K-means clustering

RADI608: Data Mining and Machine Learning
RADI602: Data Mining and Knowledge Discovery

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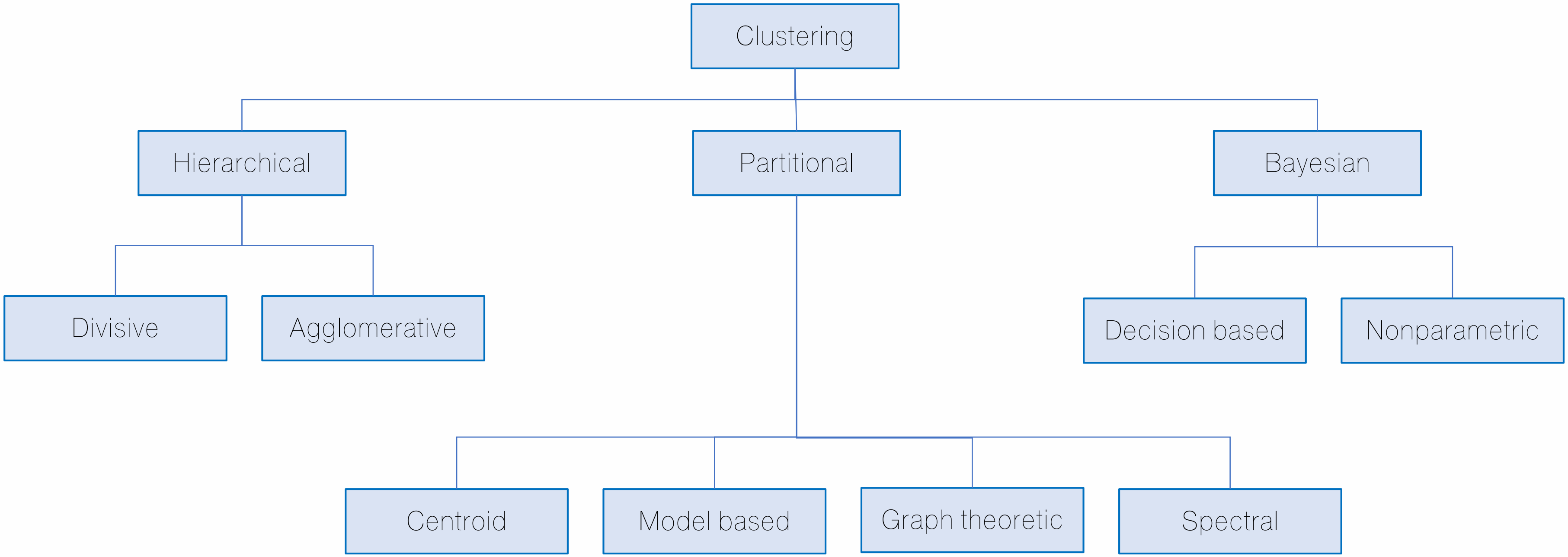
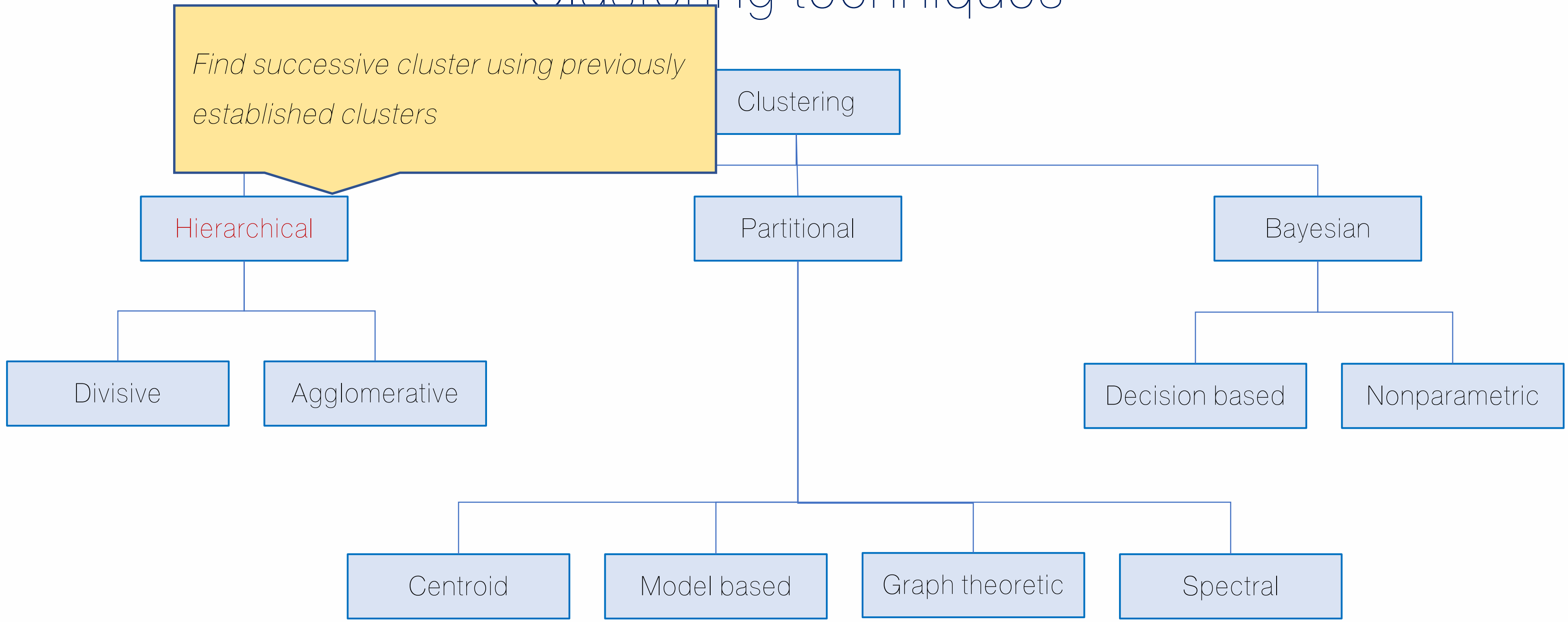
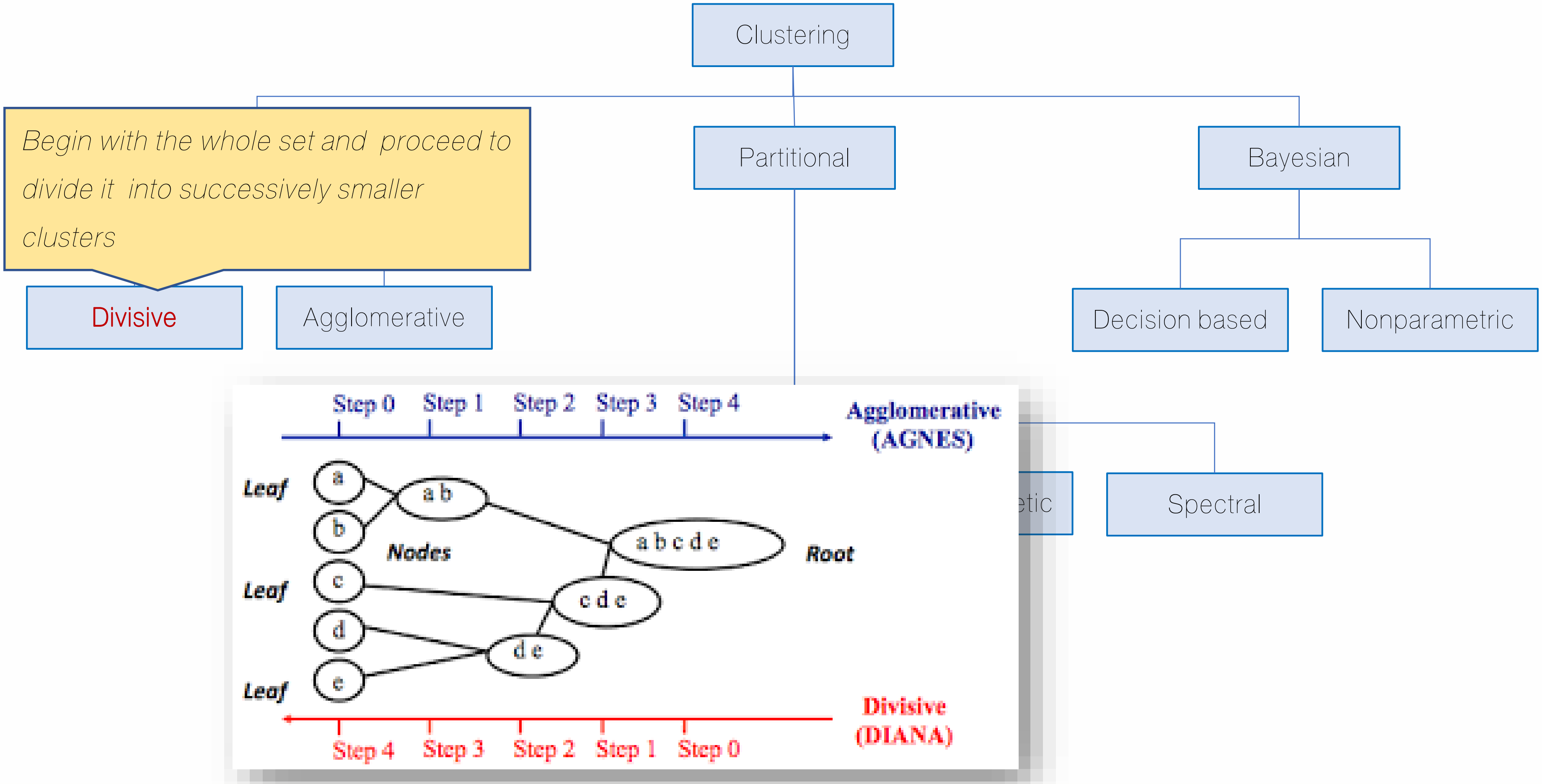
Clustering techniques



