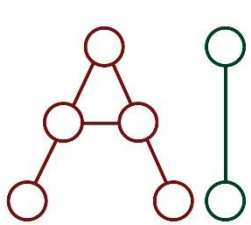


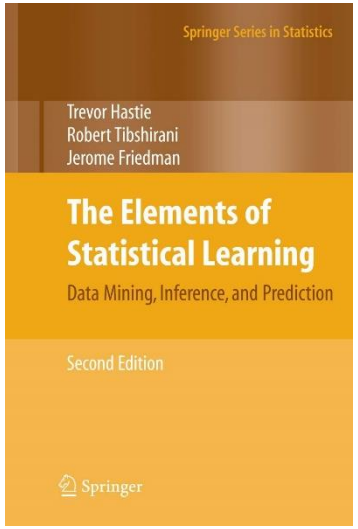
Clustering, Density Estimation, and Anomaly Detection

Assoc. Prof. Karl Ezra Pilario, Ph.D.
Process Systems Engineering Laboratory
Department of Chemical Engineering
University of the Philippines Diliman

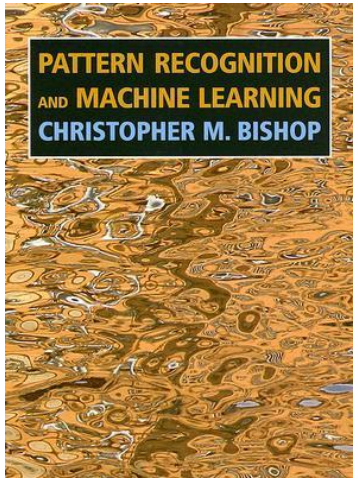
Outline

- Clustering
  - K-means Clustering
  - Hierarchical Clustering
  - Density-based Clustering
  - Gaussian Mixture Model
- Density Estimation
  - Kernel Density Estimation (KDE)
- Anomaly Detection
  - Application of KDE
  - One-class SVM
  - Local Outlier Factor
  - Isolation Forest

Hastie *et al.* (2008)
The Elements of Statistical Learning.
2nd Ed. Springer.

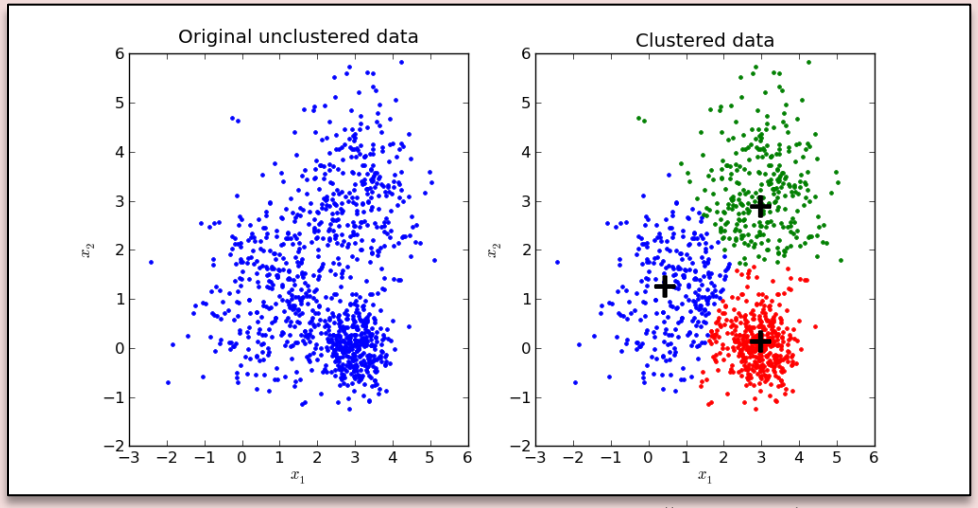


Bishop (2006)
Pattern Recognition and Machine Learning. Springer.



What is Clustering?

The problem of identifying groups or clusters of data points in a multi-dimensional space.

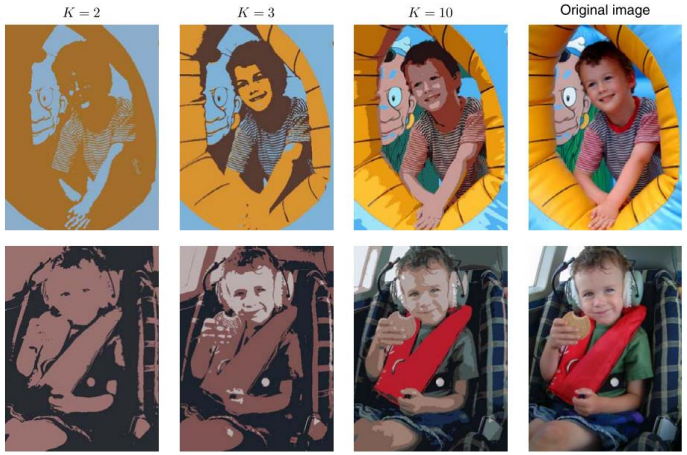


https://images.app.goo.gl/HjnuqnNrk74DRddv9

- It is NOT the same as the *classification* problem.
  - In clustering, class labels are unknown. Groupings are established solely from the locations of points.
- Interpretation: Samples within the same cluster are more *similar* to each other than those assigned to other clusters.
- The central idea is the notion of "similarity".

Some applications of Clustering:

- Customer segmentation
  - Given the attributes of your customers, can they be grouped so we can target our ads to each group of common people?
- Recommendation systems
  - It has been reported that Netflix identified 2,000 clusters of subscribers of similar taste by tracking their viewing habits. For example, *Black Mirror* is favored by Clusters 290 and 56.
  - **Source:** https://www.vulture.com/2018/06/how-netflix-swallowed-tv-industry.html
- Image compression
  - An image can be re-colored by clustering "similar" colors as one.
  - From left to right, there are 2, 3, and 10, clusters chosen. The last column is the original image.

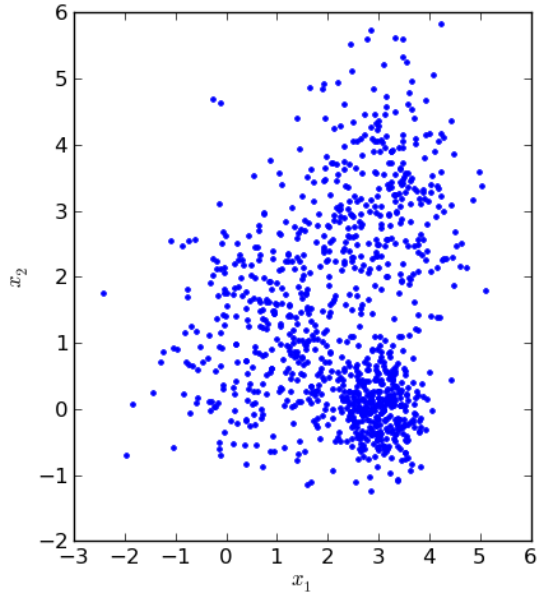


Bishop (2006). Pattern Recognition and Machine Learning. Springer.

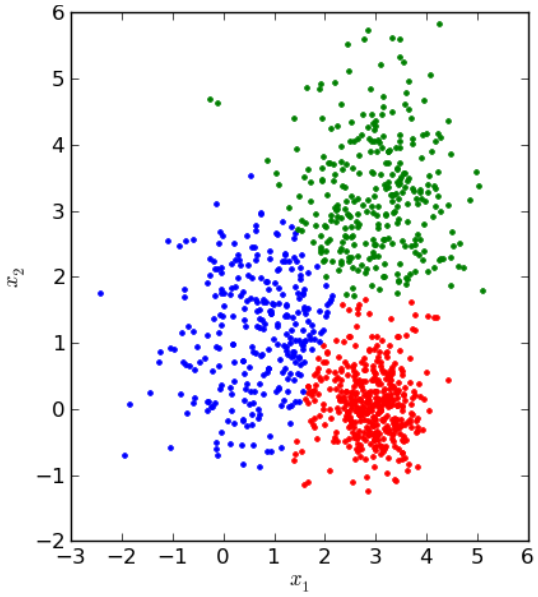
Side Note: Clustering ≠ Classification

- This is clustering:
  - Start with an unlabelled data set.
  - After clustering, points are now assigned to clusters.
  - There is no external annotator (e.g. human) defining or enforcing any labels.

Before clustering

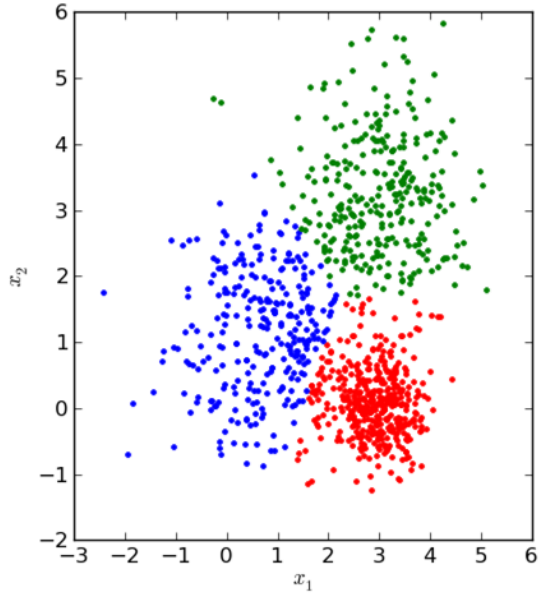


After clustering

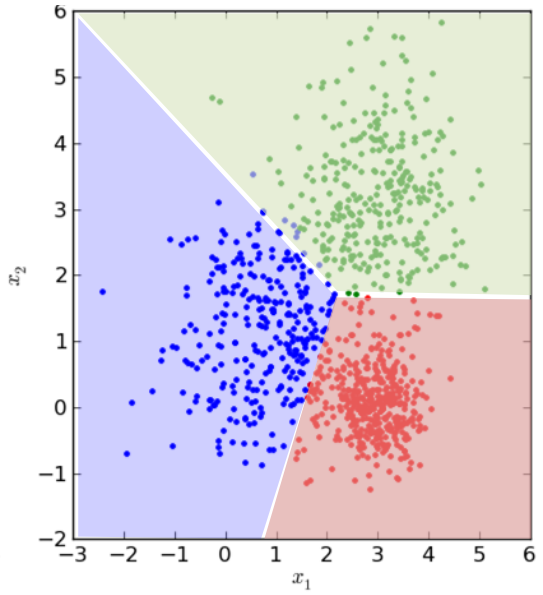


- This is classification:
  - Start with a labelled data set.
  - Labels are defined / enforced by an annotator (e.g. human).
  - After classification, the model tries to predict how the annotator labelled the data.

Before classification



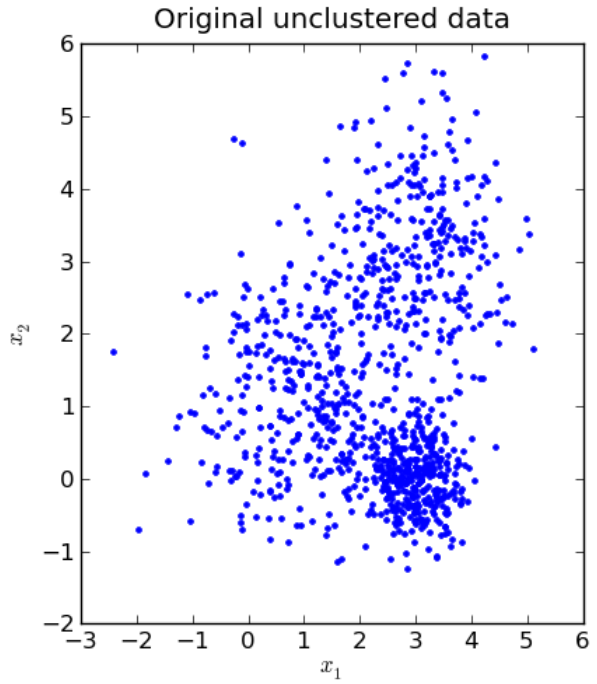
After classification

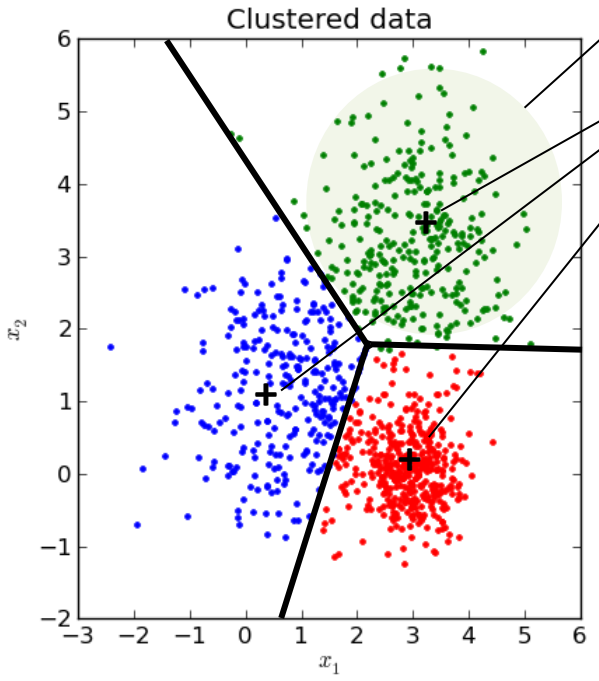


https://images.app.goo.gl/HjnuqnNrk74DRddv9

Side Note: Centroids and Voronoi Diagrams

- Typically, the result of clustering is a set of cluster centroids.
- If clusters can be visualized in 2-D, we can use Voronoi Diagrams to delineate data points that belong to different clusters.





Cell

A partitioned region of space.

Centroids

Center (mean) of each cluster cell.

Voronoi Diagram

- A partitioning of space into cells, based on a given position of centroids.
- Each separating line is the locus of points that are equidistant from the 2 nearest centroids.
- **Interpretation:**

  All points within a cell are closer to their assigned centroid than any other centroid.

https://images.app.goo.gl/HjnuqnNrk74DRddv9

K-means Clustering

Let's begin with some preliminaries.

