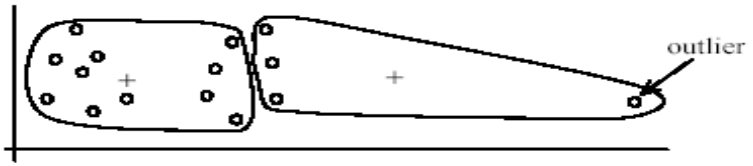
Selecting k
Using the Silhouette Coefficient

- Approach
  - Run k-means with different k values
  - Plot the Silhouette Coefficient
  - Pick the best (i.e., highest) silhouette coefficient
  - Note: silhouette coefficient does not depend on no. of clusters

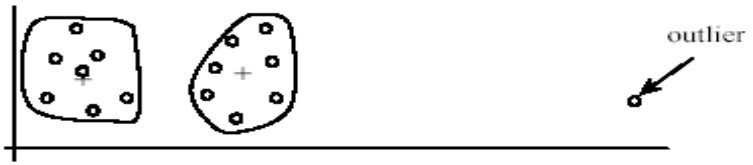


Weaknesses of K-Means: Problems with Outliers

- Possible remedy:
  - Remove data points far away from centroids
  - To be safe: monitor these possible outliers over a few iterations and then decide to remove them
- Other remedy: random sampling
  - After determining the centroids based on random samples, assign the rest of the data points (also improves runtime performance)



(A): Undesirable clusters



(B): Ideal clusters

K-Medoids

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- K-Medoids is a K-Means variation that uses the **medians** of each cluster instead of the mean
  - Medoids are the **most central existing data points** in each cluster
- K-Medoids is more robust against outliers as the median is not affected by extreme values:
  - Mean and Median of 1, 3, 5, 7, 9 is 5
  - Mean of 1, 3, 5, 7, 1009 is 205
  - Median of 1, 3, 5, 7, 1009 is 5

K-Means Clustering Summary

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- **Advantages**
  - Simple, understandable
  - Efficient time complexity: O(n * K * I * d) where
    - n = number of points
    - K = number of clusters
    - I = number of iterations
    - d = number of attributes
- **Disadvantages**
  - Need to determine number of clusters
  - All items are forced into a cluster
  - Sensitive to
    - Outliers
    - Initial seeds

Python

```
# import KMeans
from sklearn.cluster import KMeans

# create clusterer
estimator = KMeans(n_clusters = 3)

# create clustering
cluster_ids = estimator.fit_predict(dataset[['Att1', 'Att2']])
```

Density-based Clustering

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- Challenging use case for K-Means because
  - Problem 1: Non-globular shapes
  - Problem 2: Outliers / noise points

DBSCAN

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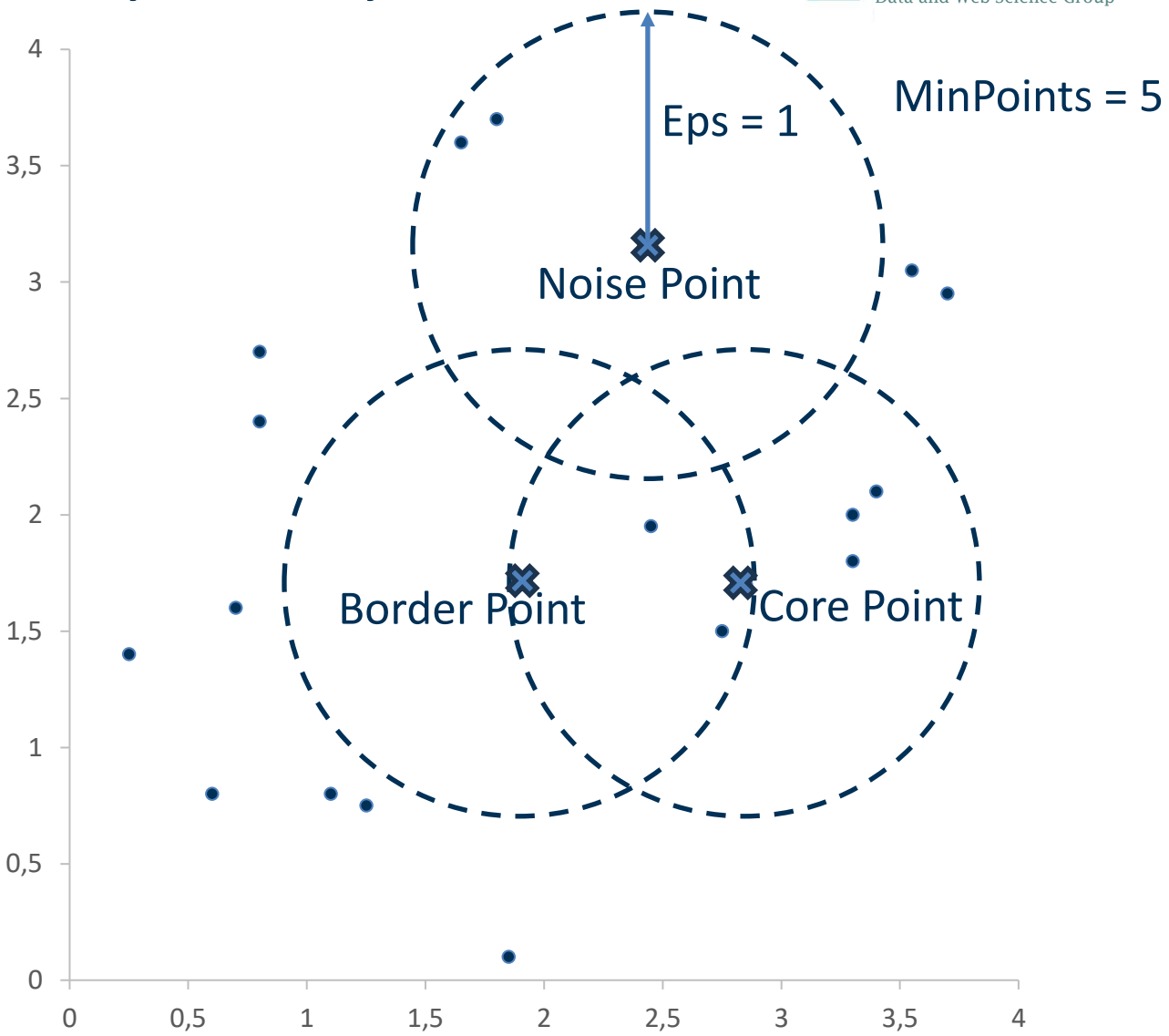
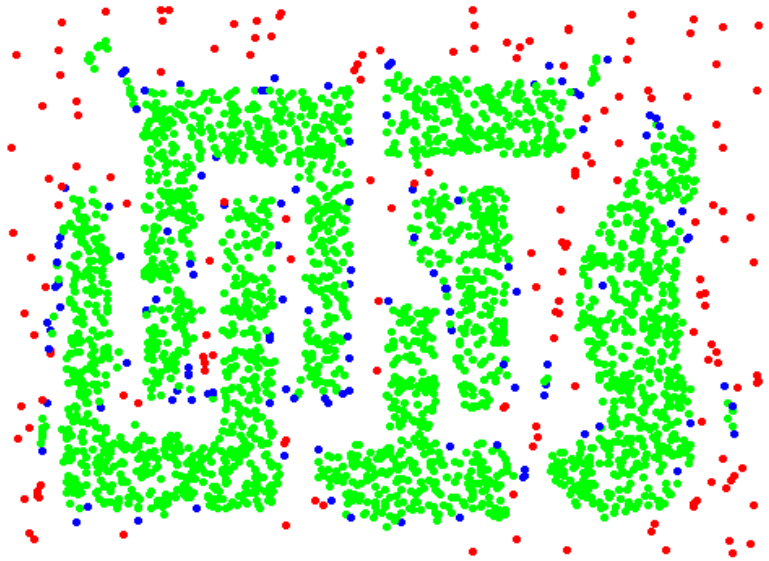
- DBSCAN is a density-based algorithm
  - **Density** = number of points within a specified radius Epsilon (Eps)
- Divides data points into three classes:
  - A point is a **core point** if it has at least a specified number of neighboring points (*MinPts*) within the specified radius *Eps*
    - the point itself is counted as well
    - these points form the interior of a dense region (cluster)
  - A **border point** has fewer points than *MinPts* within *Eps*, but is in the neighborhood of a core point
  - A **noise point** is any point that is not a core point or a border point