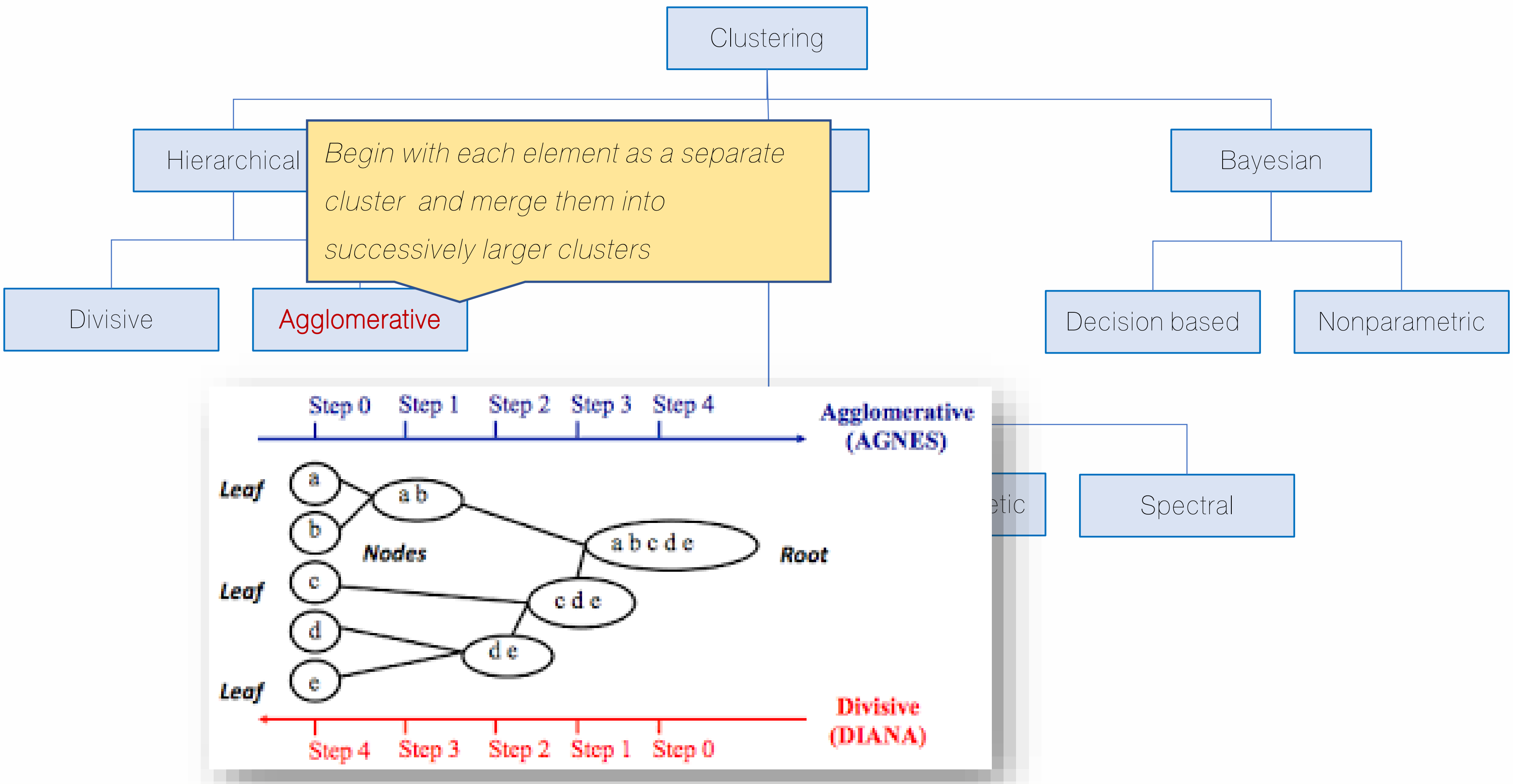
Clustering techniques



Clustering techniques



Clustering techniques



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