Let: $\boldsymbol{x}_i \in \Re^M,\ i = 1, 2, \ldots, N$ be a data set of N samples

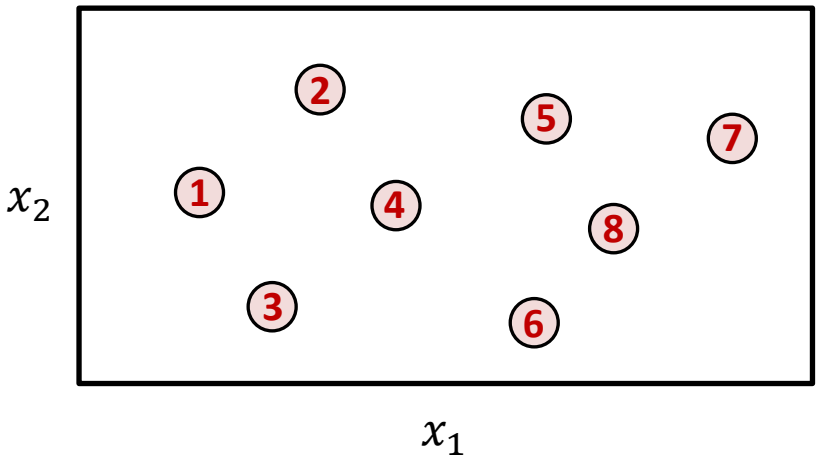
$\boldsymbol{\mu}_j \in \Re^M,\ j = 1, 2, \ldots, K$ be the locations of K centroids

$r_{ij} \in \{0, 1\},\ i = 1, 2, \ldots, N$ be an indicator

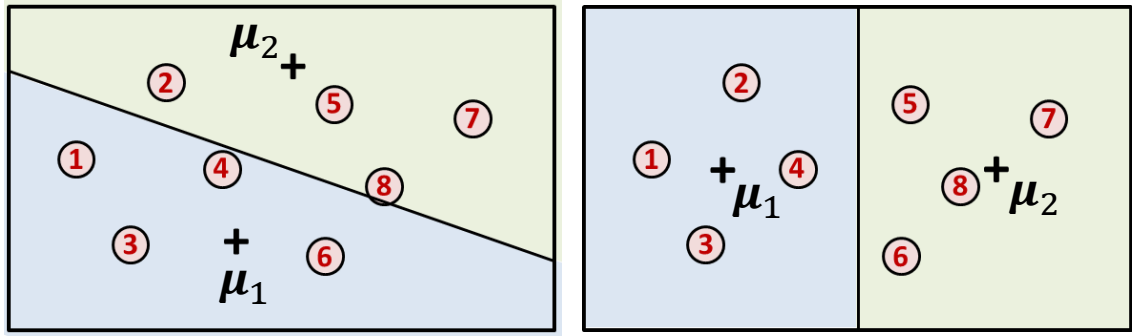
$j = 1, 2, \ldots, K$

$$\begin{cases} r_{ij} = 1 & \text{if sample } i \text{ is closest to centroid } j \\ r_{ij} = 0 & \text{otherwise} \end{cases}$$

Consider the 2-D data set to be clustered below:



An illustration of how the indicator r_{ij} works: $(N = 8, K = 2)$



r_{ij}

	Cluster $j = 1$	Cluster $j = 2$
i = 1	1	0
2	0	1
3	1	0
4	1	0
5	0	1
6	1	0
7	0	1
8	0	1

r_{ij}

	Cluster $j = 1$	Cluster $j = 2$
i = 1	1	0
2	1	0
3	1	0
4	1	0
5	0	1
6	0	1
7	0	1
8	0	1

K-means Clustering

Let: $\boldsymbol{x}_i \in \Re^M,\ i = 1, 2, \dots, N$ be a data set of N samples

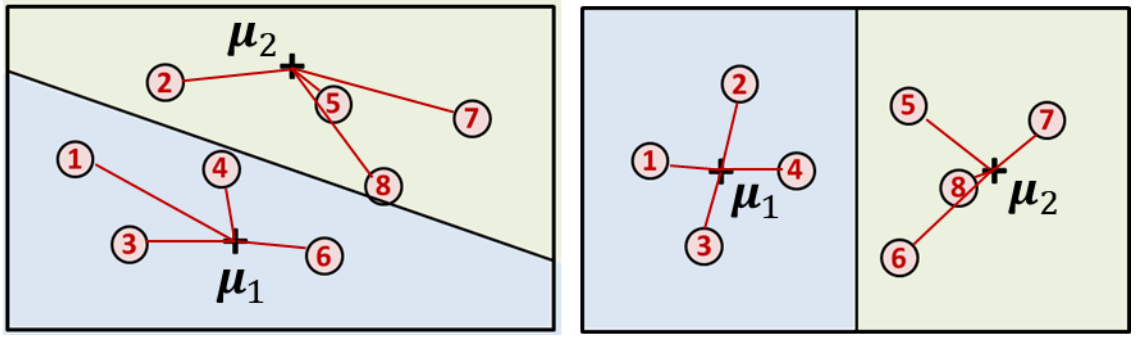
$\boldsymbol{\mu}_j \in \Re^M,\ j = 1, 2, \dots, K$ be the locations of K centroids

$r_{ij} \in \{0, 1\},\ i = 1, 2, \dots, N$, $j = 1, 2, \dots, K$ be an indicator:

$$\begin{cases} r_{ij} = 1 & \text{if sample } i \text{ is closest to centroid } j \\ r_{ij} = 0 & \text{otherwise} \end{cases}$$

In K-means clustering, the goal is to find K centroids, $\boldsymbol{\mu}_j$, that minimize the ***inertia*** or ***distortion measure***, J:

$$J = \sum_{i}^{N} \sum_{j}^{K} r_{ij} \left\| \boldsymbol{x}_i - \boldsymbol{\mu}_j \right\|^2$$



Algorithm:

Given: Data Set, $\boldsymbol{x}_i \in \Re^M,\ i = 1, 2, \dots, N$

Initialization: Set a tolerance, *tol* (e.g. 10^{-3})
Set an assumed number of clusters, *K*
Set an initial guess of *K centroids*, $\boldsymbol{\mu}_j$

1: Pre-allocate an old solution: $\boldsymbol{\mu}_j^{\text{old}} = \mathbf{0} \in \Re^{K \times M}$.

2: WHILE $\left\| \boldsymbol{\mu}_j - \boldsymbol{\mu}_j^{\text{old}} \right\| > \text{tol}$

Expectation

3: Save the old centroids: $\boldsymbol{\mu}_j^{\text{old}} \coloneqq \boldsymbol{\mu}_j$.

E-step **4**: Compute r_{ij}: Assign each $\boldsymbol{x}_i$ to the closest centroid.

M-step **5**: Compute the new centroids, $\boldsymbol{\mu}_j$:

Maximization

$$\boldsymbol{\mu}_j = \frac{\sum_i r_{ij} \boldsymbol{x}_i}{\sum_i r_{ij}}$$

Compute the new $\boldsymbol{\mu}_j$ as the average position of all data points $\boldsymbol{x}_i$ assigned to cluster j.

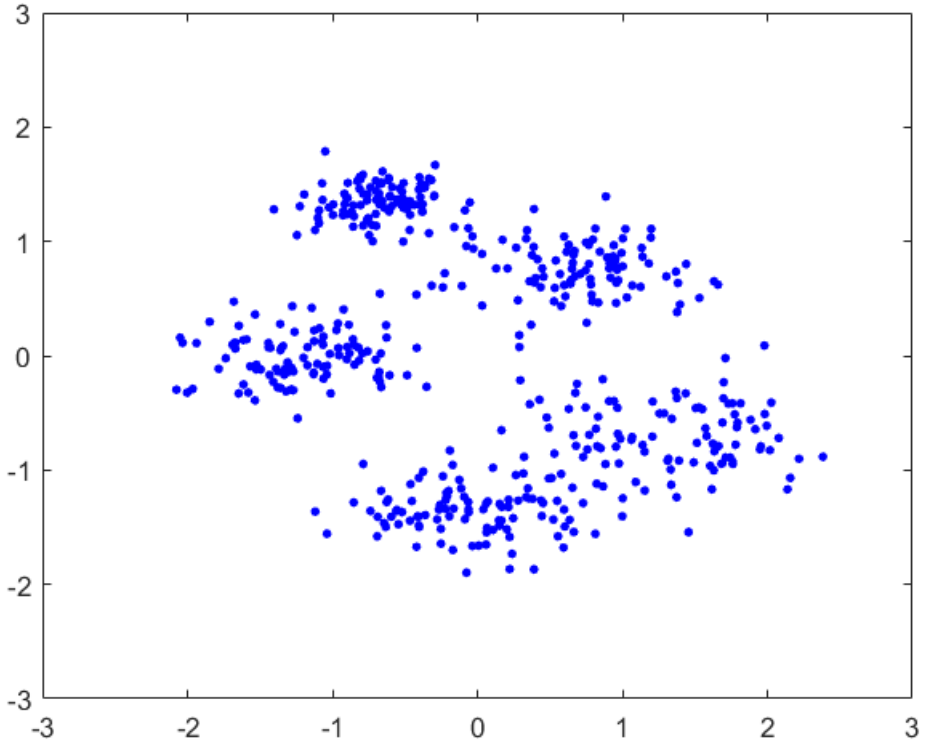
6: END WHILE

7: Report the final centroids, $\boldsymbol{\mu}_j$.

K-means Clustering

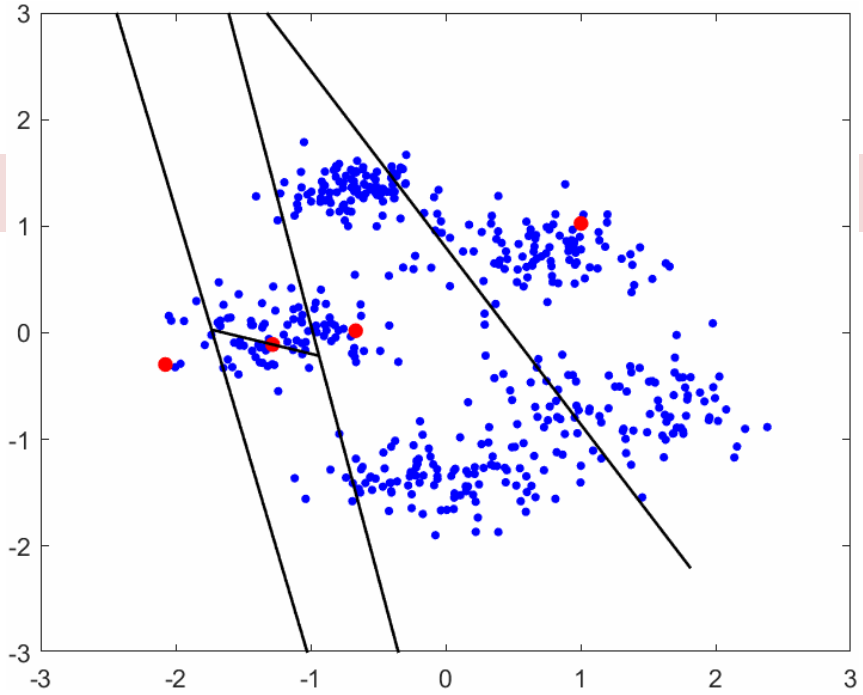
Example 1:

Find $K = 5$ clusters of samples, and their centroids, from the following data set:

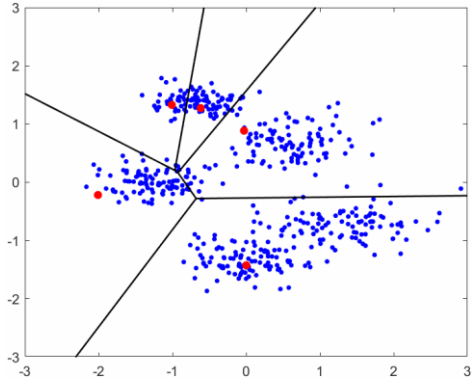


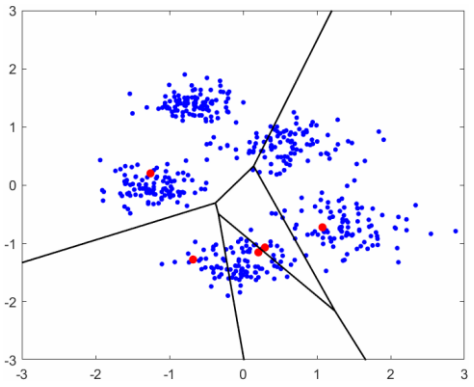
Answer:

```
( 1.3688, -0.7135)
(-0.6328,  1.2988)
(-0.0367, -1.3342)
( 0.7596,  0.7367)
(-1.2234, -0.0198)
```



However, note that different initializations may lead to local minima of J.
Solution: Try to restart K-means many times.





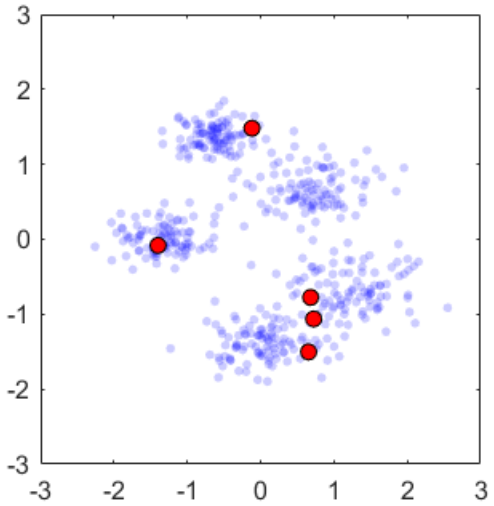
K-means Clustering

There are different ways to initialize the centroids in K-means clustering:

Forgy Initialization

Select K existing data points at random, then use them as initial guess of centroids.

sklearn: cluster.Kmeans(…init=**'random'**)

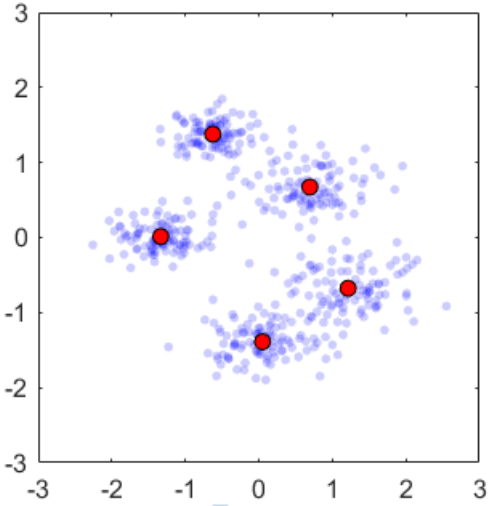


K-means++

Arthur and Vassilvitskii (2006).