Examples of Core, Border, and Noise Points



Examples of Core, Border, and Noise Points

1) Original Points



2) Point types:
core, border and noise

DBSCAN Algorithm

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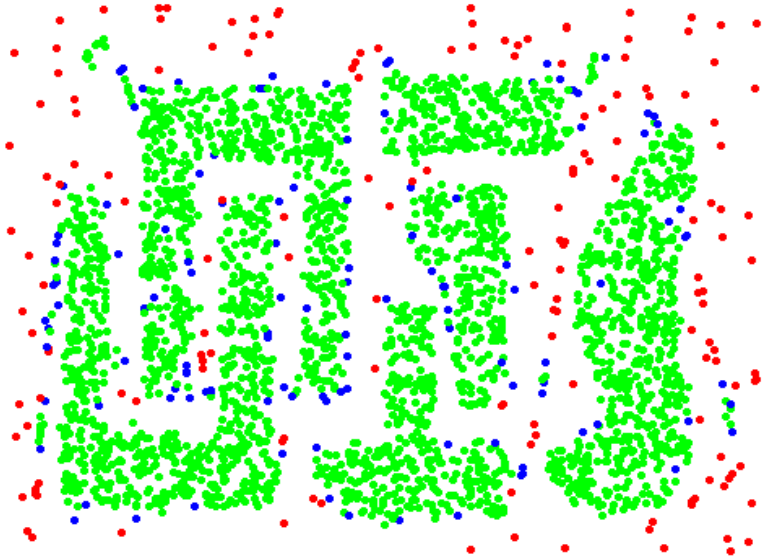
- Eliminate noise points
- Perform clustering on the remaining points

```
current_cluster_label ← 1
for all core points do
  if the core point has no cluster label then
    current_cluster_label ← current_cluster_label + 1
    Label the current core point with cluster label current_cluster_label
  end if
  for all points in the Eps-neighborhood, except i^th the point itself do
    if the point does not have a cluster label then
      Label the point with cluster label current_cluster_label
    end if
  end for
end for
```

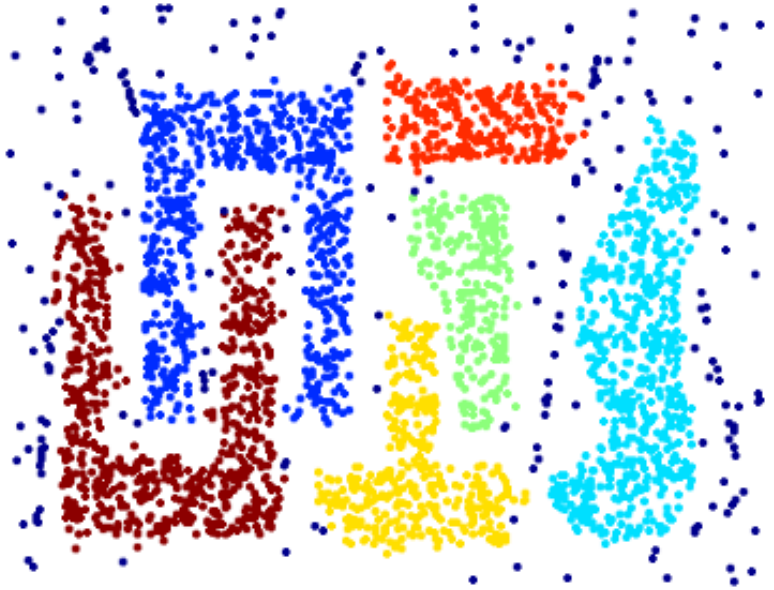
perform recursion for all points in the Eps-neighborhood of the point

Examples Clusters

1) Original Points



2) Point types:
core, border and noise



3) Clusters

When DBSCAN Does NOT Work Well

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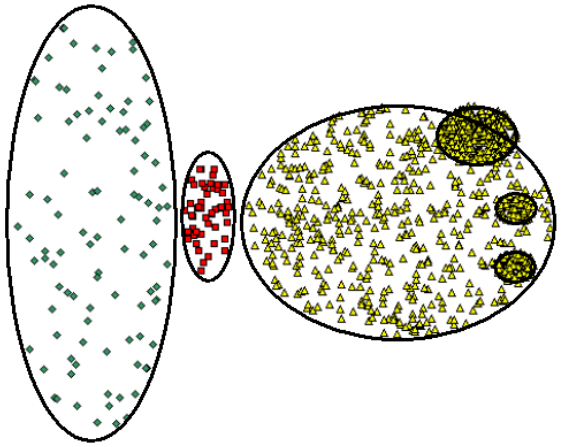
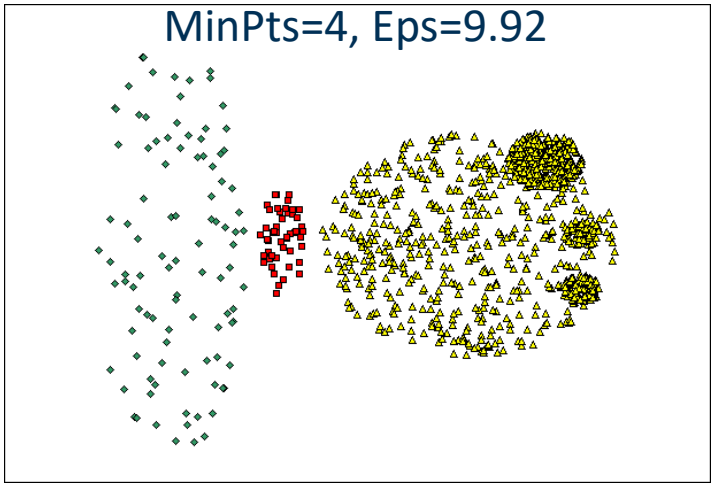
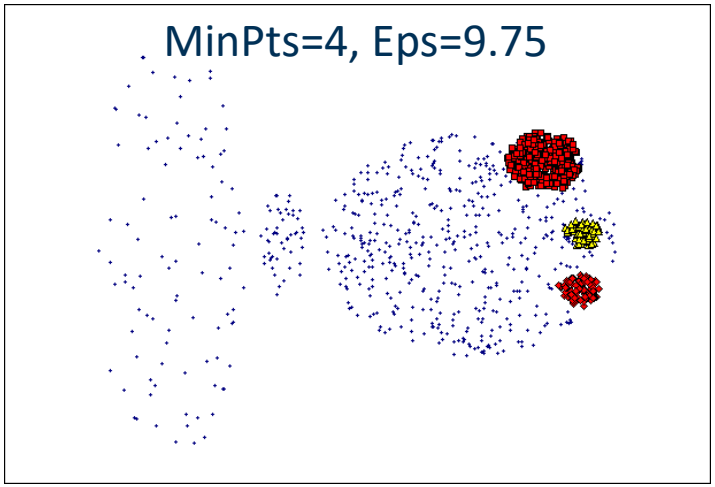
- Varing densities
- High-dimensional data



Original Points





DBSCAN: Determining EPS and MinPts

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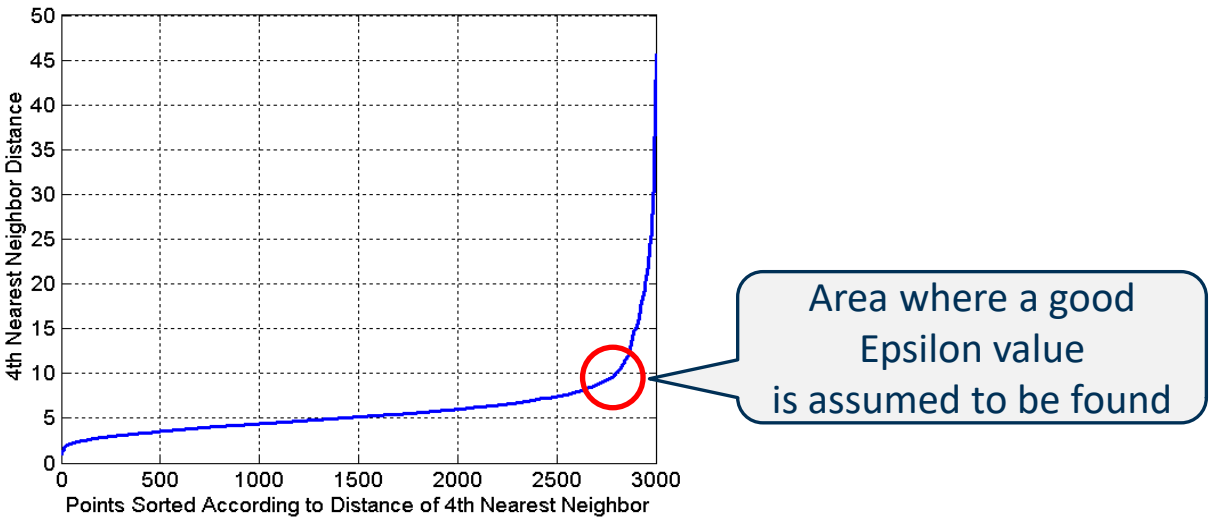
- Idea: for points in a cluster,
  their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- Plot sorted distance of every point to its k^{th} nearest neighbor



DBSCAN in Python

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Python

```python
# import DBSCAN
from sklearn.cluster import DBSCAN

# create the clusterer
clusterer = DBSCAN(min_samples=3, eps=1.5, metric='euclidean')

# create the clusters
clusters = clusterer.fit_predict(dataset[['Att1', 'Att2']])
```

Proximity Measures

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- So far, we have seen different clustering algorithms
  - All of which rely on proximity (distance, similarity, ...) measures
- Similarity
  - Numerical measure of how alike two data objects are (higher: more alike)
  - Often falls in the range [0,1]
- Dissimilarity / Distance
  - Numerical measure of how different are two data objects (higher: less alike)
  - Minimum dissimilarity is often 0
  - Upper limit varies