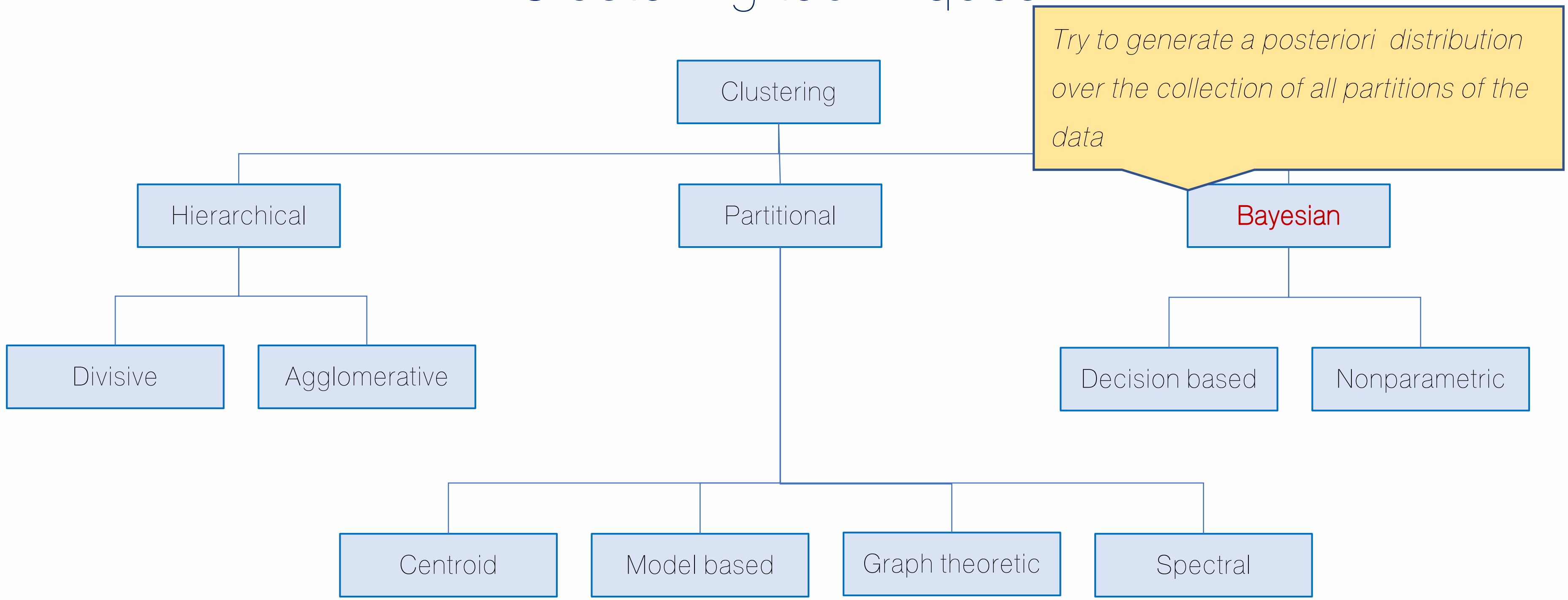
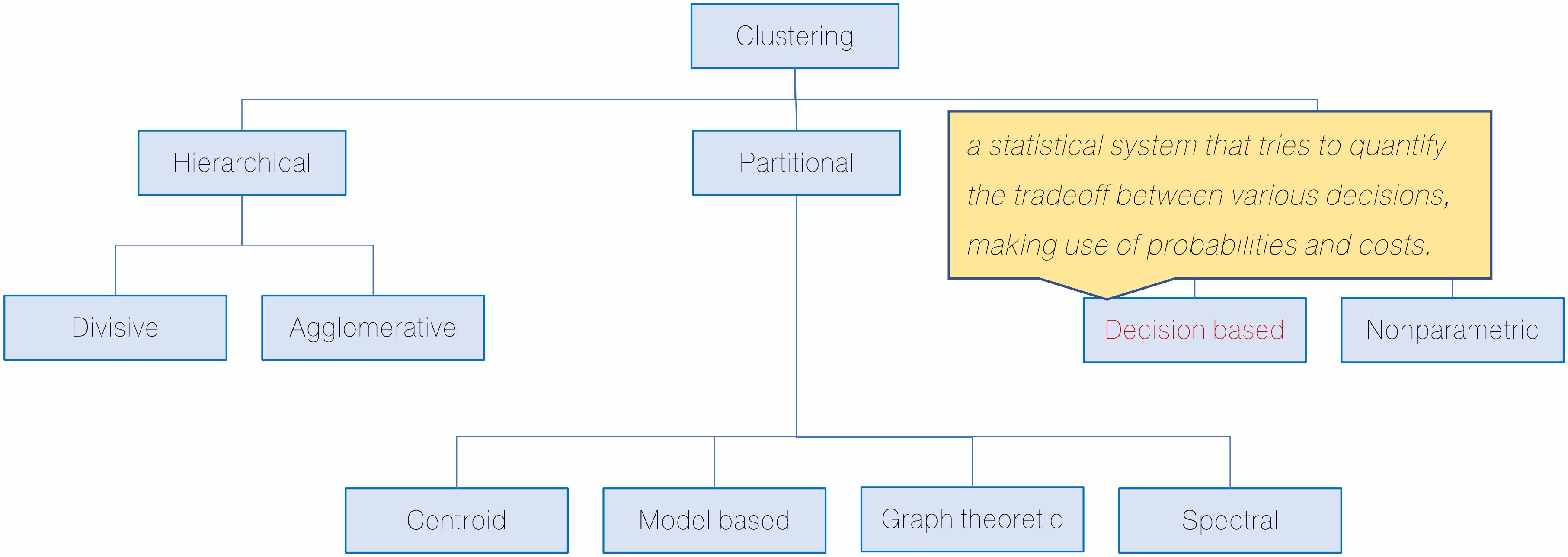
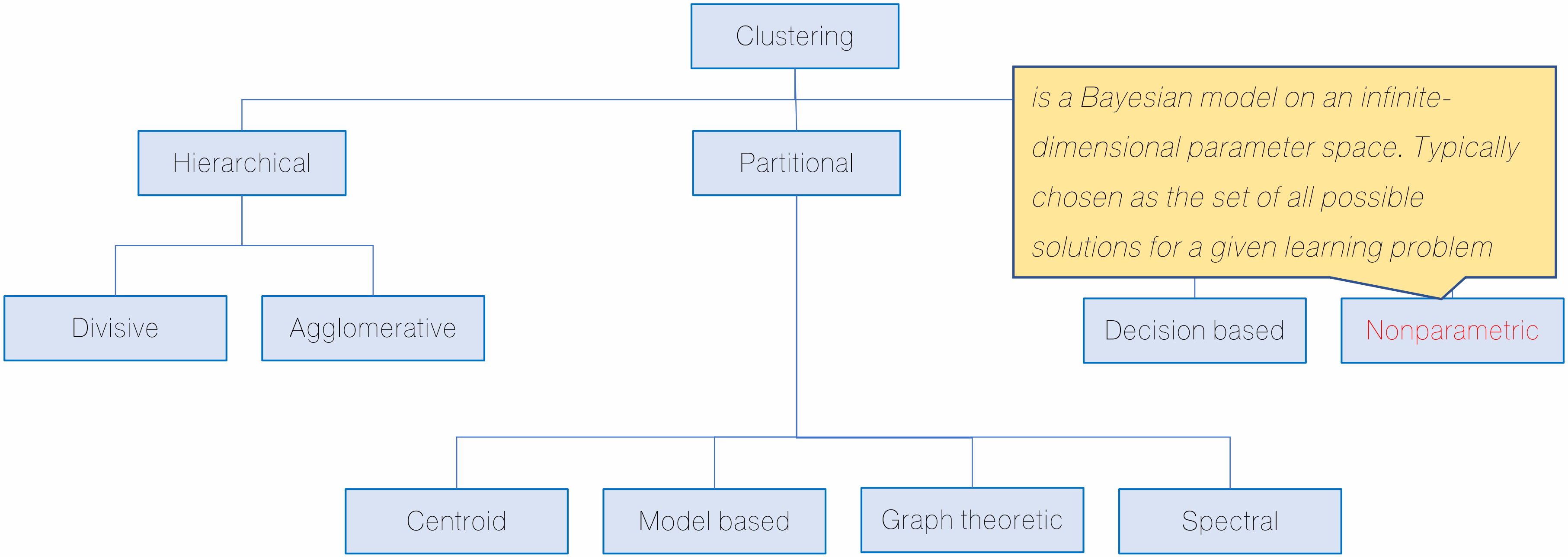
Clustering techniques