Random data points are selected one at a time and as far apart as possible, until you have K number of them.

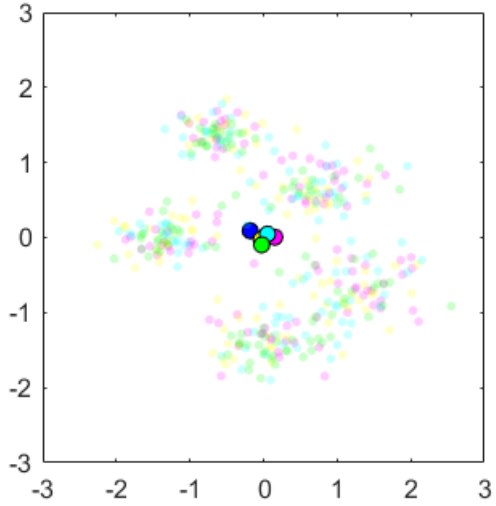
sklearn: cluster.Kmeans(…init=**'k-means++'**)



Random Partition

Assign each data point to a random cluster, then compute the means of each cluster as the initial guess.

*Not recommended



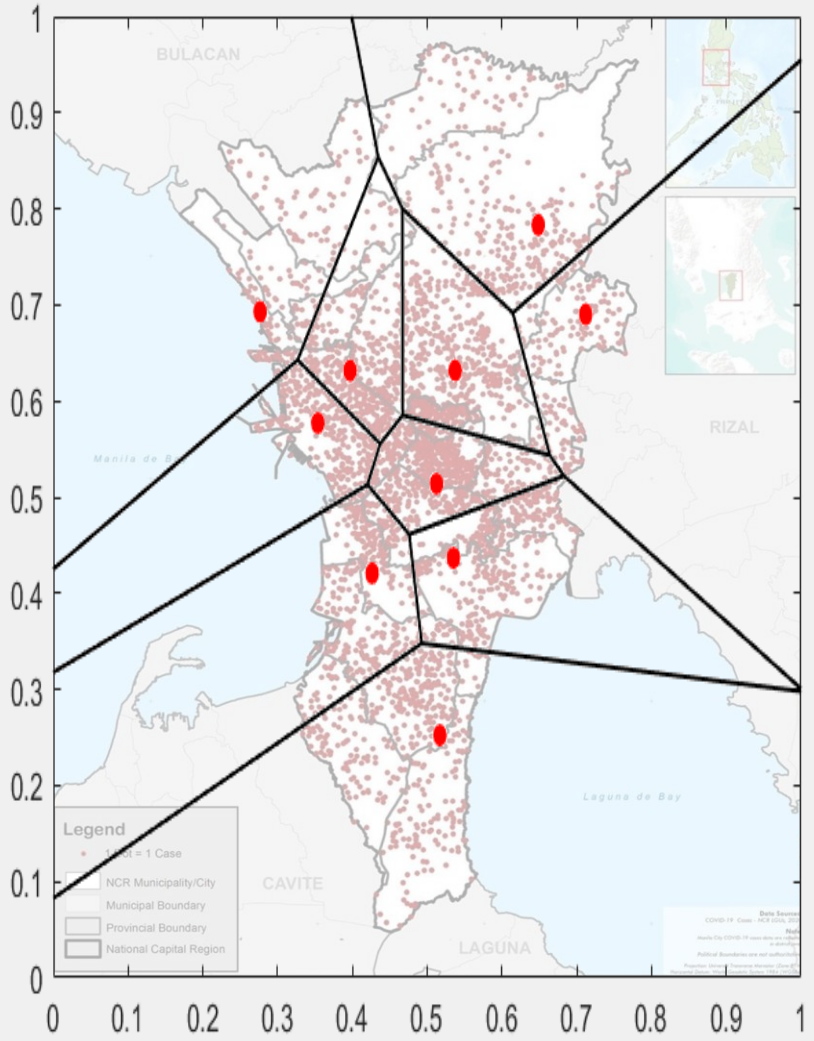
K-means Clustering

Example 2: Covid-19 Cases

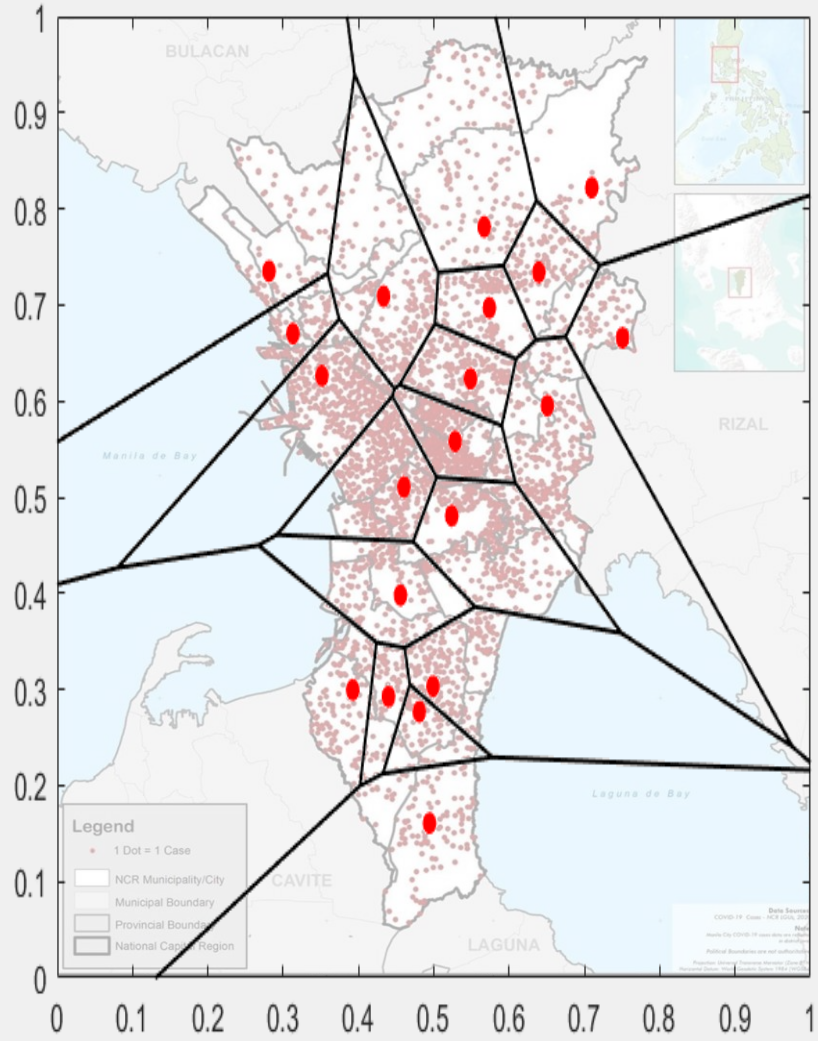
In this application, K-means clustering can be used to find *K* centroids where testing centers can be located.

Image of Covid cases from:
https://www.esquiremag.ph/politics/news/covid-19-case-distribution-map-metro-manila-a00293-20200510

Finding **10 clusters** of NCR Covid-19 cases:



Finding **20 clusters** of NCR Covid-19 cases:



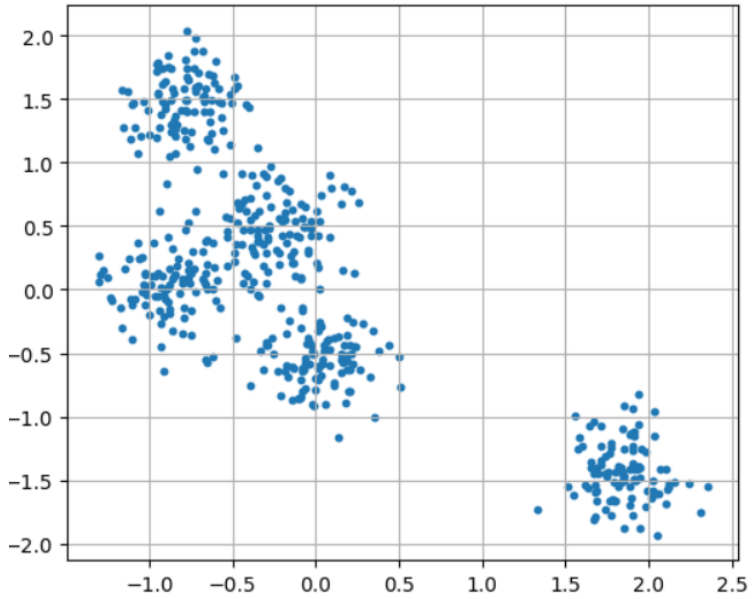
K-means Clustering

How to determine K in K-means?

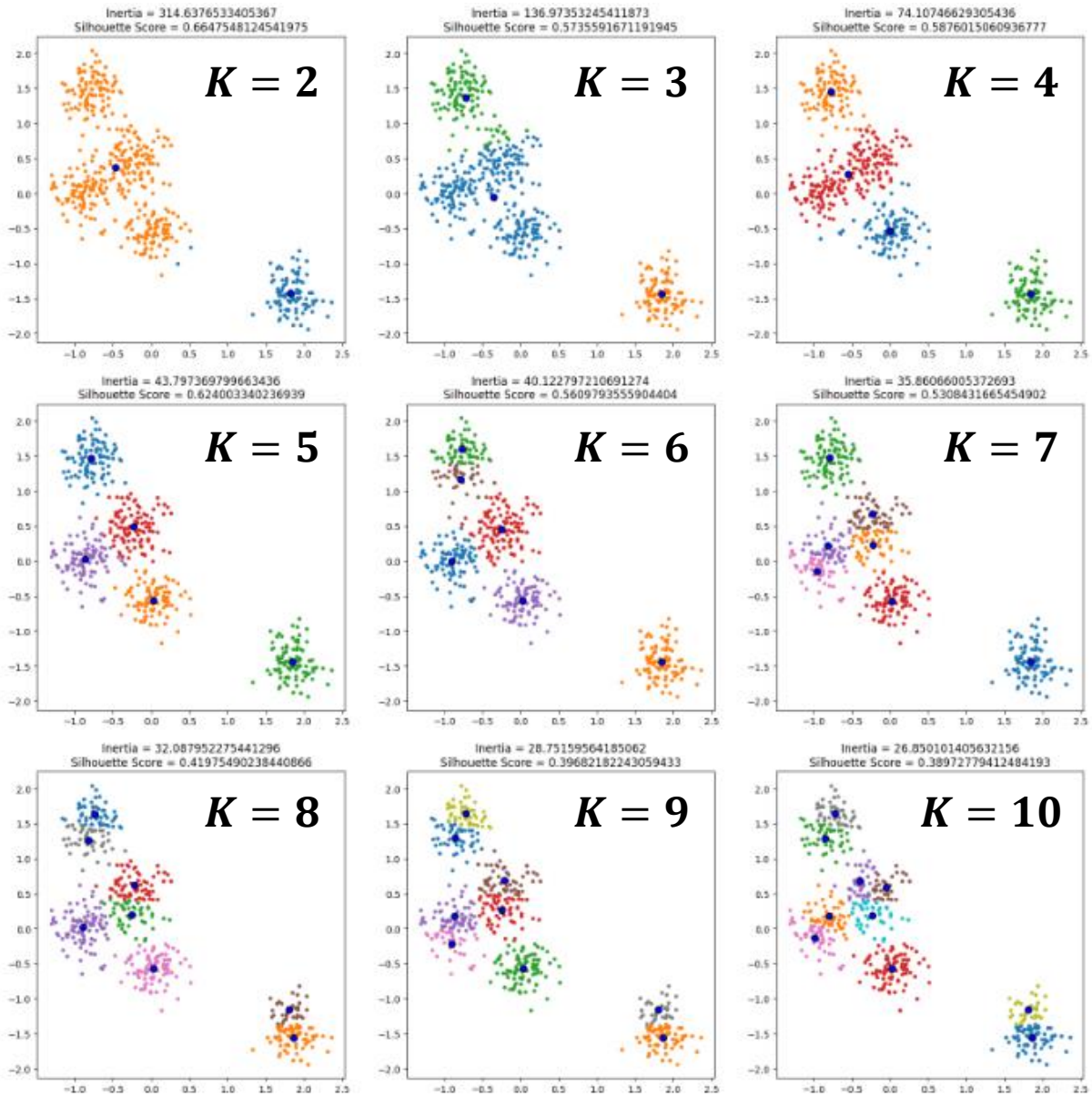
- K-means cannot automatically learn the best number of clusters, K, from the data. We have to specify it ourselves prior to running it.

- Sometimes, the number of distinct clusters, K, is obvious (especially if data set is 2D). But this is not always the case.

How many clusters are in this data set?

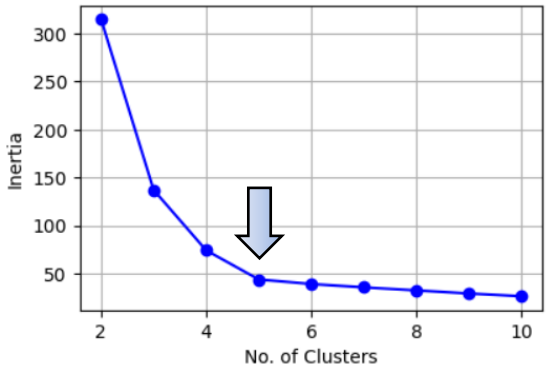


Results for various choices of K:



K-means Clustering

Elbow Method



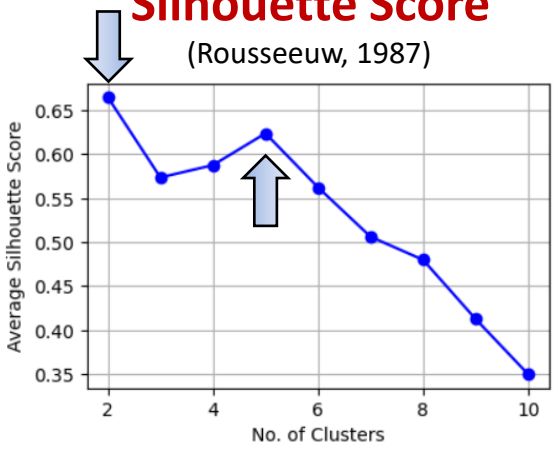
- Calculate the inertia for each K:

$$J = \sum_{i}^{N} \sum_{j}^{K} r_{ij} \left\| \boldsymbol{x}_i - \boldsymbol{\mu}_j \right\|^2$$

- Find the elbow point in the inertia plot.