- Clustering approaches heavily depend on a similarity/distance between records
  - Attributes should be **normalized**
    so that all attributes can have **equal impact** on the computation of distances

Proximity of Single Attributes

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Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Similarity and dissimilarity for simple attributes

p and q are attribute values for two data objects

Levenshtein Distance

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- Measures the dissimilarity of **two strings**
- Measures the **minimum number of edits** needed to transform one string into the other
- Allowed edit operations:
  - **Insert** a character into the string
  - **Delete** a character from the string
  - **Replace** one character with a different character
- Examples:
  - levensthein('table', 'cable') = 1 (1 substitution)
  - levensthein('Doe, Jane', 'Jane Doe') = 8 (7 substitution, 1 deletion)

Further String Similarity Measures

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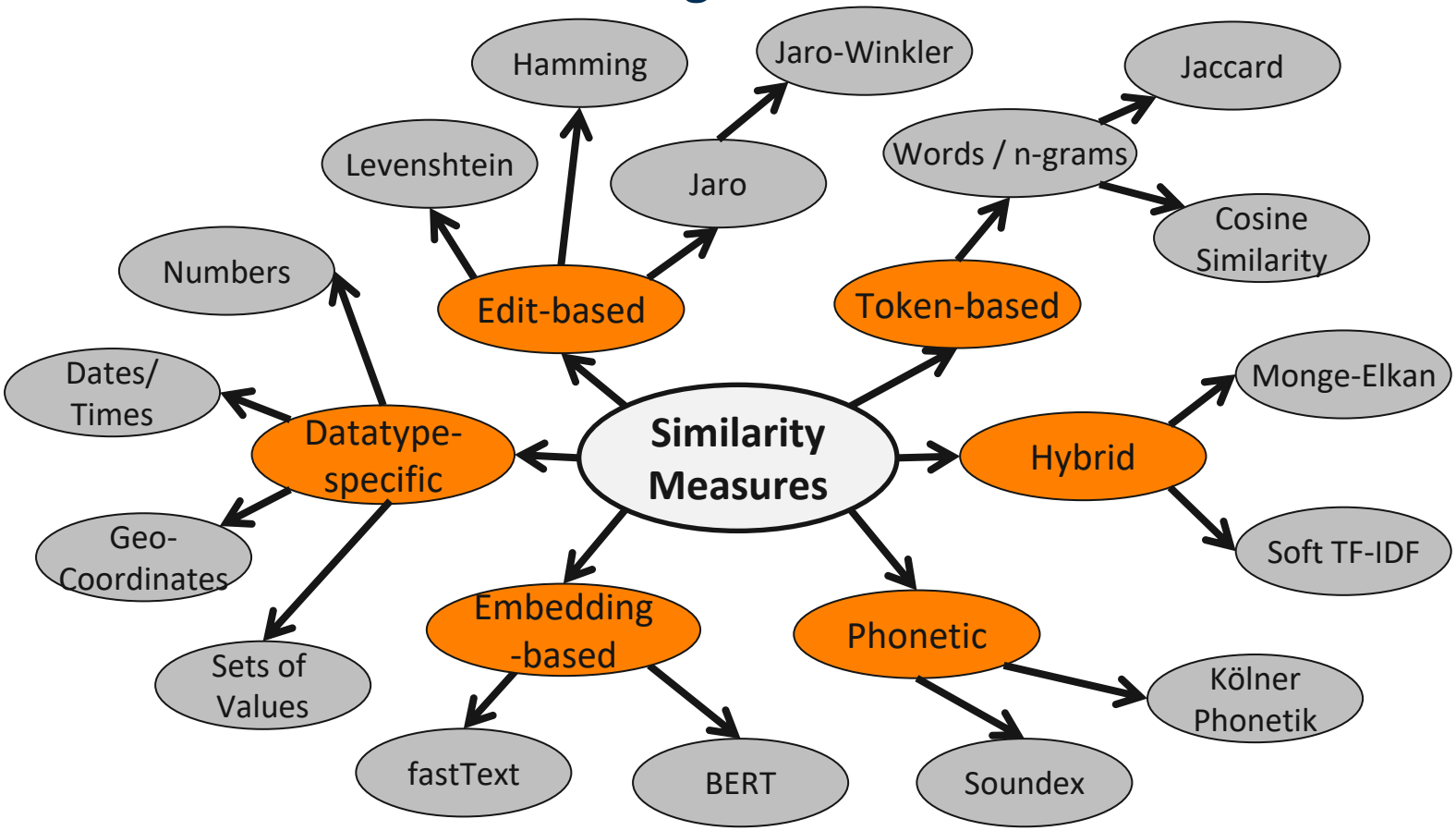
- See course: Web Data Integration



Anomaly Detection

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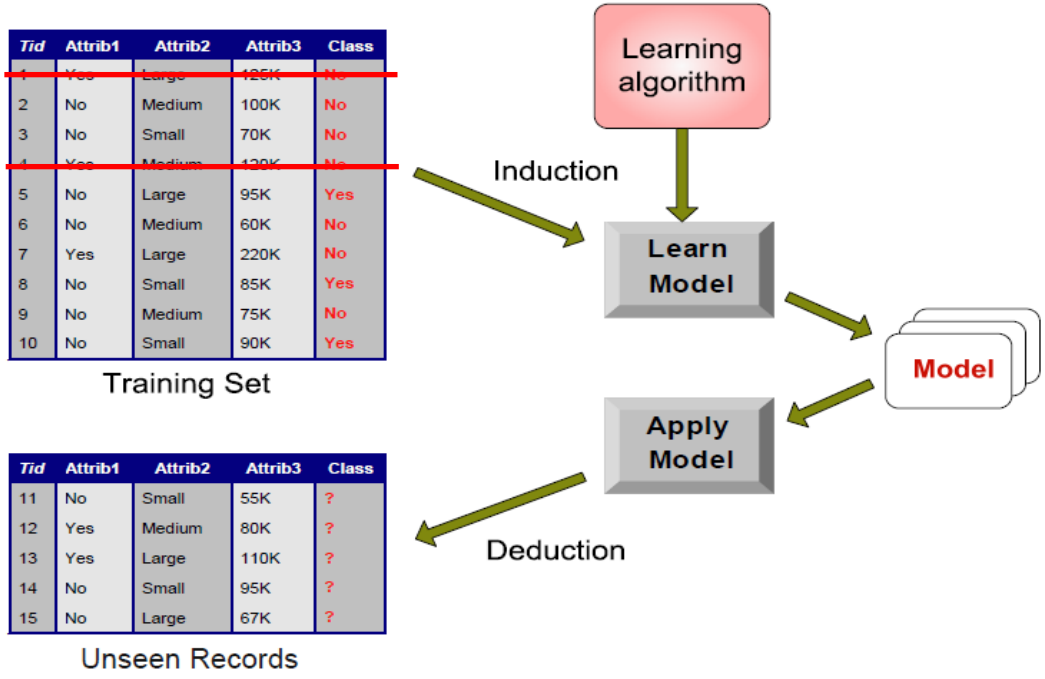
- Also known as “Outlier Detection”
- Automatically identify data points
  that are somehow different from the rest
- Working assumption:
  - There are considerably more “normal” observations than “abnormal” observations (outliers/anomalies) in the data
- Methods:
  - Statistical Approaches (IQR, MAD)
  - Distance-based Approaches
  - Density based Approaches
  - Clustering based

Pipeline

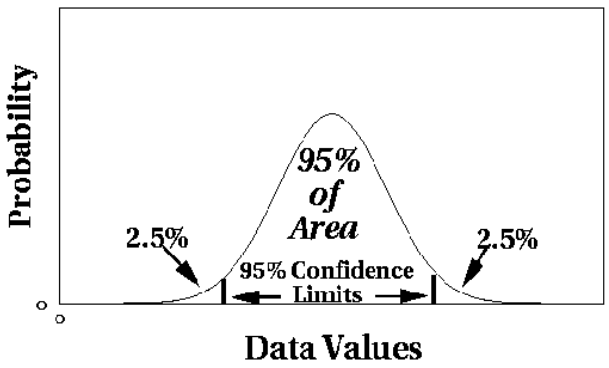
- Usage of anomaly detection in data mining pipeline
  - Remove outliers in the training set
  - **Keep the test set as it is (without removing outliers)**
    - Unless the examples are wrong (domain knowledge)



Statistical Approaches

- Assume a parametric model describing the distribution of the data (e.g., normal distribution)

- Apply a statistical test that depends on
  - Data distribution
  - Parameter of distribution (e.g., mean, variance)
  - Number of expected outliers (confidence limit)



Interquartile Range (IQR)