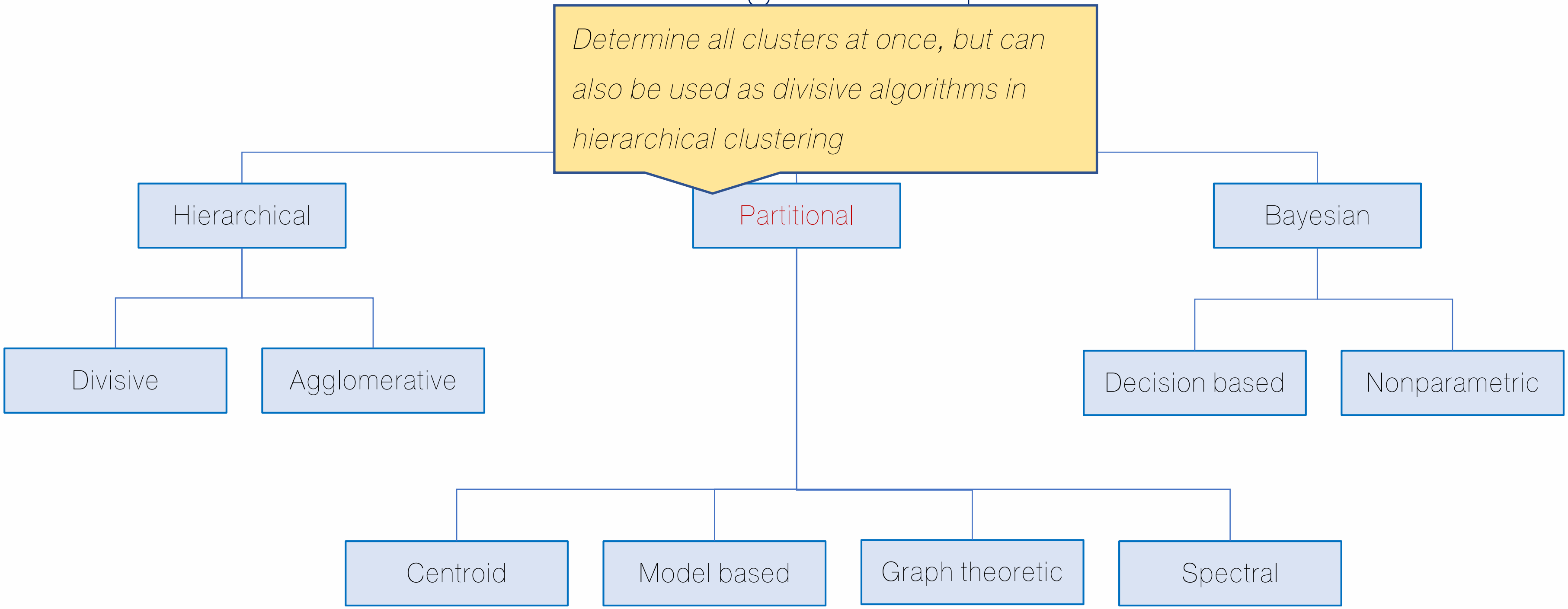
Clustering techniques



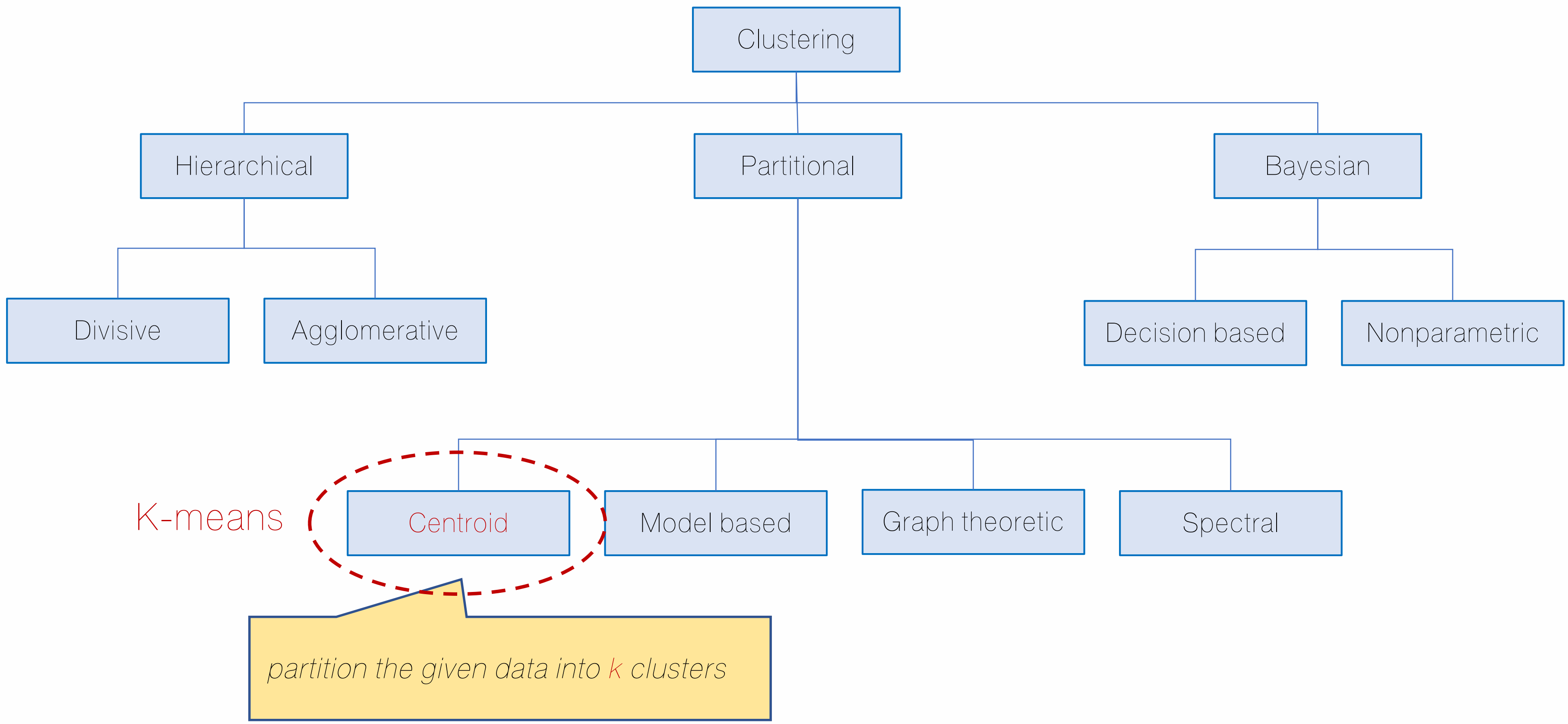
Clustering techniques



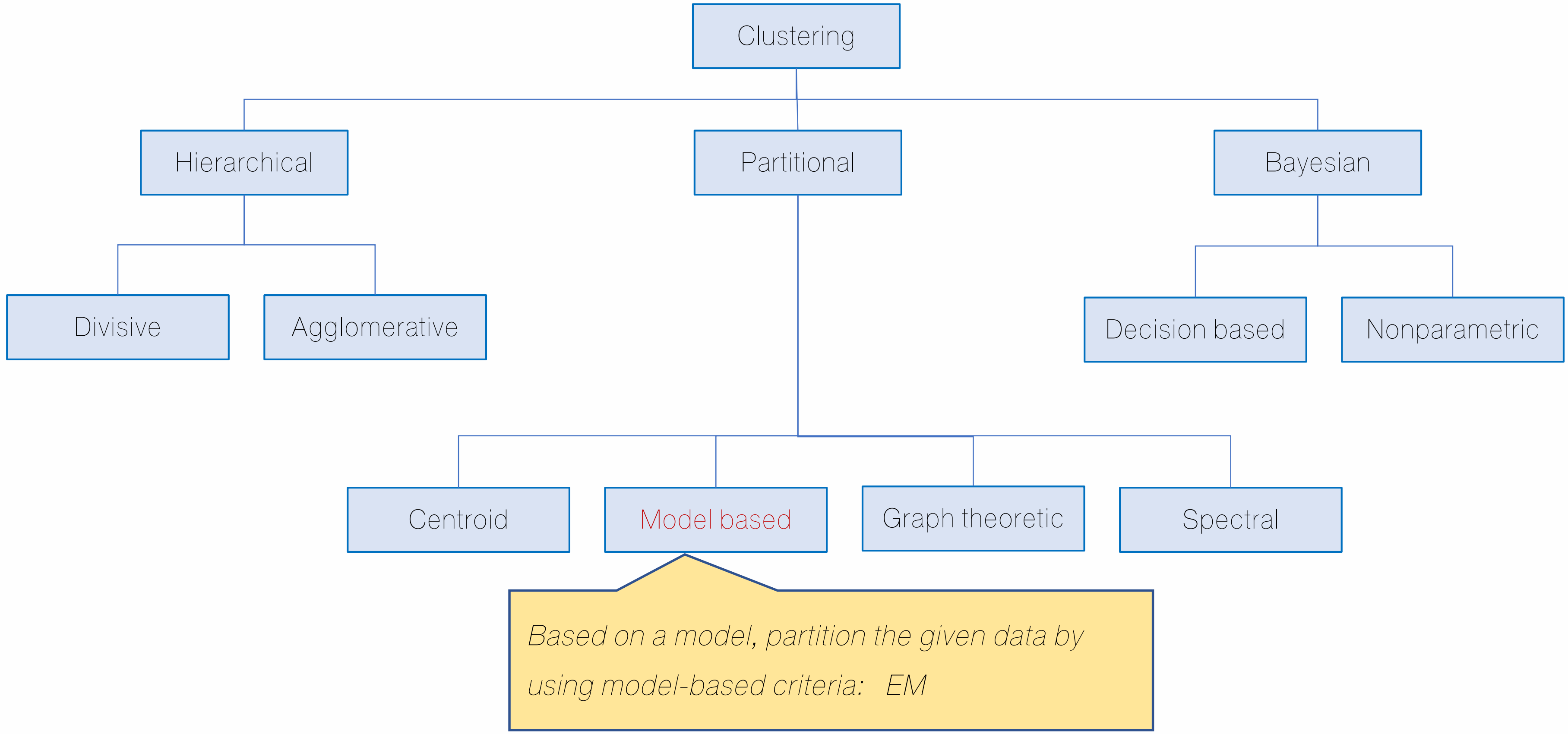
Clustering techniques



Clustering techniques

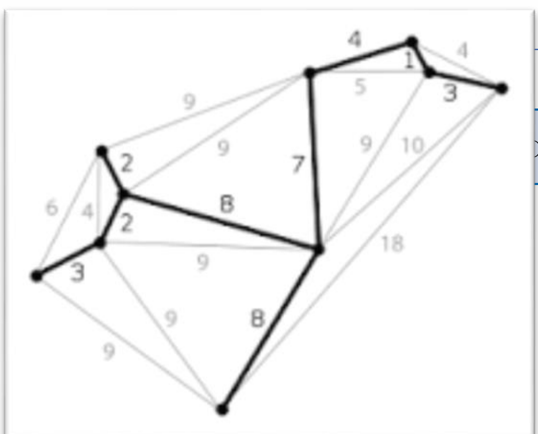


Clustering techniques



Clustering techniques

- Clustering
  - Hierarchical
    - Divisive
    - Agglomerative
  - Partitional
    - del based
    - Graph theoretic
    - Spectral
  - Bayesian
    - Decision based
    - Nonparametric

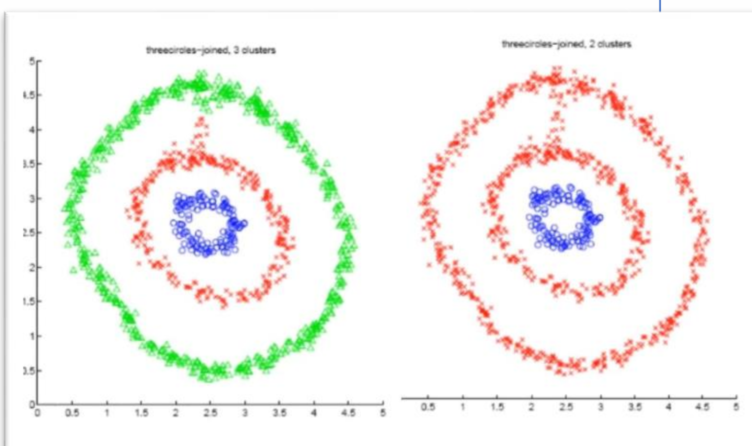


practical solutions are based on heuristics

MST: minimum spanning trees

Clustering techniques

- Clustering
  - Hierarchical
    - Divisive
    - Agglomerative
  - Partitional
    - Graph theoretic
    - Spectral
  - Bayesian
    - Decision based
    - Nonparametric



use k eigenvectors to construct k-way partitionings

K-means clustering

- K-means (MacQueen, 1967) is a partitional clustering algorithm

- Let the set of data points D be $\{x_1, x_2, \ldots, x_n\}$, where $x_i = (x_{i1}, x_{i2}, \ldots, x_{ir})$, $i=1,\ldots,n$ is a vector in $X \subseteq R_r$, and r is the number of dimensions