Silhouette Score

(Rousseeuw, 1987)



- For each K, calculate the average silhouette score:

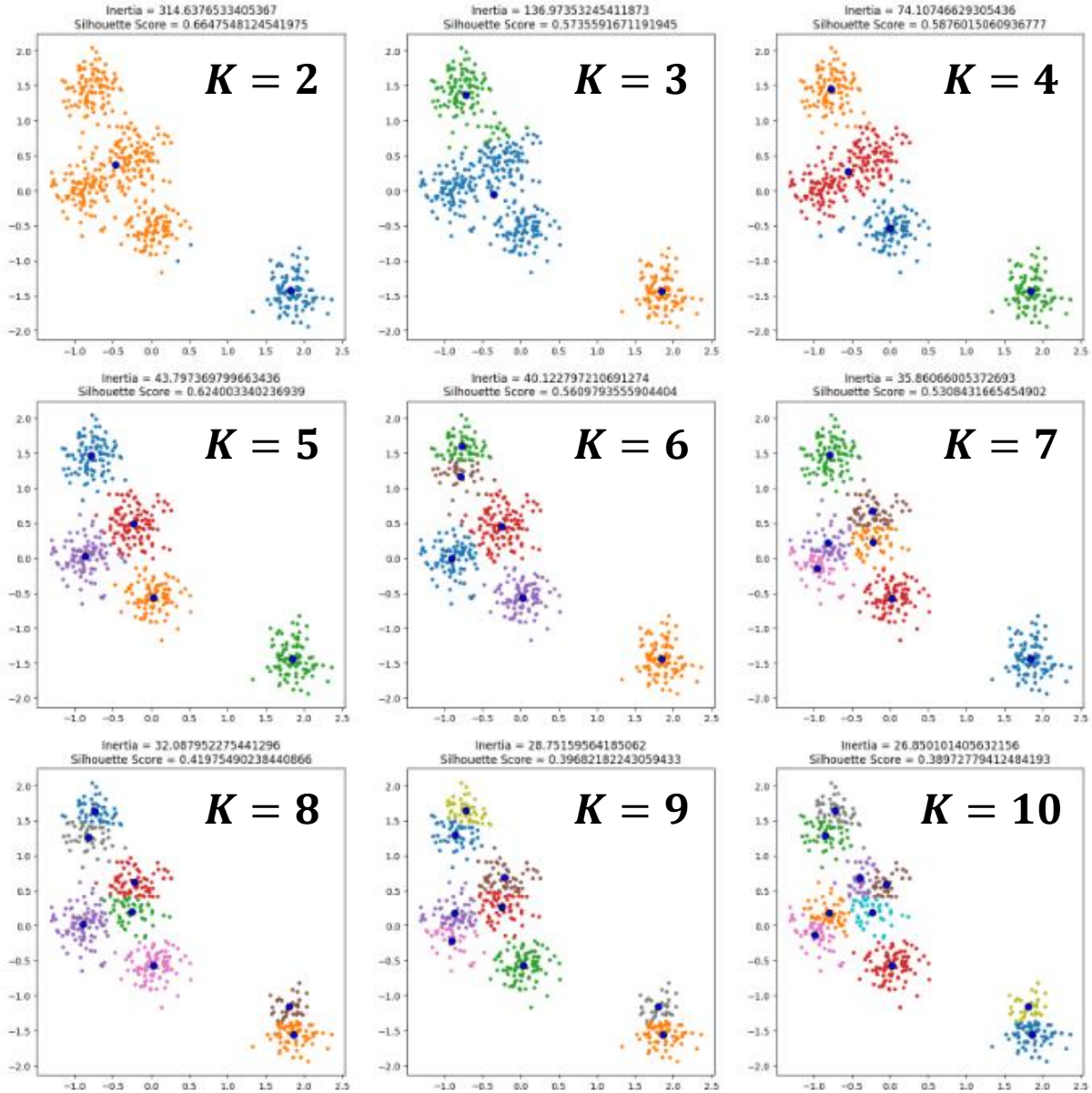
$$s(i) = \begin{cases} \dfrac{b(i) - a(i)}{\max(a(i), b(i))}, & \text{if } |C_i| > 1 \\ 0, & \text{if } |C_i| = 1 \end{cases}$$

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i} d(i,j)$$

$$b(i) = \min_{k \neq i} \frac{1}{|C_j|} \sum_{j \in C_k} d(i,j)$$

- Find the K with the maximum average silhouette score.

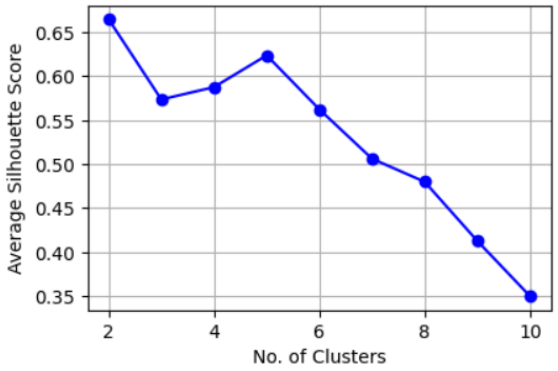
Results for various choices of K:



K-means Clustering

Silhouette Score

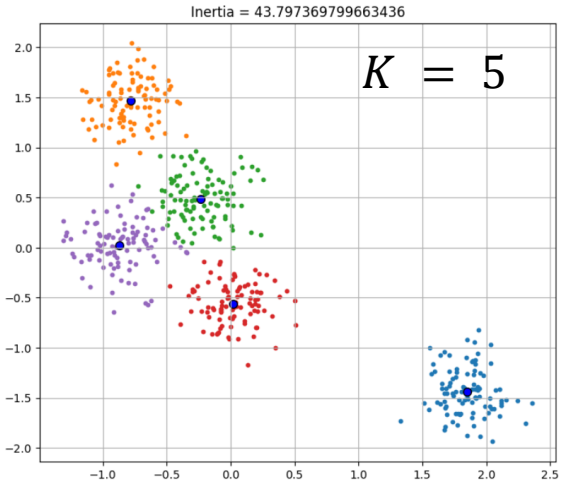
(Rousseeuw, 1987)

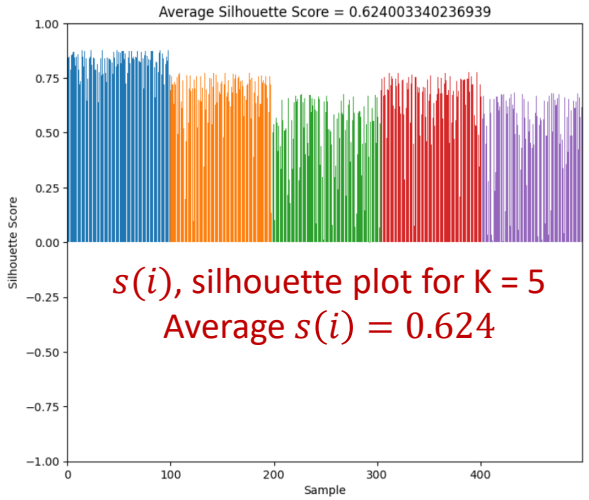


$$s(i) = \begin{cases} \dfrac{b(i) - a(i)}{\max(a(i), b(i))}, & \text{if } |C_i| > 1 \\ 0, & \text{if } |C_i| = 1 \end{cases}$$

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i} d(i,j)$$

$$b(i) = \min_{k \neq i} \frac{1}{|C_j|} \sum_{j \in C_k} d(i,j)$$





$s(i)$, silhouette plot for K = 5
Average $s(i) = 0.624$

Notation:

$d(i,j)$ = Euclidean distance of point i to point j.

$a(i)$ = mean distance between point i to all other points in the same cluster (cohesion).

$b(i)$ = mean distance between point i to all other points in the *next nearest* cluster (separation).

$|C_i|$ = no. of points assigned to cluster i.

$s(i)$ = silhouette score for point i. It ranges from -1 to 1 only.

Other performance metrics for clustering:

Internal Cluster Validity Indices

(Correct labels are *unknown*)

- Calinski-Harabasz Index
- Davies-Bouldin Index
- Dunn Index
- Negentropy Increment
- C-index

External Cluster Validity Indices

(Correct labels are *known*)

- Rand
- Adjusted Rand
- Fowlkes-Mallows
- Jaccard
- Variation of Information

See Arbelaitz, O., Gurrutxaga, I., Muguerza, J., Perez, J. M., & Perona, I. (2013). An extensive comparative study of cluster validity indices. *Pattern Recognition*, 46(1), 243–256.

K-means Clustering

Some drawbacks of K-means clustering:

1. The converged solution is not always optimal.

$$\min_{\boldsymbol{\mu}} \; J = \sum_{i}^{N} \sum_{j}^{K} r_{ij} \left\| \boldsymbol{x}_i - \boldsymbol{\mu}_j \right\|^2$$

2. If the initial centroids are poorly chosen, some clusters may end up empty.

3. If number of data points is large and high-dimensional, the algorithm can take a long time to run.

Some workarounds:

- Use a tree data structure to compute distances faster *(Moore, 2000)*.
- Use the triangle inequality instead of Euclidean distance *(Elkan, 2003)*.

Some extensions of K-means clustering:

1. Instead of the Euclidean distance, we can use a different notion of distance, $\mathcal{V}(\boldsymbol{x}_i, \boldsymbol{\mu}_j)$.

$$\min_{\boldsymbol{\mu}} \; J = \sum_{i}^{N} \sum_{j}^{K} r_{ij} \mathcal{V}(\boldsymbol{x}_i, \boldsymbol{\mu}_j)$$

2. Instead of hard clustering (each $\boldsymbol{x}_i$ is assigned to one and only one cluster), we can use soft clustering algorithms.

   Fuzzy C-means Clustering
   Fuzzy clustering by Local Approximation of MEmberships (FLAME)
   Rough K-means Clustering
   Gaussian Mixture Models

3. So far, we only have a batch version of K-means (the entire data set is used at once). Alternatively, we can use MiniBatch K-means.

We can also implement K-means clustering online: The clusters are updated as new data points arrive.

Hierarchical Clustering

The K-means algorithm only works if we know the number of clusters, K, beforehand.

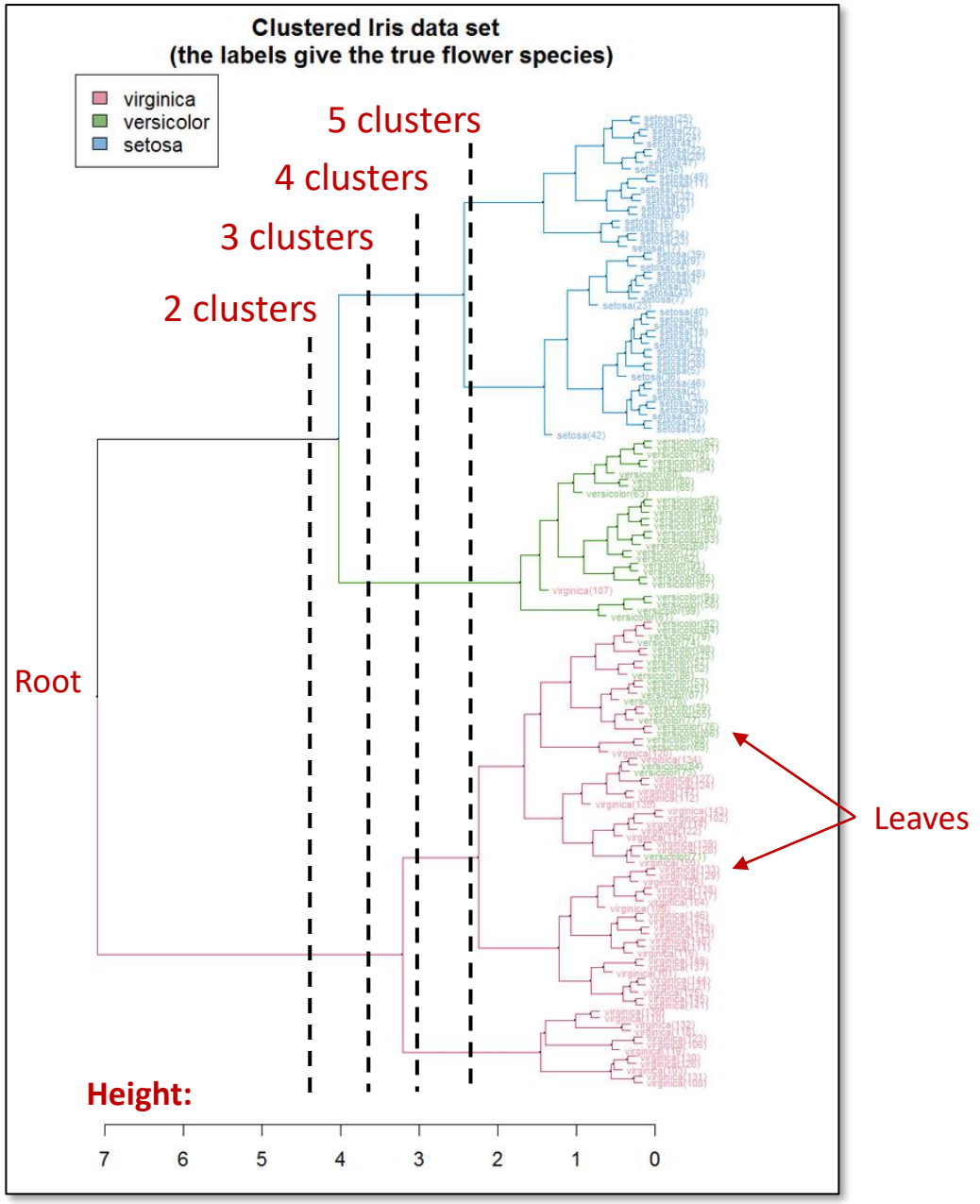
How can we view all results for any K?
What about clusters within a cluster?

One solution: **Hierarchical Clustering**

(Hierarchical Cluster Analysis)

The main result of Hierarchical Clustering is a dendrogram.