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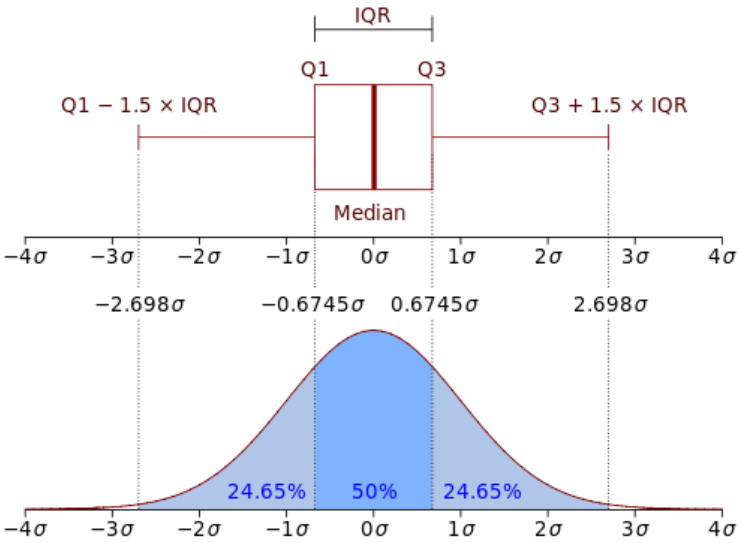

- Divides data in quartiles
  - Assumes a normal distribution
- Definitions:
  - Q1: x ≥ Q1 holds for 75% of all x
  - Q3: x ≥ Q3 holds for 25% of all x
  - IQR = Q3-Q1
- Outlier detection:
  - All values outside [Q1-1.5*IQR ; Q3+1.5*IQR]
- Example:
  - 0,1,1,3,3,5,7,42 → median=3, Q1=1, Q3=7 → IQR = 6
  - Allowed interval: [1-1.5*6 ; 7+1.5*6] = [-8 ; 16]

Thus, 42 is an outlier

https://en.wikipedia.org/wiki/File:Boxplot_vs_PDF.svg

Median Absolute Deviation (MAD)

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- MAD is the median deviation from the median of a sample, i.e.

$$\tilde{X} = median(X)$$
$$MAD = median(|X_i - \tilde{X}|)$$

- MAD can be used for outlier detection
  - All values that are k*MAD away from the median are considered to be outliers e.g., k=3
- Example:
  - X = 5, 1, 42, 0, 1, 3, 7
  - $median(X)$: 0,1,1,**3**,5,7,42 → $\tilde{X} = 3$
  - $|X_i - \tilde{X}|$ (Deviations): 3,2,2,0,2,4,39
  - MAD 0,2,2,**2**,3,4,39→ MAD = 2
  - Allowed interval: [3-3*2 ; 3+3*2] = [-3;9]

Carl Friedrich Gauss, 1777-1855

Thus, 42 is an outlier

Outliers vs. Extreme Values

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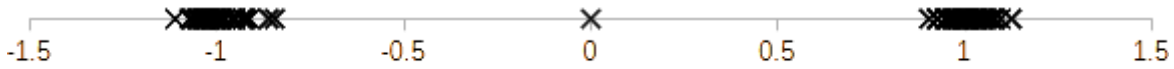
- So far, we have looked at extreme values only
  - But outliers can occur as non-extremes
  - In that case, methods like IQR fail
- IQR on the example below:
  - Q2 (Median) is 0
  - Q1 is -1, Q3 is 1

    → IQR = 2

    → everything outside [-4,+4] is an outlier

    → there are no outliers in this example



Distance-based Approaches

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- Nearest-neighbor based
  - Compute the distance between every pair of data points
  - There are various ways to define outliers:
    - Data points for which there are fewer than p neighboring points within a distance D
    - The top n data points whose distance to the k^{th} nearest neighbor is greatest
    - The top n data points whose average distance to the k nearest neighbors is greatest

Package PyOD

Density-based: LOF approach

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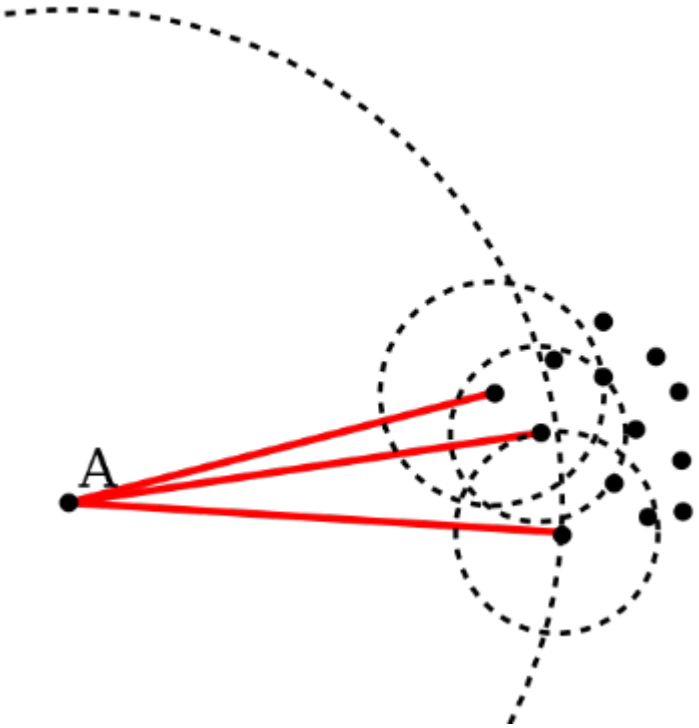
- For each point, compute the density of its local neighborhood
  - If that density is higher than the average density, the point is in a cluster
  - If that density is lower than the average density, the point is an outlier
- Compute local outlier factor (LOF) of a point A
  - Ratio of average density of A's neighbors to density of point A
- Outliers are points with large LOF value
  - Typical: larger than 1

LOF: Illustration

- Using 3 nearest neighbors
- We compute
  - the average density of A
  - the average density of A's neighbors
- If the density of A is lower than the neighbors' density
  - A might be an outlier



http://commons.wikimedia.org/wiki/File:LOF-idea.svg

DBSCAN for Outlier Detection

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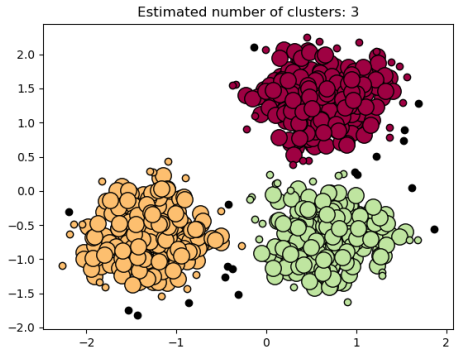
- DBSCAN directly identifies noise points
  - These are outliers not belonging to any cluster
    - In scikit-learn: label -1
  - Allows for performing outlier detection directly




```
# Apply DBSCAN with eps=0.5 and min_samples=5
dbscan = DBSCAN(eps=0.1, min_samples=5)
dbscan.fit(X)

# Identify the noise points
noise_mask = dbscan.labels_ == -1
print(noise_mask)

# Remove the noise points from the dataframe
X = X[~noise_mask]
```

Clustering-based Outlier Detection

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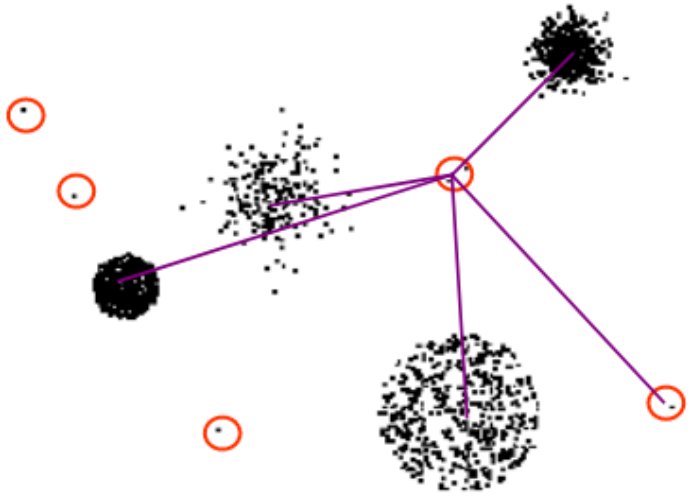
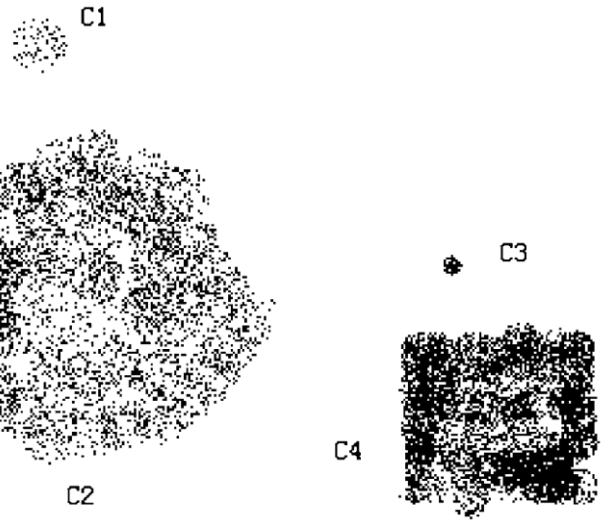
- Basic idea:
  - Cluster the data into groups of different density
  - Choose points in small cluster as candidate outliers
  - Compute the distance between candidate points and non-candidate clusters
  - If candidate points are far from all other non-candidate points, they are outliers



Clustering-based Local Outlier Factor

- Idea: anomalies are data points that are
  - In a very small cluster or
  - Far away from other clusters



- CBLOF is run on clustered data
- Assigns a score based on
  - The size of the cluster a data point is in
  - The distance of the data point to the next large cluster