- The k-means algorithm partitions the given data into k clusters:
  - Each cluster has a cluster center, called centroid
  - k is specified by the user

K-means algorithm

The k-means algorithm works as follows:

a) select the number of clusters (k) you want to identify in your data

b) Choose k (random) data points (seeds) to be the initial centroids, cluster centers

c) Assign each data point to the closest centroid

d) Re-compute the centroids using the current cluster memberships

e) If a convergence criterion is not met, repeat steps c) and d)

K-means convergence (stopping) criterion

no (or minimum) re-assignment of data points to different clusters

or

no (or minimum) change of centroids

or

Minimum decrease in the sum of squared error (SSE)

$$\mathrm{SSE} = \sum_{j=1}^{k} \sum_{X \in G_j} d(X, c_j)^2$$

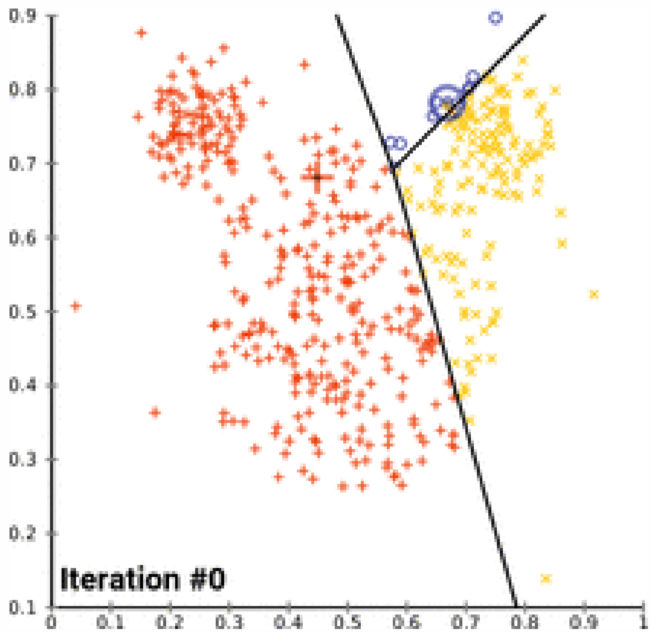
G_j is the j[th] cluster

c_j is the centroid of cluster G_j (the mean vector of all the data points in G_j)