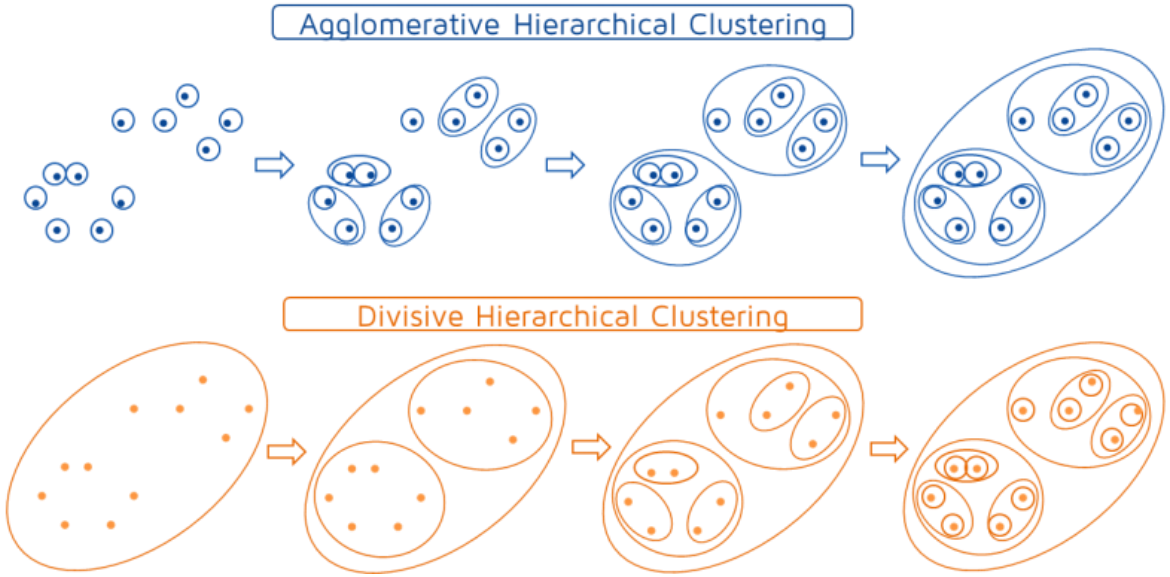
- It is a binary tree.
- The *root* represents all the data as one cluster.
- Each *leaf* represents each data point as is its own cluster.
- Onwards from the root, only one new split occurs at a time. When a split is made, two separate clusters are formed.
- The tree can be cut at any height to give any number of clusters.



https://en.wikipedia.org/wiki/Hierarchical_clustering#/media/File:Iris_dendrogram.png

Hierarchical Clustering

There are two main strategies to build the dendrogram.



https://quantdare.com/hierarchical-clustering/

Agglomerative Clustering

- Bottom-up approach
- **Algorithm:**
  1. Treat each data point as a cluster (N clusters)
  2. WHILE (No. of clusters **is not** equal to 1)
  3. Combine the 2 nearest clusters.
  4. END
  5. Report the result as a dendrogram.

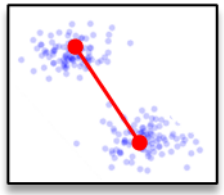
Divisive Clustering (Bisecting K-means)

- Top-down approach
- **Algorithm:**
  1. Treat the entire data set as 1 cluster.
  2. WHILE (No. of clusters **is not** equal to N)
  3. Identify new clusters using K-means.
  4. END
  5. Report the result as a dendrogram.

Hierarchical Clustering

Different ways to **merge** clusters:

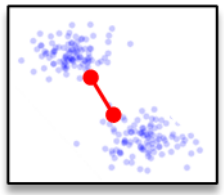
- Merges are determined in a greedy manner.
- Two clusters are merged if they are the "closest" pair to each other.
- The term "closest" can be defined in many ways:
  - Centroid-linkage
  - Single-linkage
  - Complete-linkage
  - Average-linkage
  - Ward's method



Centroid-linkage

- Two clusters are "closest" if their *centroids* are closest.

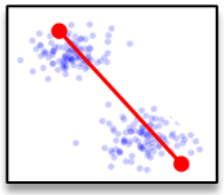
$$D(c_1, c_2) = D\left(\frac{1}{|c_1|}\sum_{\boldsymbol{x}\in c_1}\boldsymbol{x}, \frac{1}{|c_2|}\sum_{\boldsymbol{x}\in c_2}\boldsymbol{x}\right)$$



Single-linkage (SLINK)

- Two clusters are "closest" if the *two nearest points* between them is closest.
- Favors long chains of clusters.

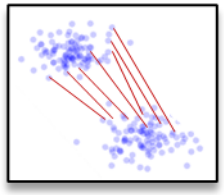
$$D(c_1, c_2) = \min_{\boldsymbol{x}_1\in c_1,\ \boldsymbol{x}_2\in c_2} D(\boldsymbol{x}_1, \boldsymbol{x}_2)$$



Complete-linkage (CLINK)

- Two clusters are "closest" if the *two farthest points* between them is closest.
- Favors spherical clusters with consistent diameter.

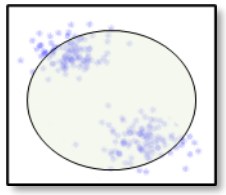
$$D(c_1, c_2) = \max_{\boldsymbol{x}_1\in c_1,\ \boldsymbol{x}_2\in c_2} D(\boldsymbol{x}_1, \boldsymbol{x}_2)$$



Average-linkage

- Two clusters are "closest" if the *average distance* between all pairs of points is closest.
- Less affected by outliers.

$$D(c_1, c_2) = \frac{1}{|c_1|}\frac{1}{|c_2|}\sum_{\boldsymbol{x}_1\in c_1}\sum_{\boldsymbol{x}_2\in c_2} D(\boldsymbol{x}_1, \boldsymbol{x}_2)$$



Ward's Method

- Two clusters are merged if there is a minimum increase in total within-cluster variance after merging.

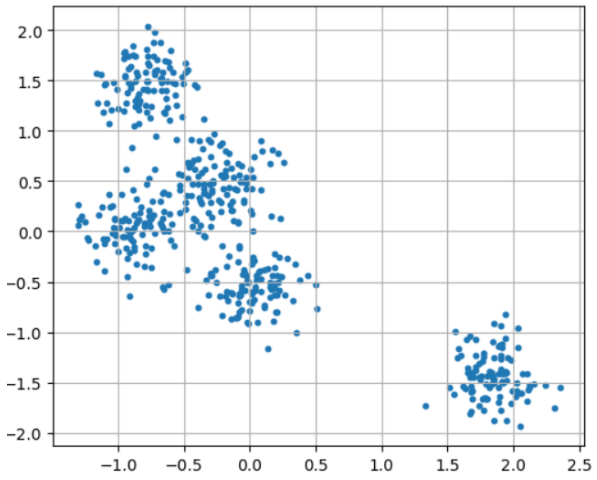
$$D(c_1, c_2) = \sum_{\boldsymbol{x}\in c_1\cup c_2} D\left(\boldsymbol{x}, \boldsymbol{\mu}_{c_1\cup c_2}\right)^2$$

Reference: https://www.youtube.com/watch?v=vg1w5ZUF5lA

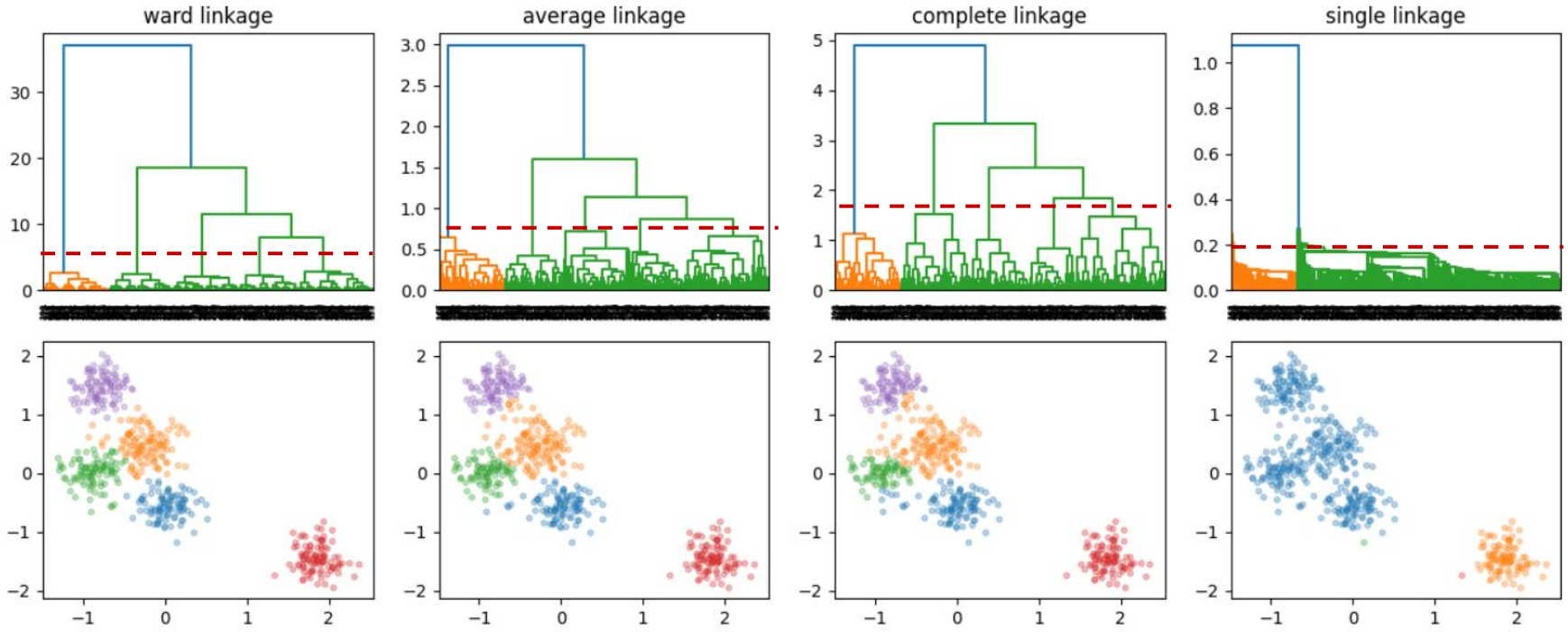
Hierarchical Clustering

In our example, Ward's method shows the most intuitive dendrogram.

Ward's method is the *default* method for Agglomerative Clustering in `sklearn`.



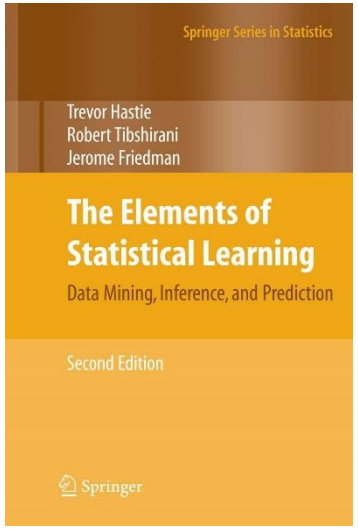
Dendrograms (top) and Cluster Visualizations (bottom)



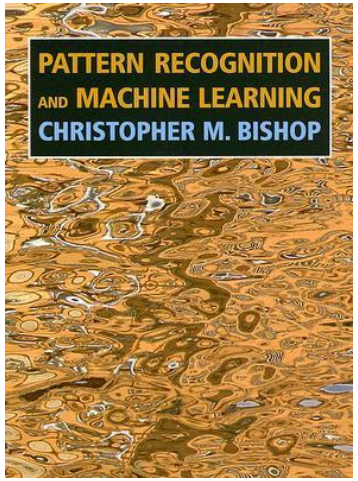
Outline

- Clustering
  - K-means Clustering
  - Hierarchical Clustering
  - Density-based Clustering
  - Gaussian Mixture Model
- Density Estimation
  - Kernel Density Estimation (KDE)
- Anomaly Detection
  - Application of KDE
  - One-class SVM
  - Local Outlier Factor
  - Isolation Forest

Hastie *et al.* (2008)
The Elements of Statistical Learning.
2nd Ed. Springer.



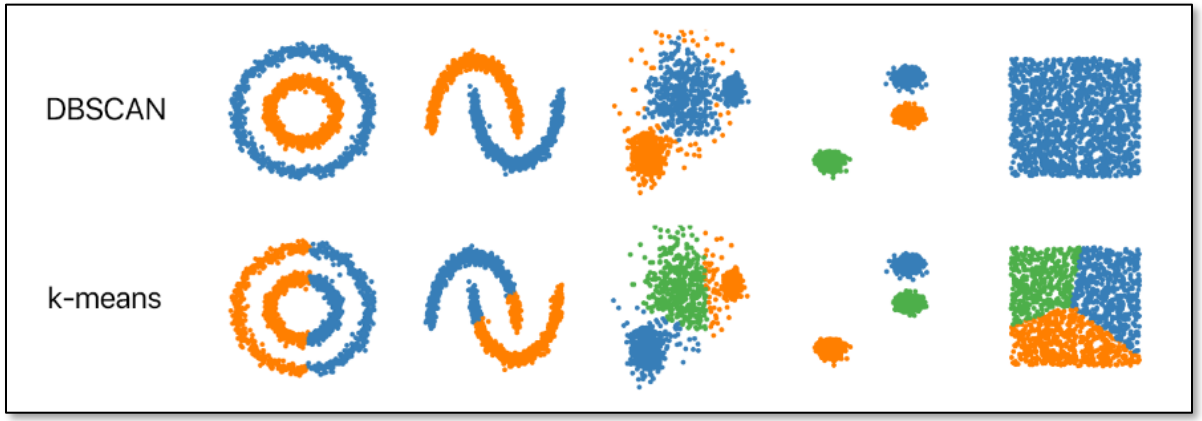
Bishop (2006)
Pattern Recognition and Machine Learning. Springer.



Density-based Clustering

Two famous algorithms for density-based clustering are DBSCAN and OPTICS.