Clustering-based Local Outlier Factor

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- General process:
  - First, run a clustering algorithm (of your choice)
  - Then, apply CBLOF

Package PyOD

- Result: data points with outlier score

```
from sklearn.cluster import KMeans
from pyod.models.cblof import CBLOF
# clustering
clust = KMeans()
# outlier detection
detector = CBLOF(n_clusters=8,clustering_estimator=clust)
detector.fit(X)
# removal
noise_mask =detector.predict(X) == 1
X = X[~noise_mask]
```

Isolation Forest

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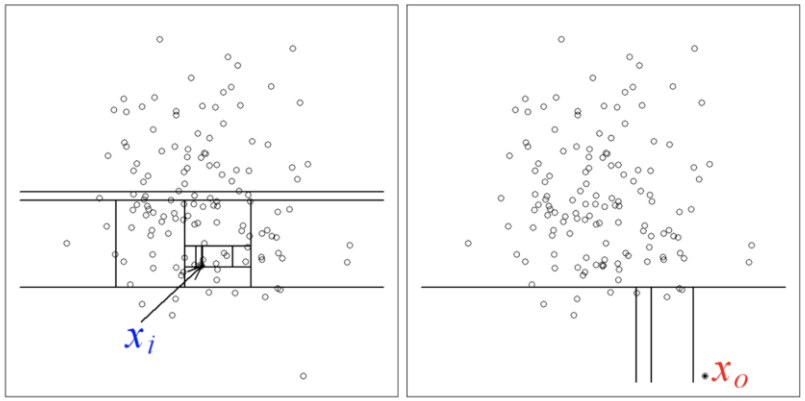
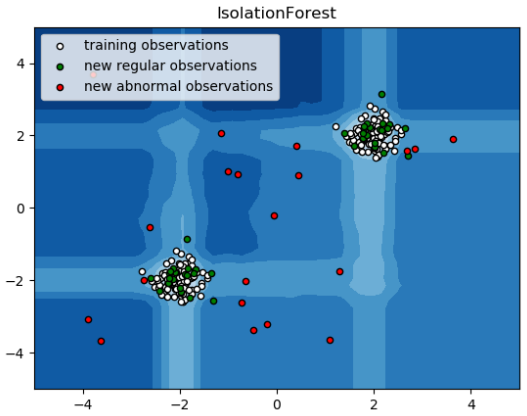
- Isolation tree:
  - A decision tree that has only leaves with one example each
- Isolation forests:
  - Train a set of random isolation trees
- Idea:
  - Path to outliers in a tree is shorter than path to normal points
  - Across a set of random trees, average path length is an outlier score

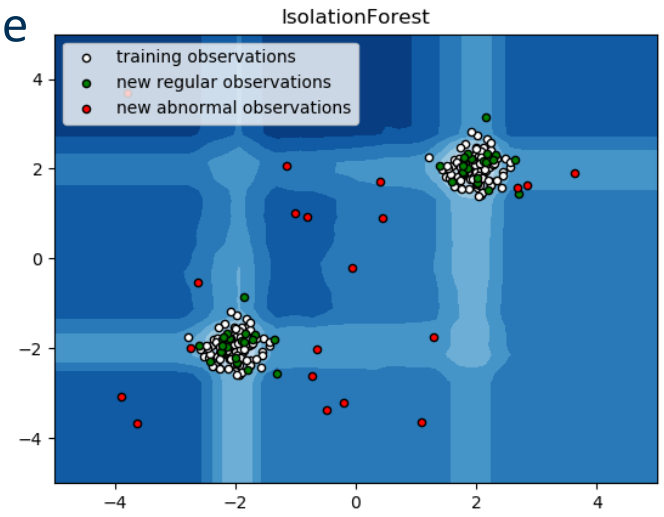




https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

- Training a single isolation tree
  - For each leaf node w/ more than one data point
    - Pick an attribute Att and a value V at random
    - Create inner node with test Att<V
      - Train isolation tree for each subtree
- Output
  - A tree with just one instance per (leaf) node
  - Usually, an upper limit on height is used



https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

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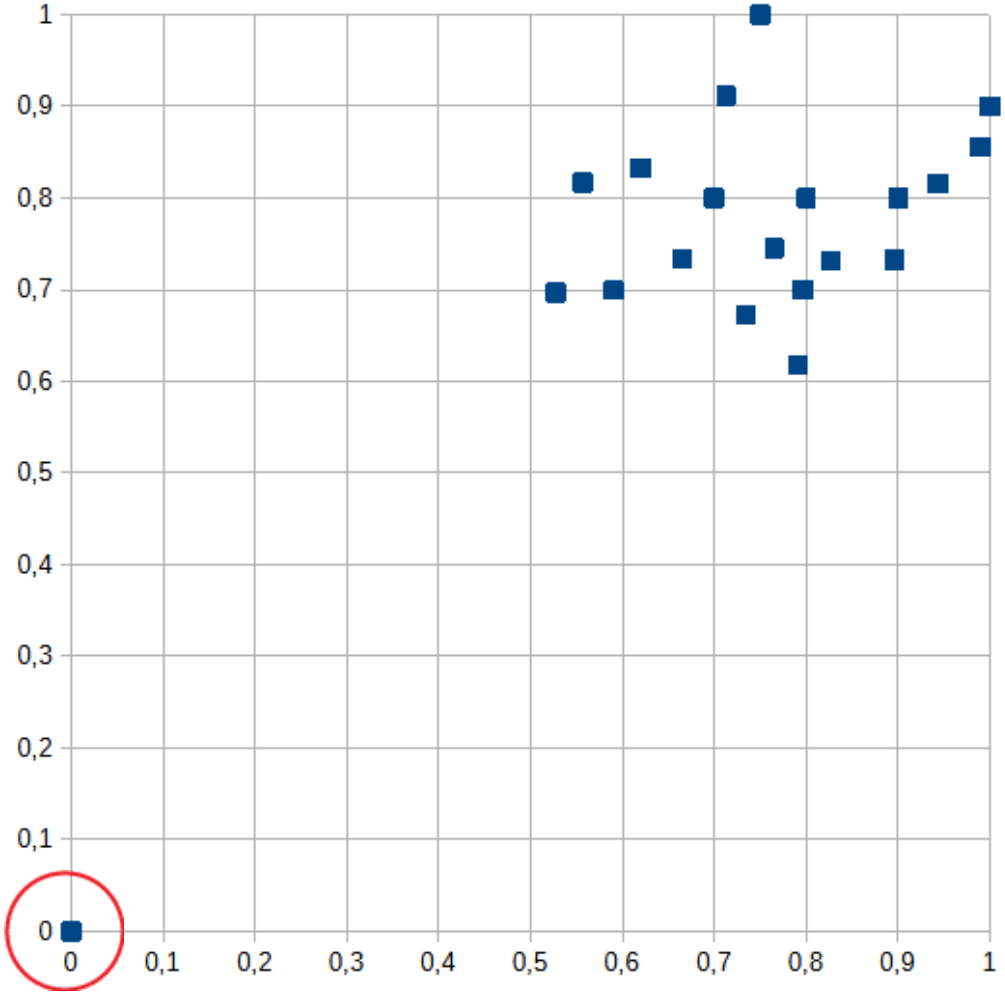
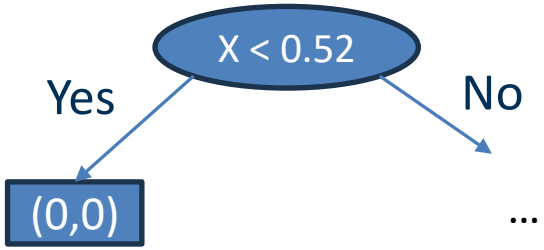
- Probability of (0,0) ending in a leaf at height 1