$d(X, c_j)$ is the (Euclidean) distance between data point X and centroid c_j

K-means algorithm

Try to minimize the difference within each cluster and maximize the difference between clusters.



https://en.wikipedia.org/wiki/K-means_clustering

An example of K-means clustering

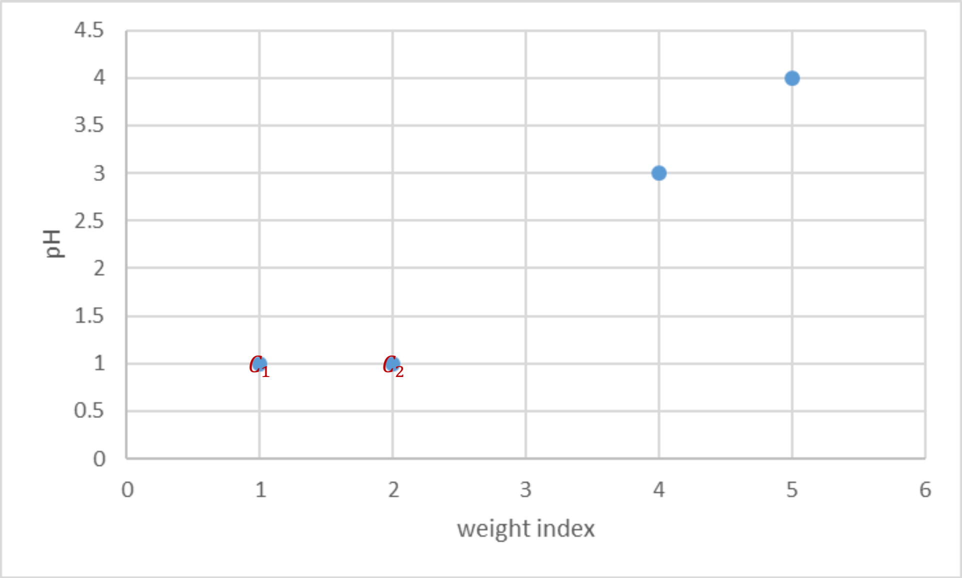
We have 4 types of medicines (samples) with 2 features (weight index and pH).

We have to group these samples into k = 2 group of medicine.

	medicine A	medicine B	medicine C	medicine D
weight index	1	2	4	5
pH	1	1	3	4

http://people.revoledu.com/kardi/tutorial/kMean/NumericalExample.htm

An example of K-means clustering



1. From k = 2,
2. we initialized centroid of group 1: C_1 = (1, 1) and centroid of group 2: C_2 = (2, 1)
3. Calculate the distance between cluster centroid to each object (use a Euclidean distance)

Remarks: a distance can calculate by using another methods such as, manhattan distance, etc.

	medicine A	medicine B	medicine C	medicine D
weight index	1	2	4	5
pH	1	1	3	4

An example of K-means clustering

Euclidean distance = d(a, b) = d(b, a) , $\sqrt{(q_1 - p_1)^2 + \cdots + (q_n - p_n)^2}$

Iteration - 0

$$D^0 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \begin{matrix} C_1 = (1, 1) & group\ 1 \\ C_2 = (2, 1) & group\ 2 \end{matrix}$$

Distance between C_1 = (1, 1) and $Medicine\ A$ = (1, 1) :

= $\sqrt{(1-1)^2 + (1-1)^2}$

= 0

Distance between C_2 = (2, 1) and $Medicine\ A$ = (1, 1) :

= $\sqrt{(1-2)^2 + (1-1)^2}$

= 1

	medicine A	medicine B	medicine C	medicine D
weight index	1	2	4	5
pH	1	1	3	4

An example of K-means clustering

Euclidean distance = d(a, b) = d(b, a) , $\sqrt{(q_1 - p_1)^2 + \cdots + (q_n - p_n)^2}$

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$$D^0 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \begin{array}{ll} C_1 = (1, 1) & group\ 1 \\ C_2 = (2, 1) & group\ 2 \end{array}$$

Distance between C_1 = (1, 1) and $Medicine\ B$ = (2, 1) :

= $\sqrt{(2-1)^2 + (1-1)^2}$

= 1

Distance between C_2 = (2, 1) and $Medicine\ B$ = (2, 1) :

= $\sqrt{(2-2)^2 + (1-1)^2}$

= 0

	medicine A	medicine B	medicine C	medicine D
weight index	1	2	4	5
pH	1	1	3	4

An example of K-means clustering

Euclidean distance = d(a, b) = d(b, a) , $\sqrt{(q_1 - p_1)^2 + \cdots + (q_n - p_n)^2}$

Iteration - 0

$$D^0 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \begin{matrix} C_1 = (1, 1) & group\ 1 \\ C_2 = (2, 1) & group\ 2 \end{matrix}$$

Distance between C_1 = (1, 1) and *Medicine* C (4, 3) :

= $\sqrt{(4-1)^2 + (3-1)^2}$

= 3.61

Distance between C_2 = (2, 1) and *Medicine C* (4, 3) :

= $\sqrt{(4-2)^2 + (3-1)^2}$

= 2.83

	medicine A	medicine B	medicine C	medicine D
weight index	1	2	4	5
pH	1	1	3	4

An example of K-means clustering

Euclidean distance = d(a, b) = d(b, a) , $\sqrt{(q_1 - p_1)^2 + \cdots + (q_n - p_n)^2}$

Iteration - 0

$$D^0 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \begin{array}{l} C_1 = (1, 1) \quad group\ 1 \\ C_2 = (2, 1) \quad group\ 2 \end{array}$$

Distance between C_1 = (1, 1) and *medicine D* (5, 4) :

= $\sqrt{(5-1)^2 + (4-1)^2}$

= 5

Distance between C_2 = (2, 1) and *medicine D* (5, 4) :