Difference between DBSCAN and K-means Clustering:



https://www.mygreatlearning.com/blog/dbscan-algorithm/

K-means Clustering

- Distance-based
- Cluster shapes tend to be ***spherical*** around the centroids.
- Each point will eventually belong to a cluster
- Sensitive to outliers

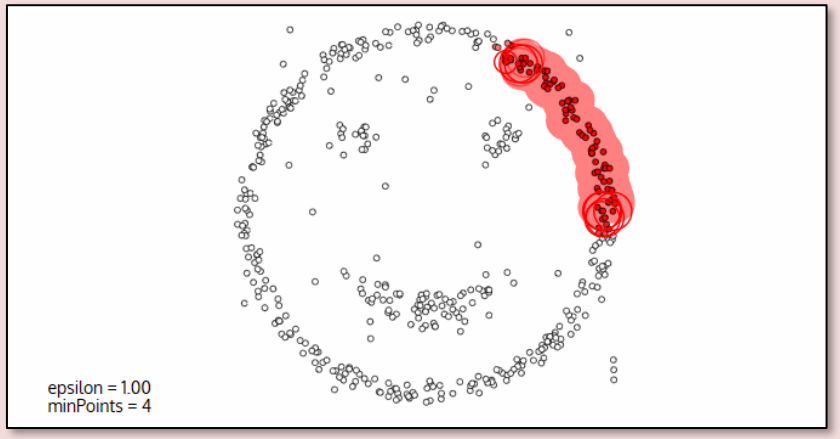
DBSCAN

- Density-based
- Clusters can be ***any shape*** of connected data points.
- Some points will be un-clustered (outliers)
- Robust to outliers

DBSCAN

(Density-based Spatial Clustering of Applications with Noise)

This illustrates DBSCAN on a toy data set:
(https://www.kdnuggets.com/2020/04/dbscan-clustering-algorithm-machine-learning.htm)



DBSCAN parameters: minPts and Epsilon (ε)

If there are at least 'minPts' points within a radius of 'ε' to a point, then we consider all these points to be part of the same cluster.

Gaussian Mixture Models

- A soft-clustering version of K-means.
- Assumes that each cluster is Gaussian-distributed.
- The entire data set is then clustered as a mixture of K Gaussian distributions. K must be known.

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

π_k = weight of kth cluster
K = total number of clusters
$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ = kth Gaussian dist.

Recall: K-means clustering algorithm

Given: Data Set, $\boldsymbol{x}_i \in \Re^M,\ i = 1, 2, \ldots, N$

Initialization: Set a tolerance, *tol* (e.g. 10^{-3})
Set an assumed number of clusters, *K*
Set an initial guess of *K centroids*, $\boldsymbol{\mu}_j$

1: Pre-allocate an old solution: $\boldsymbol{\mu}_j^{\text{old}} = \mathbf{0} \in \Re^{K \times M}$.

2: WHILE $\|\boldsymbol{\mu}_j - \boldsymbol{\mu}_j^{\text{old}}\| > \text{tol}$

3: Save the old centroids: $\boldsymbol{\mu}_j^{\text{old}} := \boldsymbol{\mu}_j$.

4: Compute r_{ij}: Assign each $\boldsymbol{x}_i$ to the closest centroid.

5: Compute the new centroids, $\boldsymbol{\mu}_j$:

$$\boldsymbol{\mu}_j = \frac{\sum_i r_{ij} \boldsymbol{x}_i}{\sum_i r_{ij}}$$

Compute the new $\boldsymbol{\mu}_j$ as the average position of all data points $\boldsymbol{x}_i$ assigned to cluster j.

6: END WHILE

7: Report the final centroids, $\boldsymbol{\mu}_j$.

The algorithm for GMMs is similar to K-means.

EM = Expectation Maximization
(Dempster et al., 1997)

- **E-step:** Calculate the responsibilities, r_{ij}, of each $\boldsymbol{x}$ to each $\boldsymbol{\mu}$.

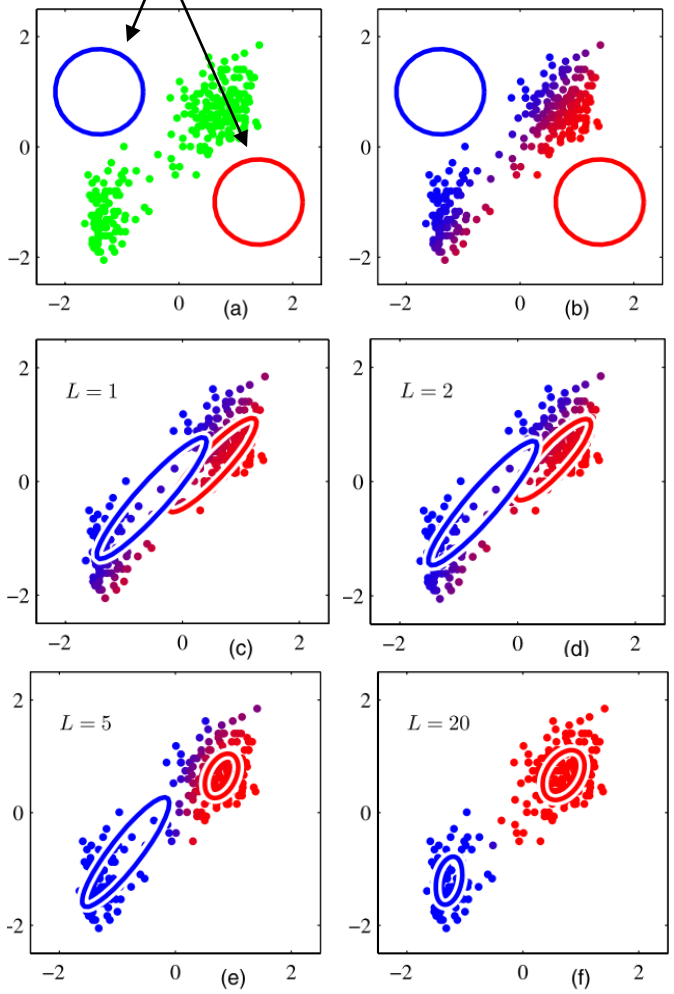
$$r_{ij} = \frac{\pi_j \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}$$

- **M-step:** Update new $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.

$$\boldsymbol{\mu}_j = \frac{\sum_i r_{ij} \boldsymbol{x}_i}{\sum_i r_{ij}} \qquad \boldsymbol{\Sigma}_j = \frac{1}{N_j} \sum_{n=1} r_{nj} (\boldsymbol{x}_n - \boldsymbol{\mu}_j)^2$$

How the EM algorithm works:

2-D Gaussian PDFs
$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$



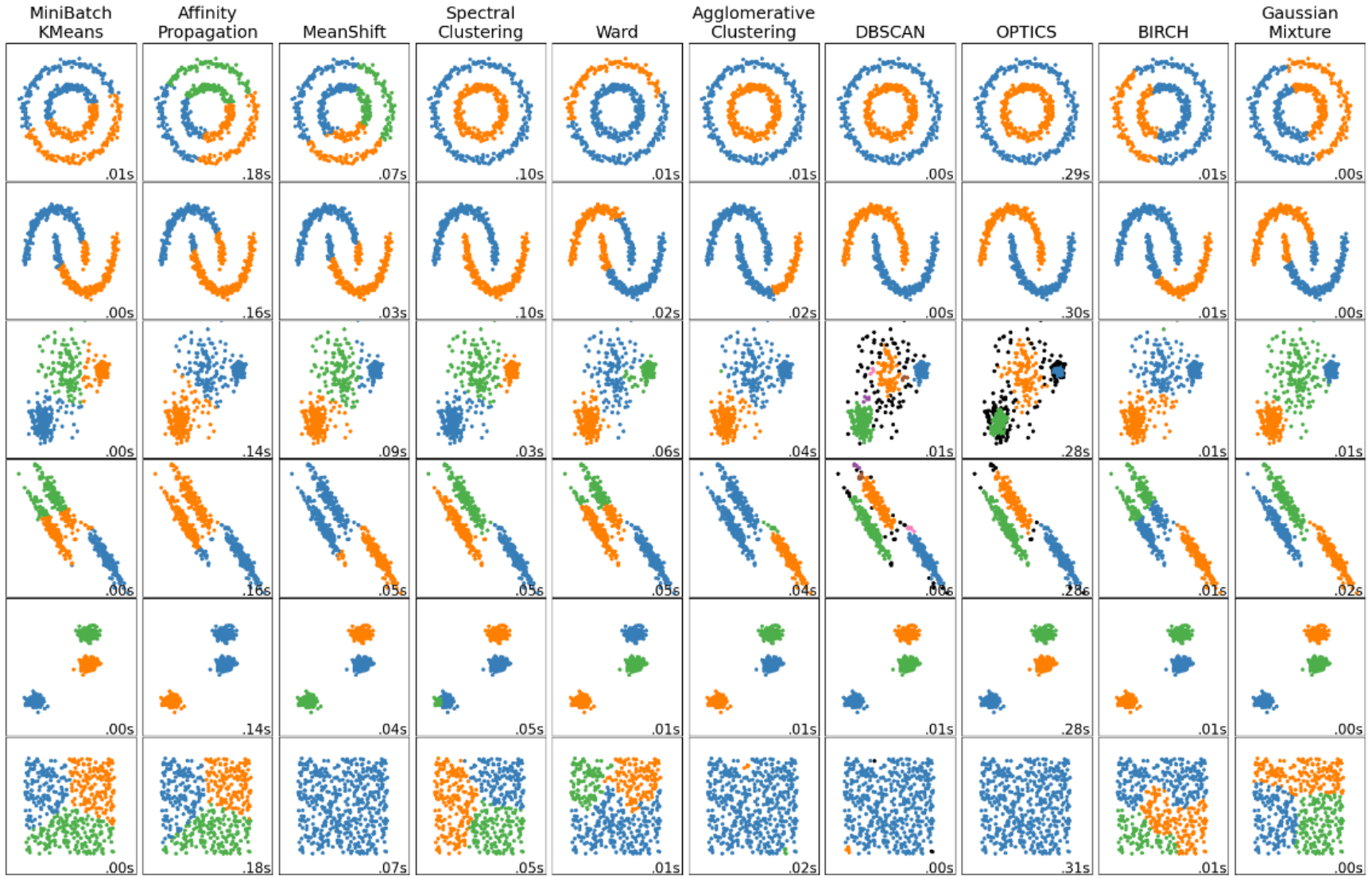
A Comparison of Clustering Methods

So far, we discussed only:

- K-means
- Mini-batch K-means
- Hierarchical Clustering
  - Ward
- DBSCAN
- Gaussian Mixture

In scikit-learn, other clustering algorithms are available.

You can apply a performance metric (e.g. silhouette score) on all these results in order to compare them quantitatively.



A comparison of the clustering algorithms in scikit-learn

Outline

- Clustering
  - K-means Clustering
  - Hierarchical Clustering
  - Density-based Clustering
  - Gaussian Mixture Model
- **Density Estimation**
  - **Kernel Density Estimation (KDE)**
- **Anomaly Detection**
  - **Application of KDE**
  - **One-class SVM**
  - **Local Outlier Factor**
  - **Isolation Forest**

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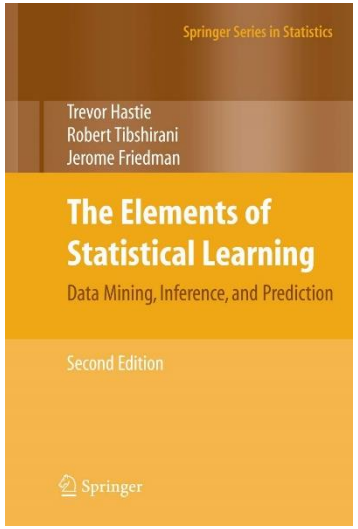

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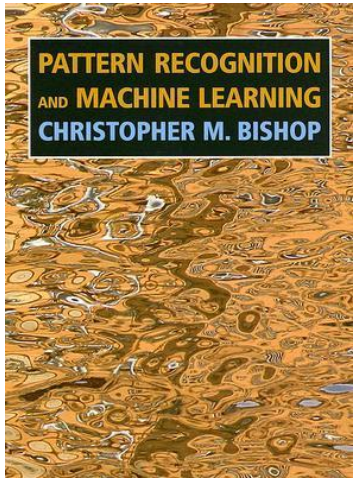
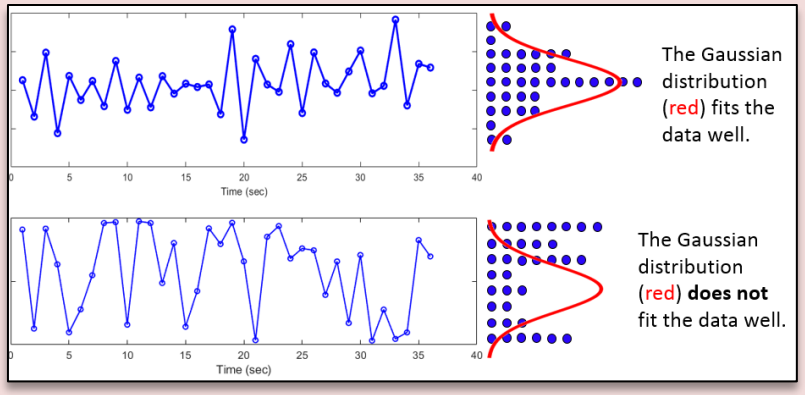


Density Estimation

- Refers to the estimation of an unobservable underlying probability density function given only observed data.
- Usually, we only assume that the data is Gaussian-distributed. However, if the data is multi-modal or non-Gaussian, then we need to perform density estimation.