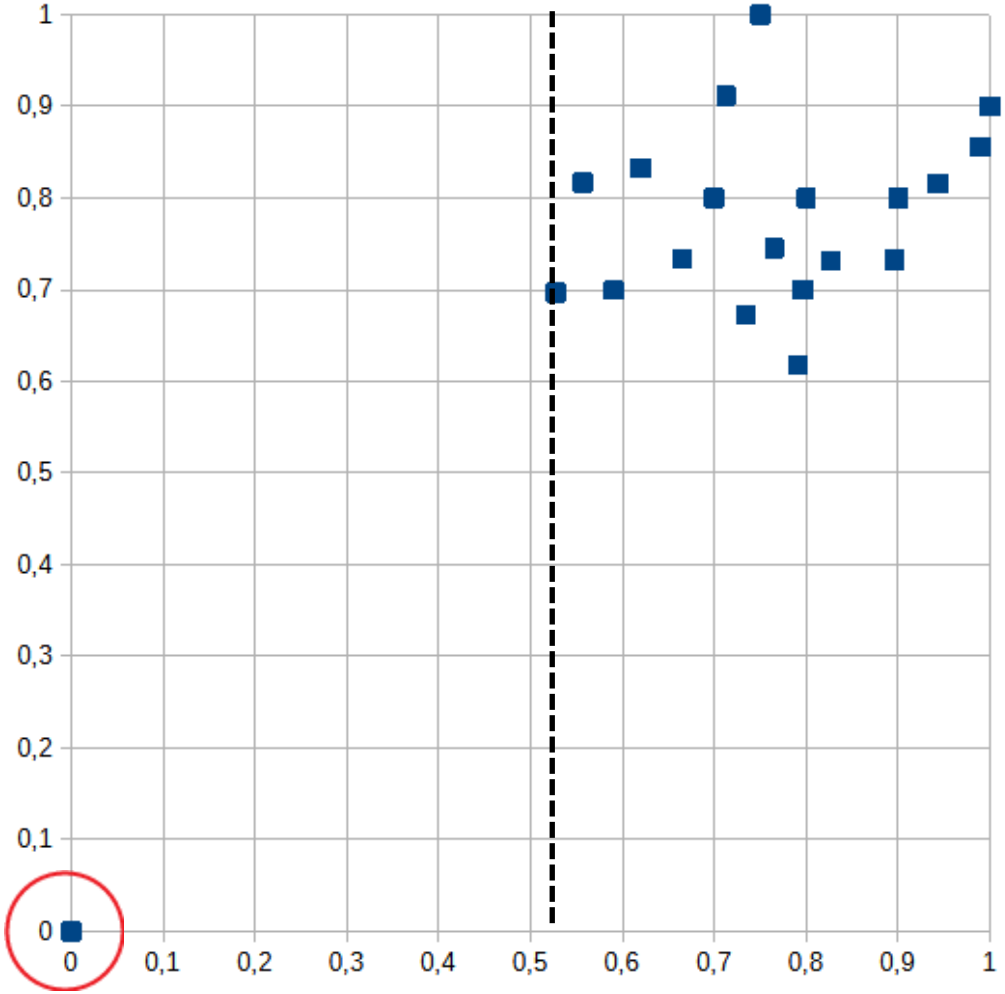


https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

- Probability of (0,0) ending in a leaf at height 1
  - pick Att X, pick X<0.52



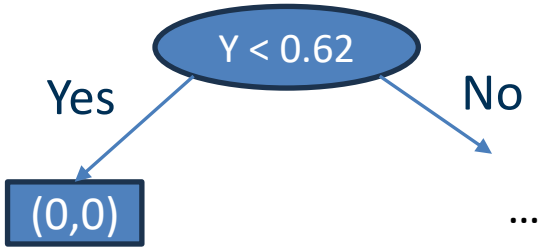


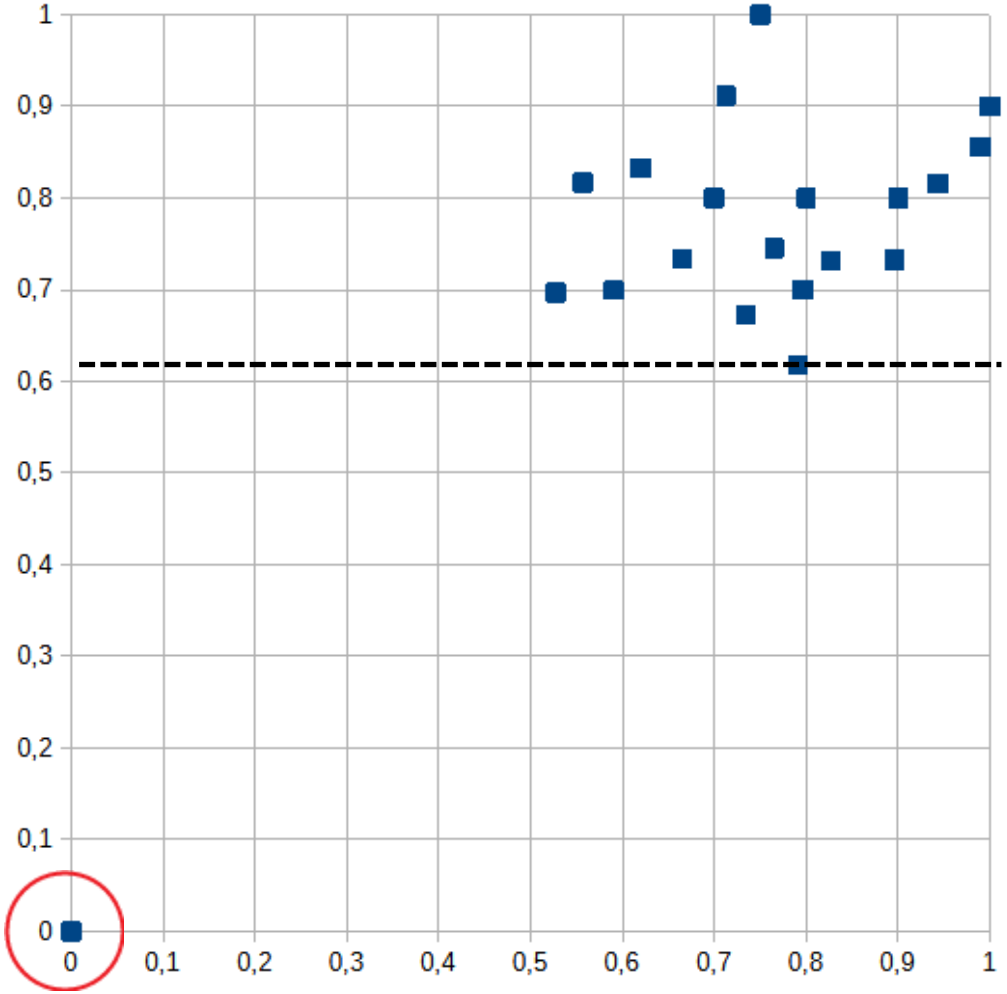
https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

- Probability of (0,0) ending in a leaf at height 1
  - pick Att X, pick X<0.52

    OR
  - pick Att Y, pick Y<0.62

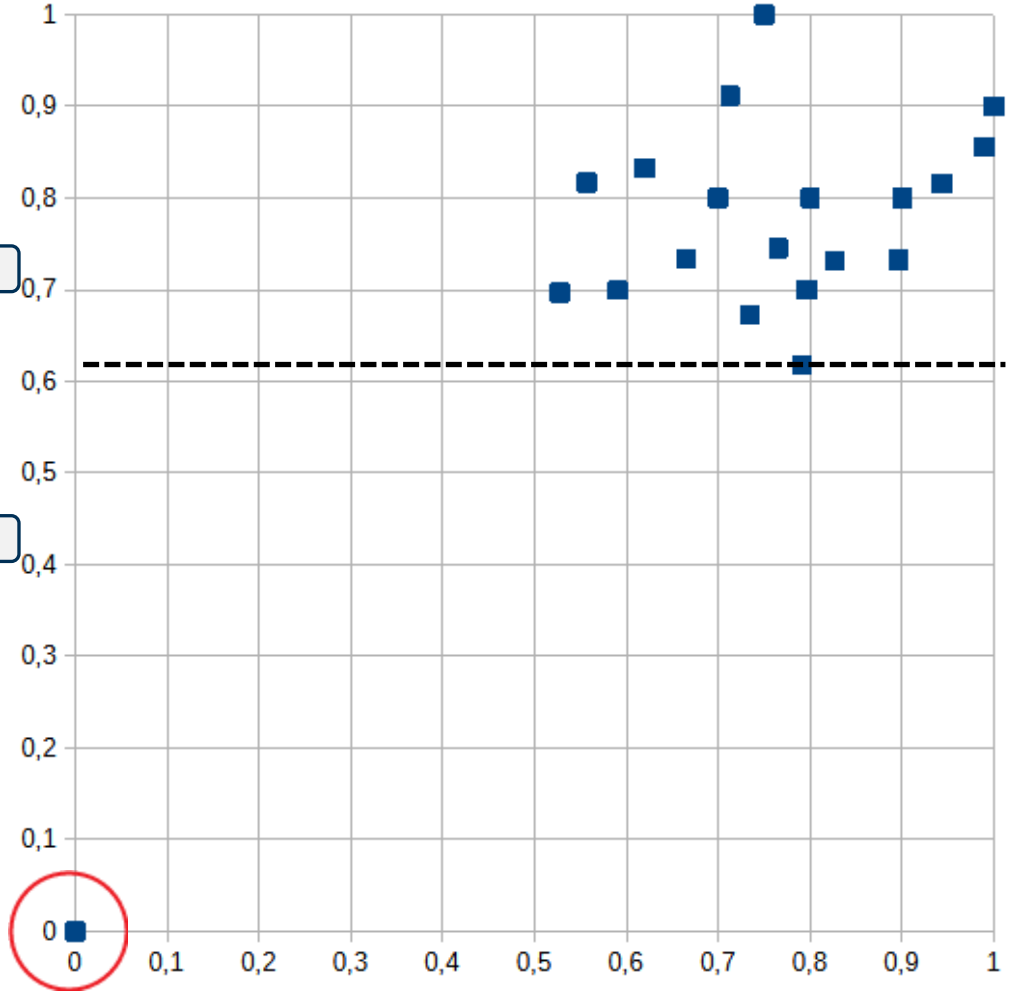




https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

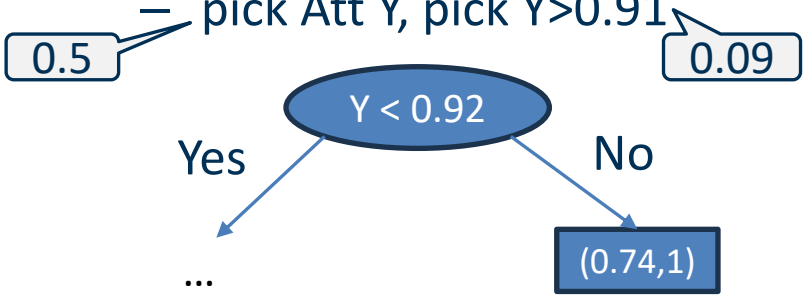
- Probability of (0,0) ending in a leaf at height 1
  - pick Att X, pick X<0.52 (0.5 × 0.52)
  - OR
  - pick Att Y, pick Y<0.62 (0.5 × 0.62)
- 0.5*0.52 + 0.5*0.62 → 0.57