Gaussian vs. Non-Gaussian Data



Kernel Density Estimation

Estimate the probability, $p(\boldsymbol{x})$, as a sum of kernel functions $K(\boldsymbol{x})$:

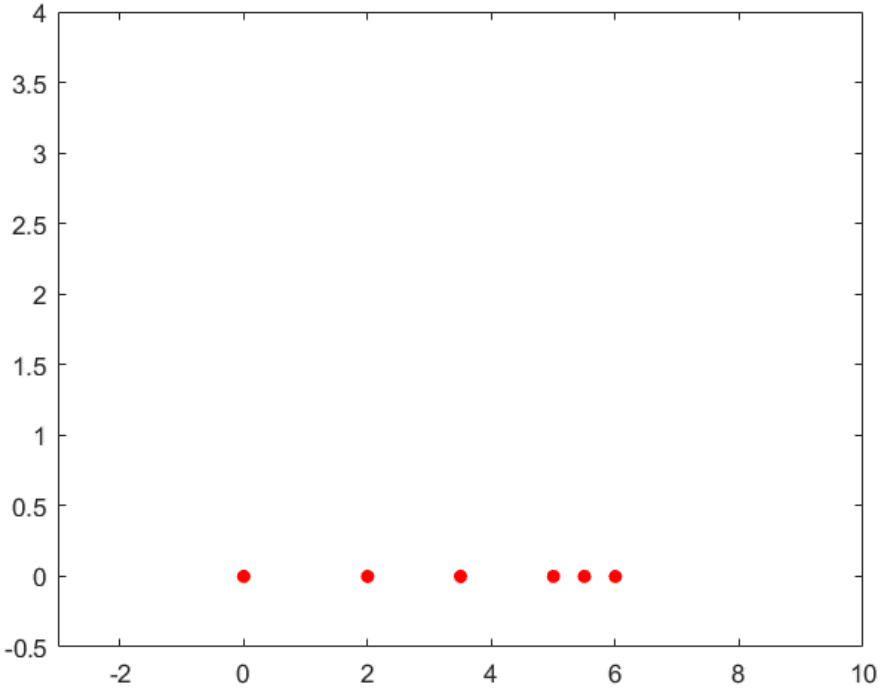
$$p(\boldsymbol{x}) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{h^D}\,K\left(\frac{\boldsymbol{x}-\boldsymbol{x}_i}{h}\right)$$

h = bandwidth
D = dimensions of the data
N = no. of data points
$k(\cdot)$ = kernel function
$\boldsymbol{x}_i$ = training data
$\boldsymbol{x}$ = any new query data

Example:

Estimate the probability distribution of the following univariate non-Gaussian data:

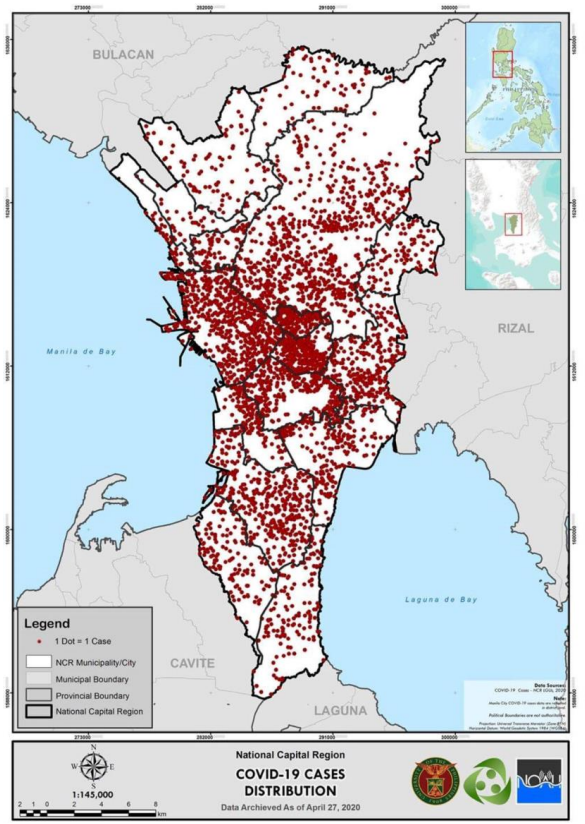
0.0,
2.0,
3.5,
5.0,
5.5,
6.0



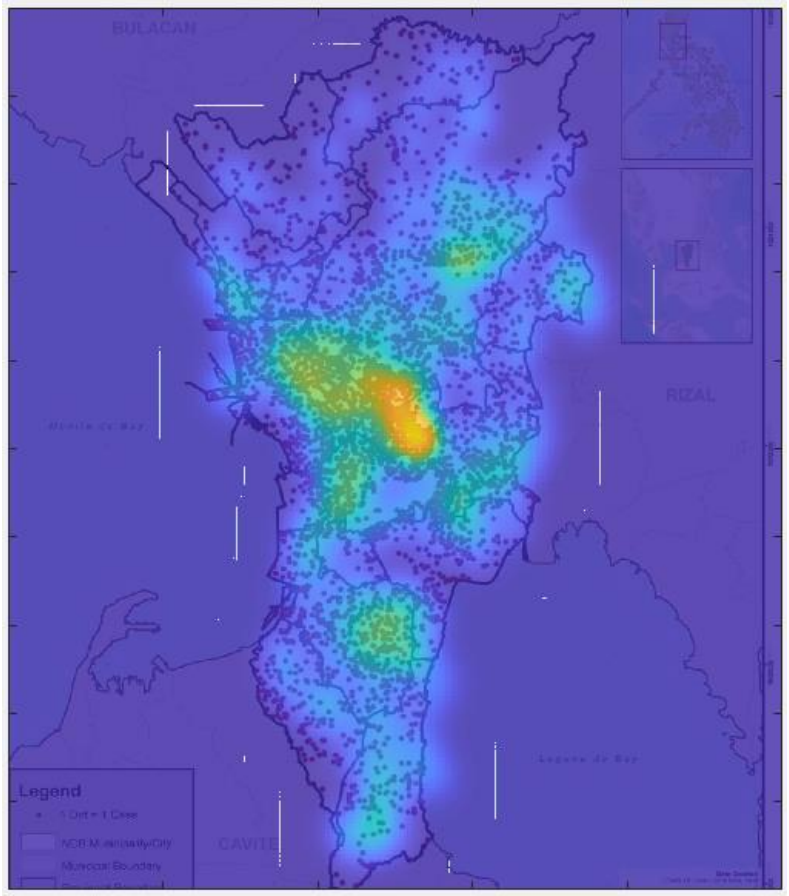
Density Estimation

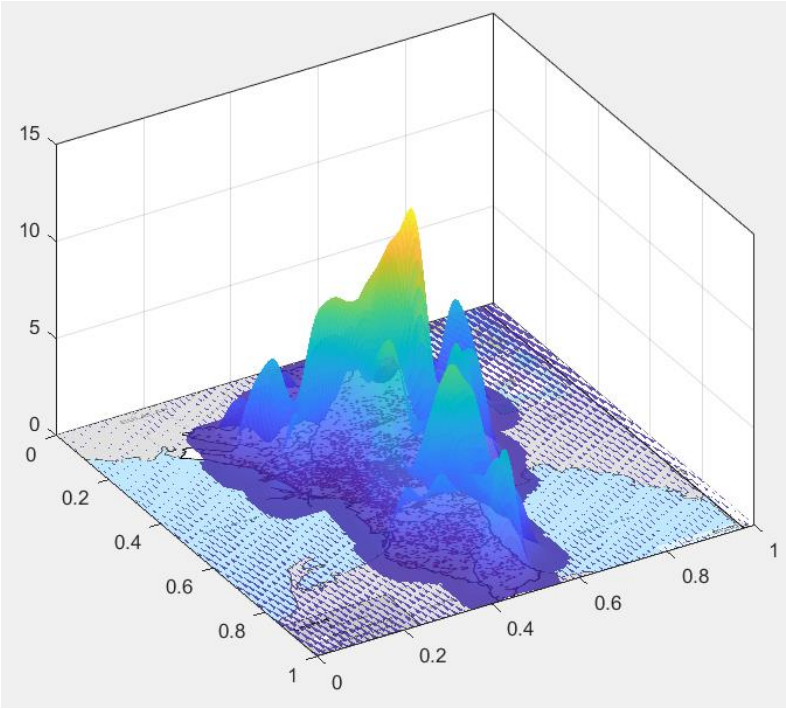
Example:

Use the bivariate kernel density estimator to find the distribution of Covid cases using a bandwidth of $h = [0.02, 0.02]$ and the Gaussian kernel.



Answer:





The areas with high density of cases will have higher peaks in the estimated distribution.

Anomaly Detection

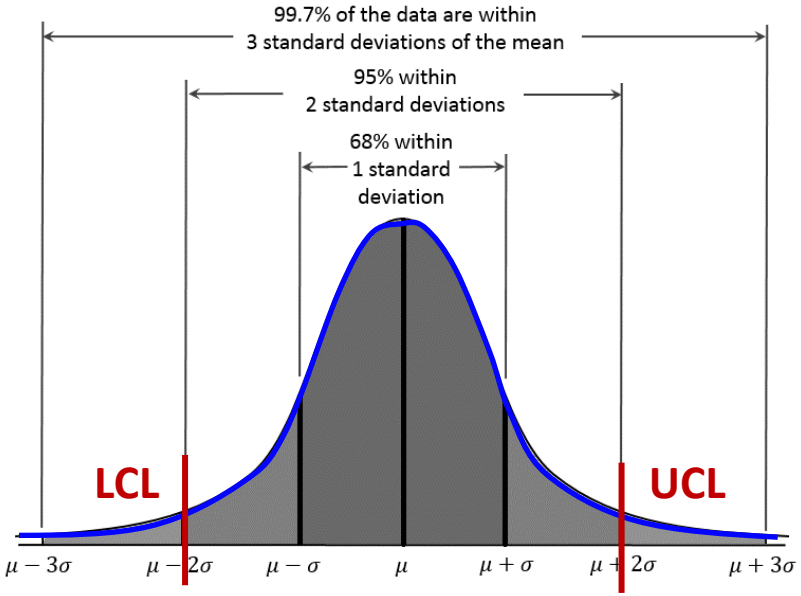
One important application of KDE is *anomaly detection*:
Finding data points that deviate from the expected distribution.

Practical uses of anomaly detection:

- Fault detection in any industrial system
- Defect detection in products
- Fraud detection in financial transactions
- Detecting cyber-attacks, network intrusions
- Detecting fake data (images, texts, etc.)
- Detecting anomalies in medical data
- Outliers and change points detection in time series
- Detecting unusual human behavior*

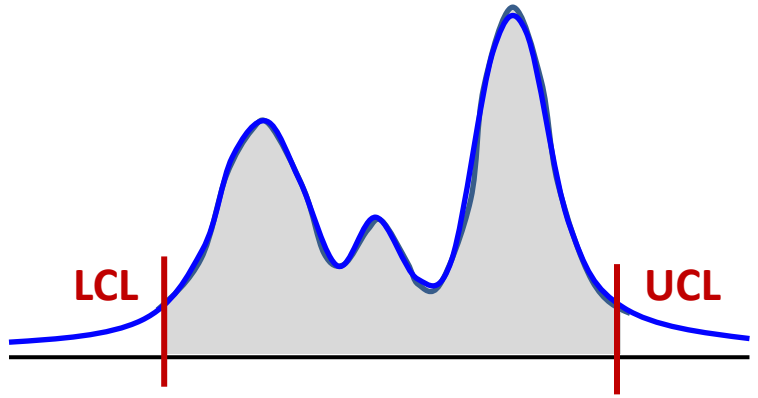
If the data is Gaussian-distributed:
(Use Elliptic Envelope or just Quantiles)

- Fit a Gaussian distribution to the data. Find $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.
- Establish a confidence level, α, e.g. 95%.
- Calculate the thresholds at which the area under the distribution is a fraction of α.
- Use the thresholds as upper control limit and lower control limit.



If the data is <u>not</u> Gaussian-distributed:
(Use KDE)

- Fit a distribution to the data using Kernel Density Estimation (KDE).
- Do the same steps as above.



Other Anomaly Detection Methods

One-Class SVM

Support Vector Data Description (SVDD)

Tax and Duin (2004)

- Minimize the volume of a *hyper-sphere* around the data points.
- All points outside the *hyper-sphere* are outliers.

$$\min_{R,\boldsymbol{a}} R^2 + C\sum_{i=1}^{n}\epsilon_i$$

$$\|x_i - \boldsymbol{a}\|^2 \leq R^2 + \epsilon_i \quad \forall i = 1, 2, \dots, n$$
$$\epsilon_i \geq 0 \quad \forall i = 1, 2, \dots, n$$

sklearn.svm.OneClassSVM

Support Vector Method for Novelty Detection

Scholkopf *et al.* (1999)

- Separate the data points from the origin by maximizing the distance of a *hyper-plane* to the origin.
- All points outside the *hyper-plane* are outliers.

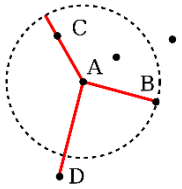
$$\min_{\boldsymbol{w},\epsilon_i,\rho} \frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{1}{\nu n}\sum_{i=1}^{n}\epsilon_i - \rho$$

$$\langle \boldsymbol{w}, \phi(\boldsymbol{x}_i)\rangle \geq \rho - \epsilon_i \quad \forall i = 1, 2, \dots, n$$
$$\epsilon_i \geq 0 \quad \forall i = 1, 2, \dots, n$$

Local Outlier Factor

Breunig (2000)

- Similar to DBSCAN in that it is density-based.
- Relevant Formula:
  - Reachability Distance (RD)



RD(A,B) and **RD(A,C)** are the same since B and C belong to the k-nearest neighbors of A. Meanwhile, **RD(A,D)** = $\text{dist}(A, D)$ since D is not a neighbor of A.

  - Local Reachability Density (LRD)

$$LRD(A) = \frac{1}{\frac{1}{|N_k(A)|}\sum_{B\in N_k(A)} RD(A,B)}$$

$N_k(A)$ is the set of k-nearest neighbors of A.

- **Local Outlier Factor (LOF)**

$$LOF(A) = \frac{\sum_{B\in N_k(A)} LRD(B)}{|N_k(A)| \cdot LRD(A)}$$

Higher LOF, more likely an outlier

"Average LRD of the neighbors of point A divided by A's own LRD"

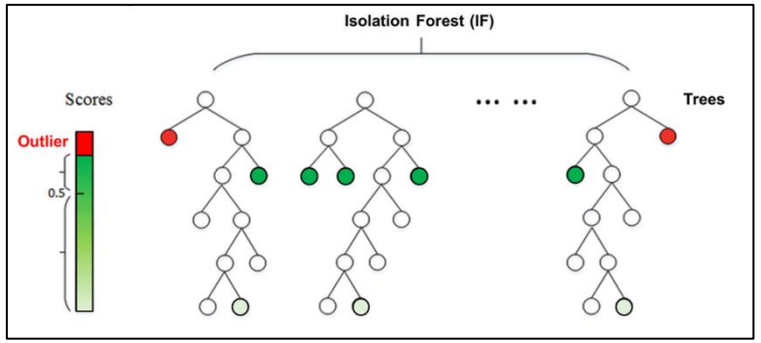
sklearn.neighbors.LocalOutlierFactor

Isolation Forest

Liu *et al.* (2008)

- Build a typical forest of Decision Trees.
- The shorter the average paths from the root to a leaf, the more likely the leaf is an outlier.

Source: https://wiki.datrics.ai/isolation-forest-model



sklearn.ensemble.IsolationForest

Anomaly Score

$$Score(x, n) = 2^{\frac{-E(h(x))}{c(n)}}$$

Higher score, more likely an outlier

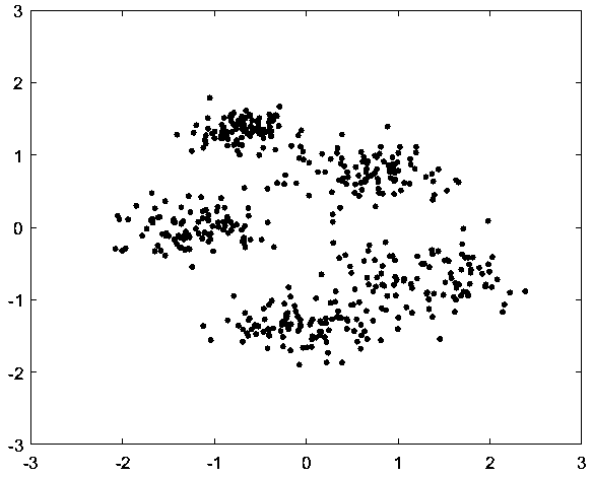
Path length $h(x)$ is the number of edges traversed from the root to a leaf node x.

$c(n)$ = average path length of all leaves as if searched via a Binary Search Tree.

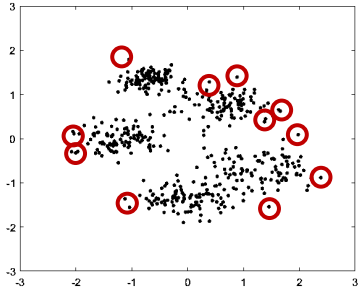
Side Note: Outlier Detection vs. Novelty Detection

- Anomalies can be: outliers that contaminate the *existing* training data.
- Anomalies can also be: novel test data that do not conform to a given training data.

Training Data

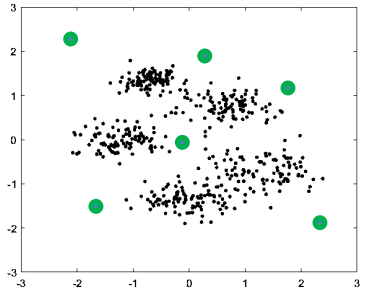


Outlier Detection only



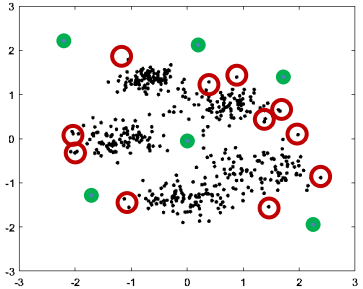
- Only training data are analyzed.
- There are no new test data.
- Which training data points are outliers?

Novelty Detection only



- Only test data are analyzed.
- All training data are treated as *normal* or *uncontaminated by anomalies*.
- Which test data points are novel with respect to the training set?

Detecting both outliers and novel data points



- Both training data and new test data are analyzed.
- Which training data points are outliers? Which test data points are novel?

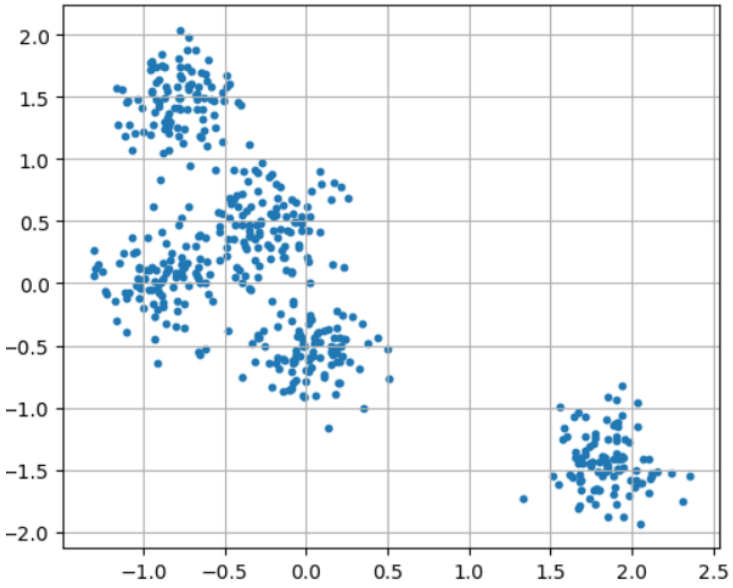
Outlier Detection = unsupervised anomaly detection
Novelty Detection = semi-supervised anomaly detection

Anomaly Detection

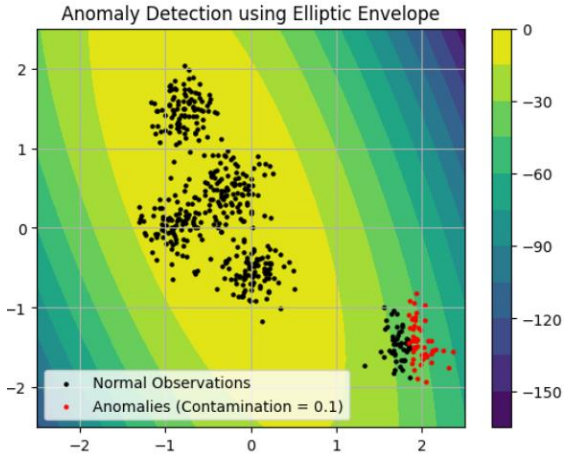
Example:

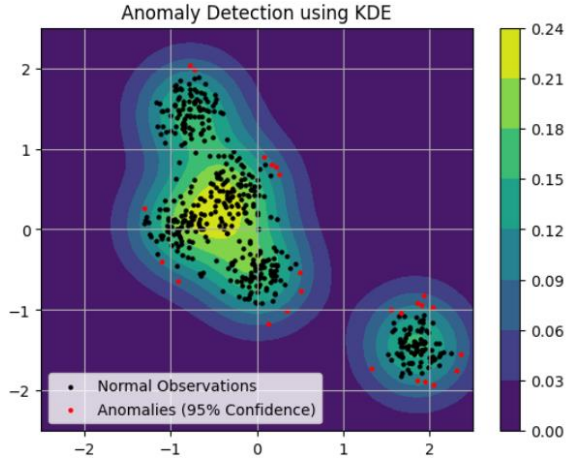
Identify outliers from this 2D data set using the following methods:

- Elliptic Envelope (contamination = 0.1)
- KDE at 95% confidence
- One-class SVM ($\nu = 0.05, \gamma = 1$)
- Local Outlier Factor (no. of neighbors = 5)
- Isolation Forest (contamination = 0.1)



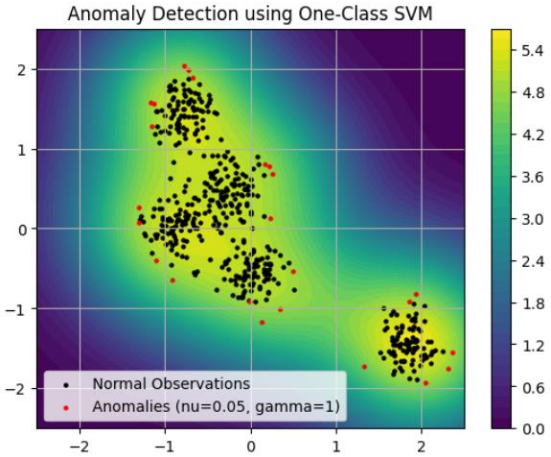
Elliptic Envelope

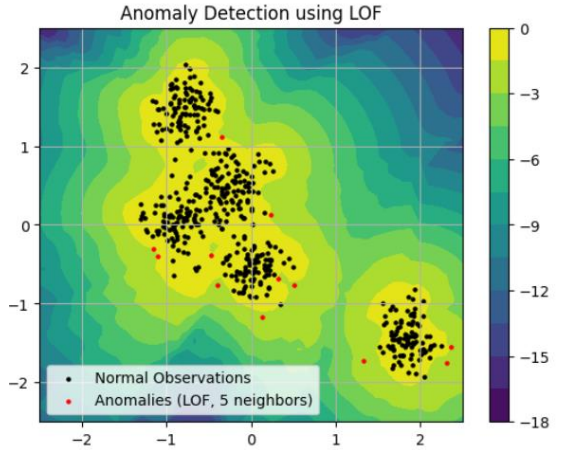




Kernel Density Estimation

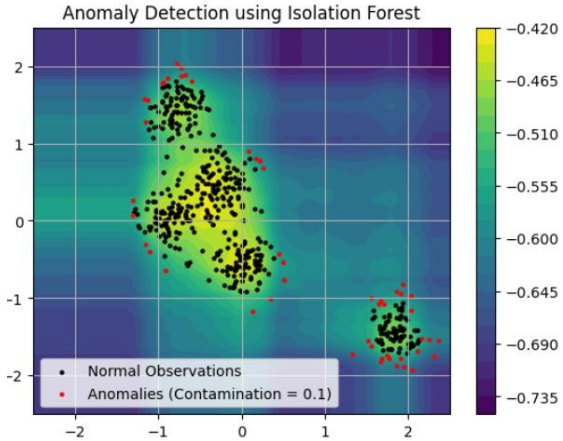
One-Class SVM





Local Outlier Factor

Isolation Forest

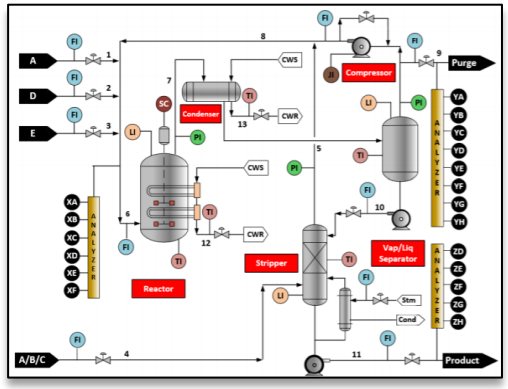


Note: Generating the contour map of anomaly scores is a *novelty* detection task.

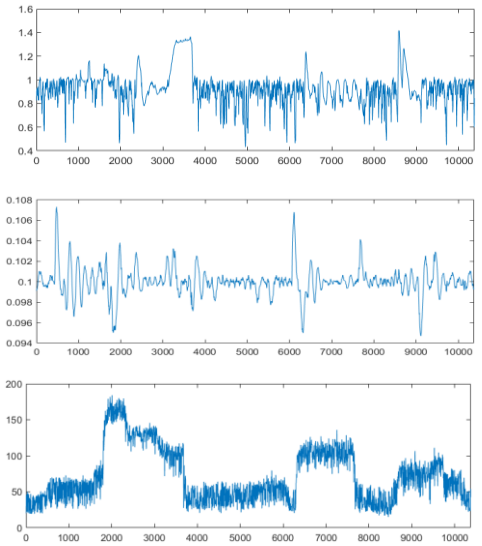
Side Note: Anomaly Detection in Multivariate Data

In industry, statistical control charts are used to detect outliers / abnormal events.

Industrial System



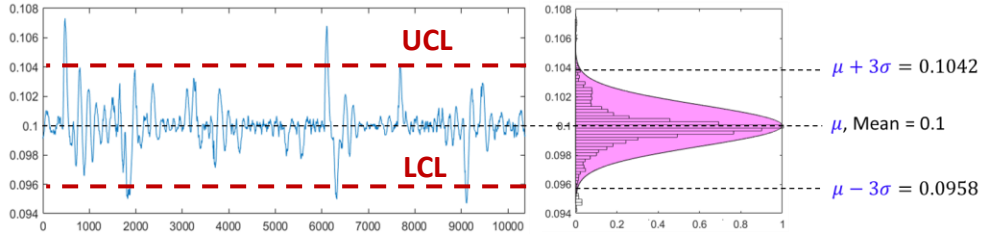
Multivariate Data (Time Series)



Time
(1 sample per second)

Univariate Control Charts

Pressure (MPa) at bottom separator



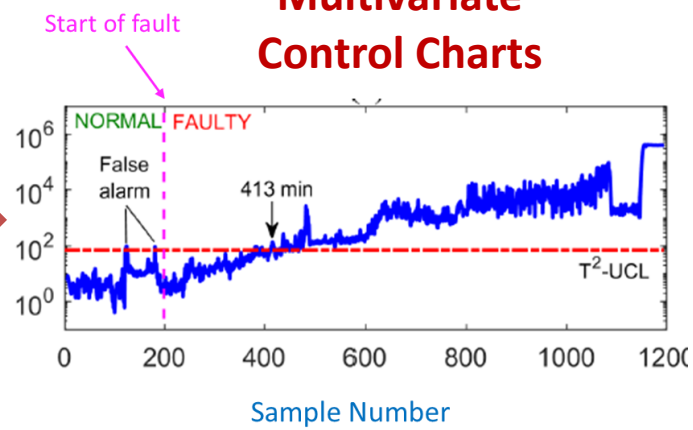
Feature Extraction
(e.g. PCA, ICA, Deep Learning)

Health Indicator
(e.g. Hotelling's T^2 statistic)

Threshold Setting
(e.g. KDE, LOF, OC-SVM, etc.)

All steps involve only unsupervised learning because abnormal data is scarce in industry.

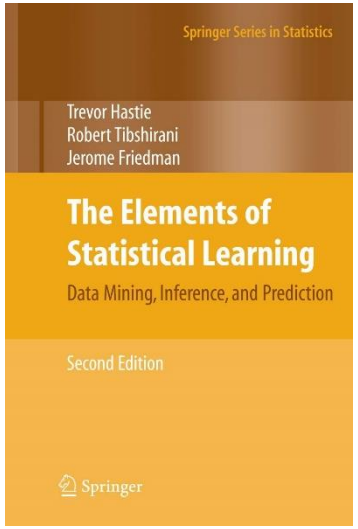
Multivariate Control Charts



Outline

- Clustering
  - K-means Clustering
  - Hierarchical Clustering
  - Density-based Clustering
  - Gaussian Mixture Model
- Density Estimation
  - Kernel Density Estimation (KDE)
- Anomaly Detection
  - Application of KDE
  - One-class SVM
  - Local Outlier Factor
  - Isolation Forest

Hastie *et al.* (2008)
The Elements of Statistical Learning.
2nd Ed. Springer.



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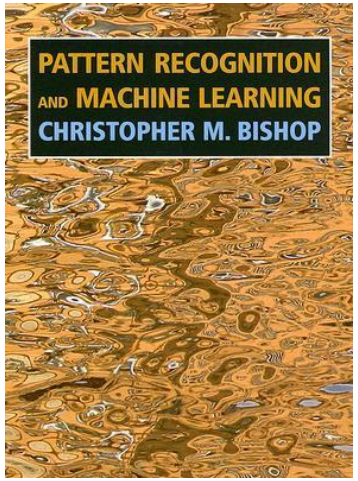

Further Reading

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