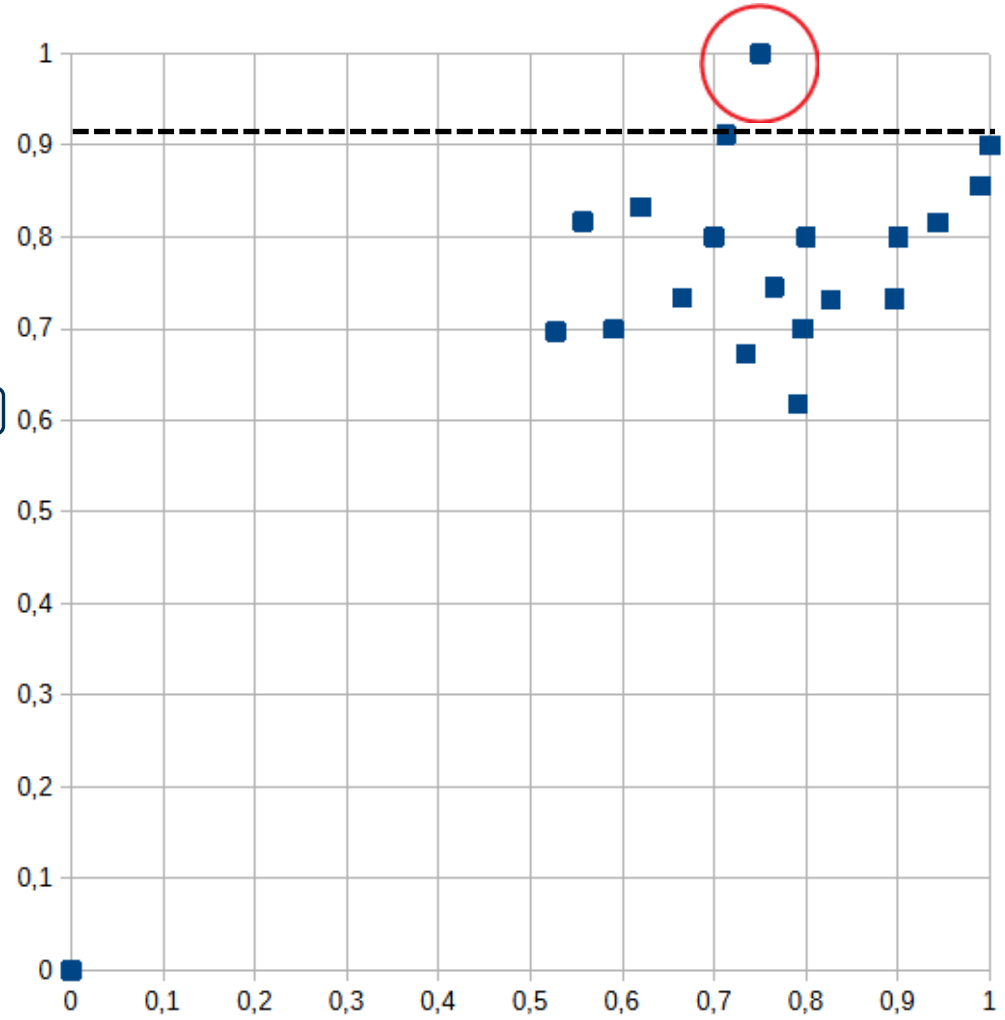
https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

- Probability of **(0.74,1)** ending in a leaf at height 1
  - pick Att Y, pick Y>0.91



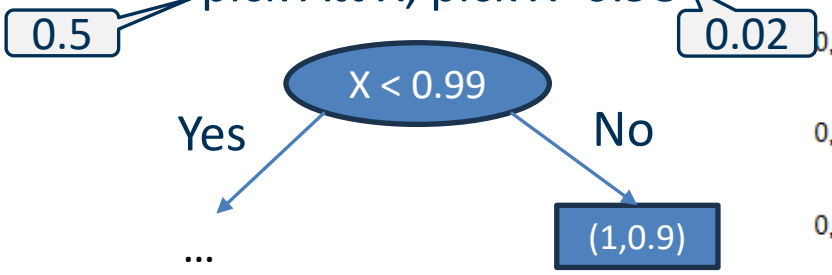
- 0.5 * 0.09
  → 0.045



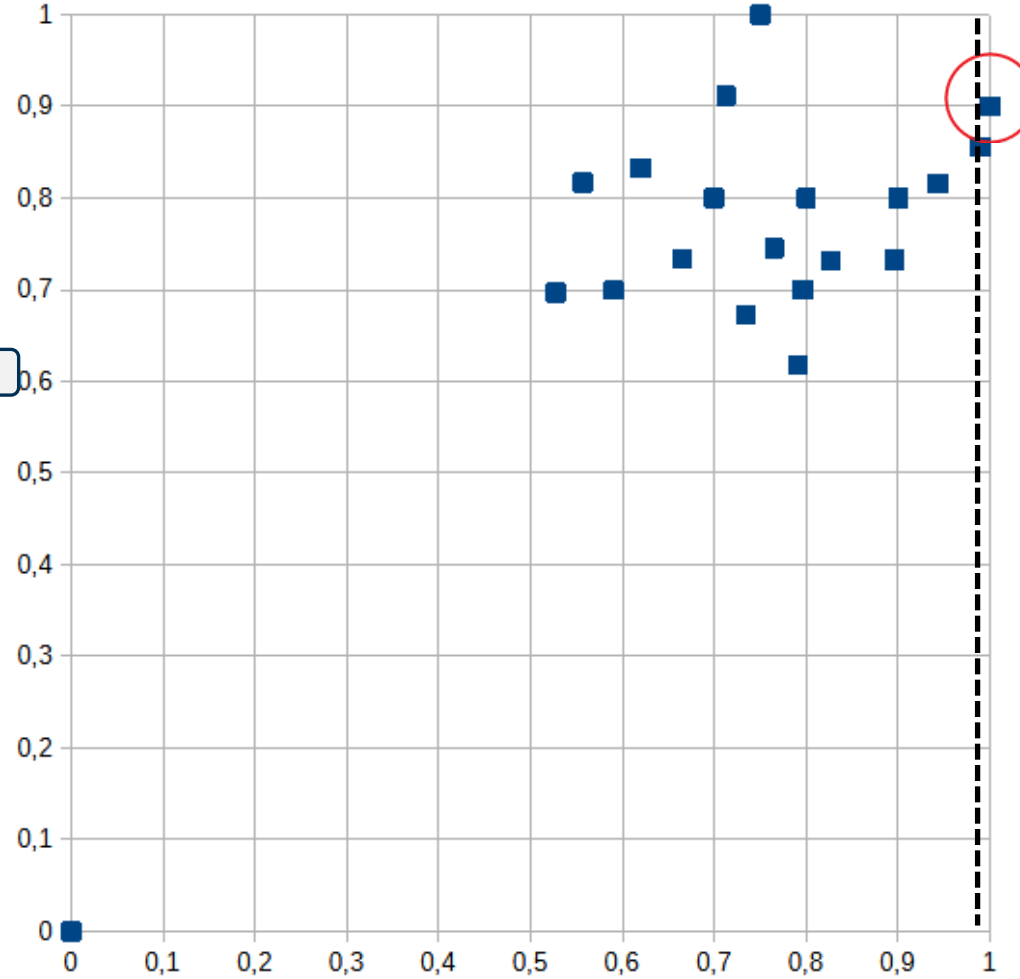
https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

- Probability of **(1,0.9)** ending in a leaf at height 1
  - pick Att X, pick X>0.98



- 0.5 * 0.02
  → 0.01



https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

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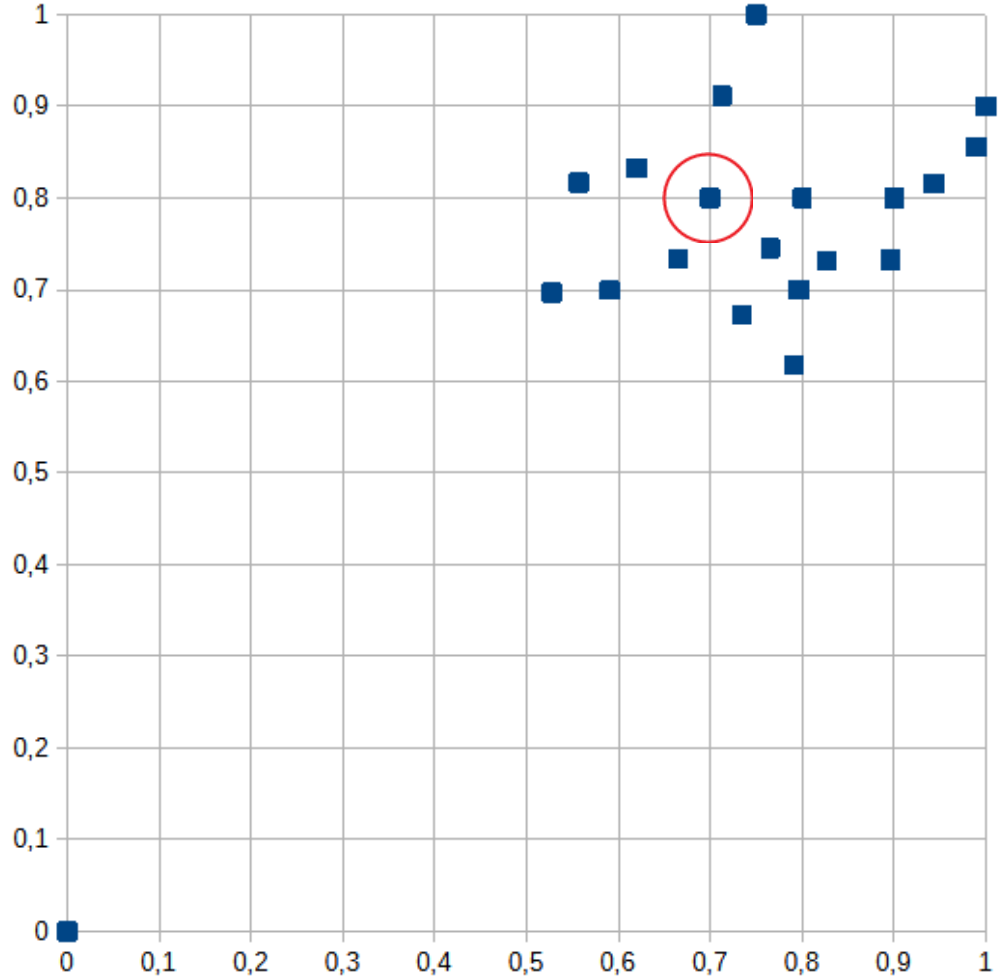
- Probability of any other data point ending in a leaf at height 1
  - This is not possible!
  - At least two tests are necessary



https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Isolation Forest

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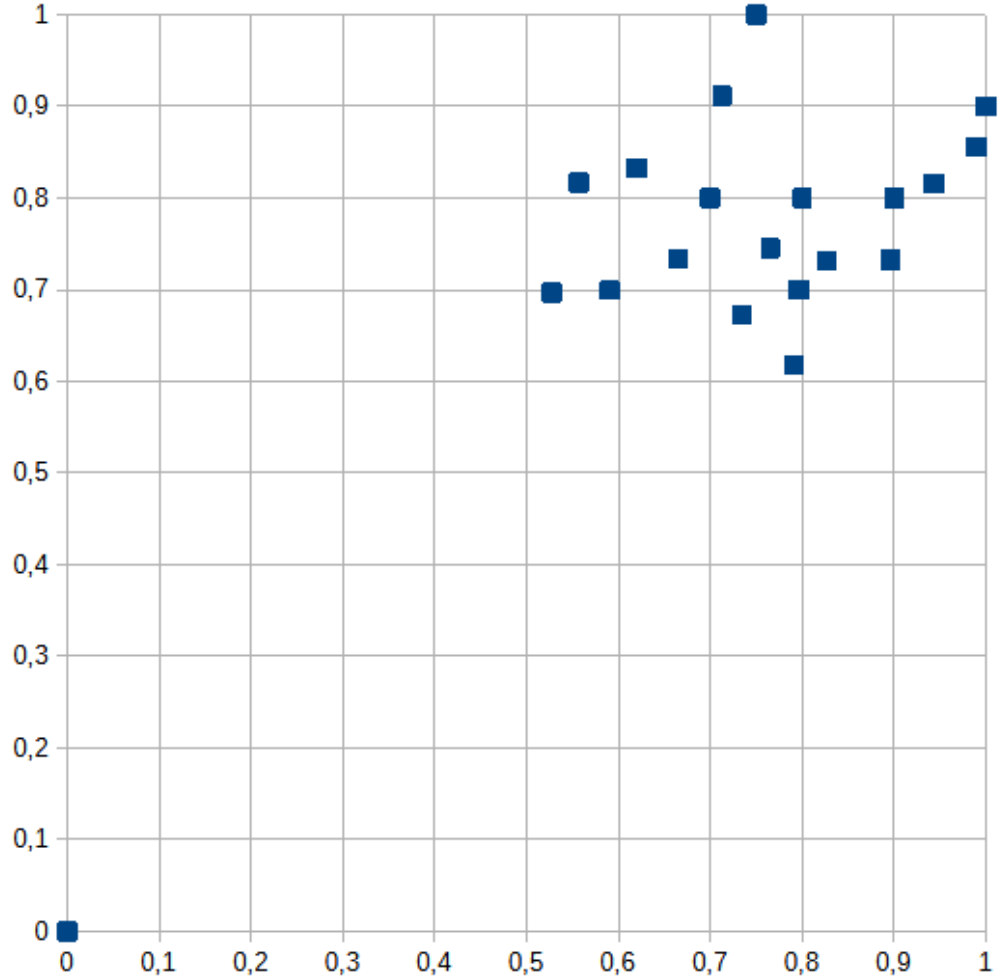
- Observations
  - Data points in dense areas need more tests
    - i.e., they end up deeper in the trees
  - Data points far away from the rest have a higher probability to be isolated earlier
    - i.e., they end up *higher* in the trees



https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Questions?

Online Lectures

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- This week additional material is about hierarchical clustering
- Online lectures are exercise and exam relevant

Week	Monday(Offline Lecture)	Online Lecture (see Ilias Course)	Thursday (Exercise)
01.09.2025	no lecture		Introduction to Python (13:45–15:15)
08.09.2025	Introduction to Data Mining (PDF, 3 MB)		Intro
15.09.2025	Preprocessing (PDF, 2 MB)		Preprocessing
22.09.2025	Classification 1 (PDF, 2 MB) + Intro to Student Project	Nearest Centroids	Classification 1
29.09.2025	Classification 2	Comparing Classifiers	Classification 2
06.10.2025	Regression	Ensembles	Regression
13.10.2025	Clustering and Anomalies	Hierarchical Clustering	Clustering
20.10.2025	Feedback on project outlines	Time Series	Time Series
27.10.2025	Association Analysis and Subgroup Discovery	Multi Modal Data	Association Analysis
03.11.2025	Project feedback session		Project Work
10.11.2025	Project feedback session		Project Work
17.11.2025	Project feedback session		Project Work
24.11.2025	Project feedback session		Project Work
01.12.2025	Q&A		**Project Presentations**

Literature for this Slideset

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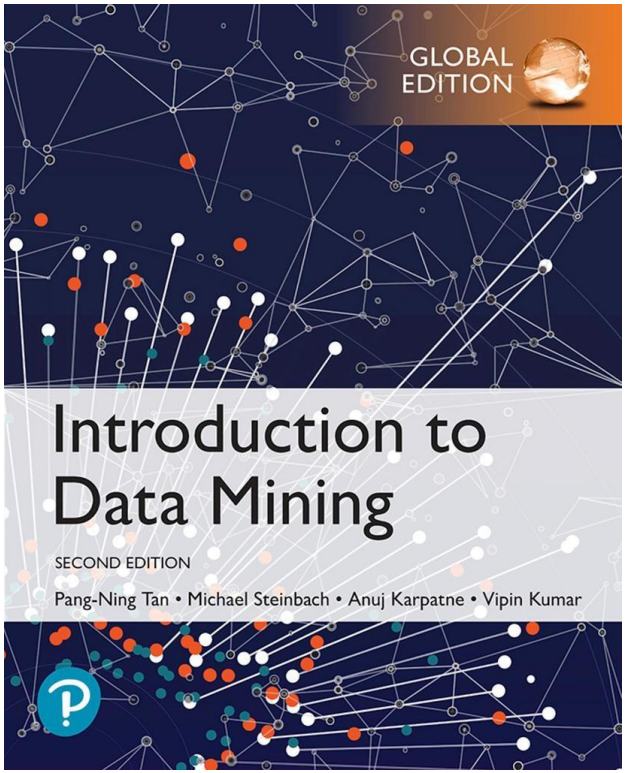
- Pang-Ning Tan, Michael Steinbach, Karpatne,Vipin Kumar: Introduction to Data Mining. 2nd Edition. Pearson.



- Chapter 5: Cluster Analysis
  - Chapter 5.2: K-Means
  - Chapter 5.3: Agglomerative Hierarchical Clustering
  - Chapter 5.4: DBSCAN
- Chapter 2.4: Measures of Similarity and Dissimilarity