= $\sqrt{(5-2)^2 + (4-1)^2}$

= 4.24

An example of K-means clustering

4. Object clustering: assign each object based on the minimum distance. A assign to group 1, B, C, D assign to group 2

Iteration - 0

$$D^0 = \begin{array}{c} \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \\ \begin{matrix} A & \quad B & \quad C & \quad D \end{matrix} \end{array} \begin{matrix} C_1 = (1, 1) & group\ 1 \\ C_2 = (2, 1) & group\ 2 \end{matrix}$$

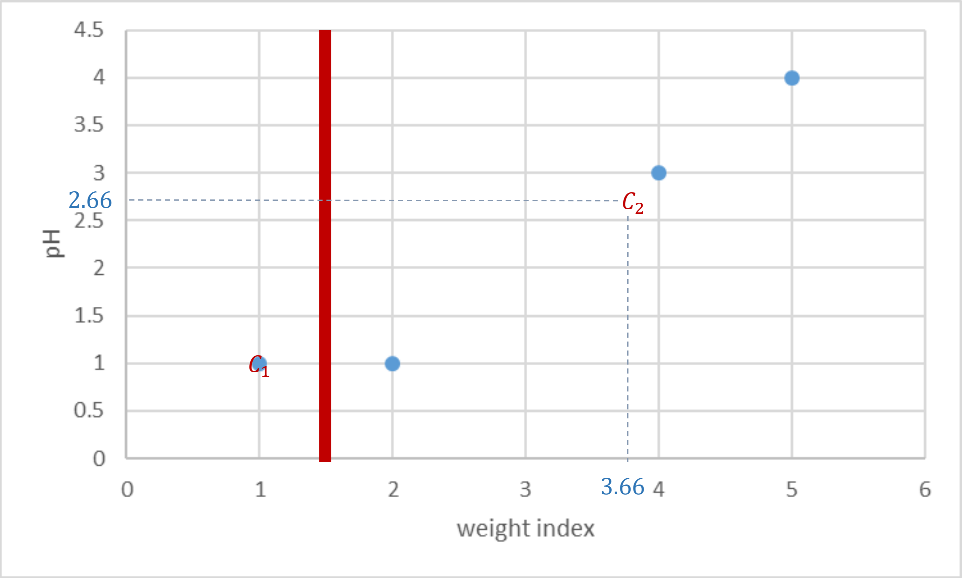
$$G^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \end{bmatrix} \begin{matrix} group\ 1 \\ group\ 2 \end{matrix}$$

5. Determine centroids for interation-1: calculate new centroid of each group

group 1 has one member, then centroid $C_1 = (1, 1)$

group 2 has three members, then $C_2 = \left(\frac{2+4+5}{3}, \frac{1+3+4}{3}\right) = \left(\frac{11}{3}, \frac{8}{3}\right)$

An example of K-means clustering



$$C_1 = (1, 1) \text{ and } C_2 = \left(\frac{11}{3}, \frac{8}{3}\right)$$

Iteration - 1

An example of K-means clustering

Iteration - 1

$$D^1 = \begin{array}{c} \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 3.14 & 2.36 & 0.47 & 1.89 \end{bmatrix} \\ \begin{matrix} A & \quad B & \quad C & \quad D \end{matrix} \end{array} \begin{array}{ll} C_1 = (1, 1) & group\ 1 \\ C_2 = (11/3,\ 8/3) & group\ 2 \end{array}$$

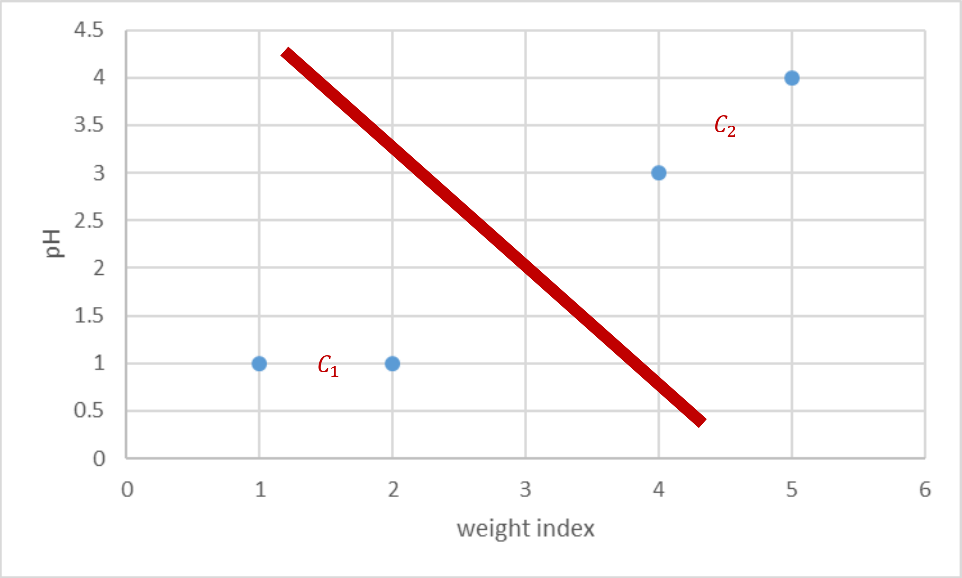
$$G^1 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{array}{l} group\ 1 \\ group\ 2 \end{array}$$

new centroid of each group

group 1 has two members, then centroid $C_1 = (\frac{1+2}{2}, \frac{1+1}{2}) = (1\frac{1}{2}, 1)$

group 2 has two members, then $C_2 = (\frac{4+5}{2}, \frac{3+4}{2}) = (4\frac{1}{2}, 3\frac{1}{2})$

An example of K-means clustering



$$C_1 = (1\tfrac{1}{2}, 1) \text{ and } C_2 = (4\tfrac{1}{2}, 3\tfrac{1}{2})$$

Iteration - 2

An example of K-means clustering

Iteration - 2

$$D^2 = \begin{bmatrix} 0.50 & 0.50 & 3.20 & 4.61 \\ 4.30 & 3.54 & 0.71 & 0.71 \end{bmatrix} \begin{array}{l} C_1 = (1\frac{1}{2}, 1) \quad group\ 1 \\ C_2 = (4\frac{1}{2}, 3\frac{1}{2}) \quad group\ 2 \end{array}$$

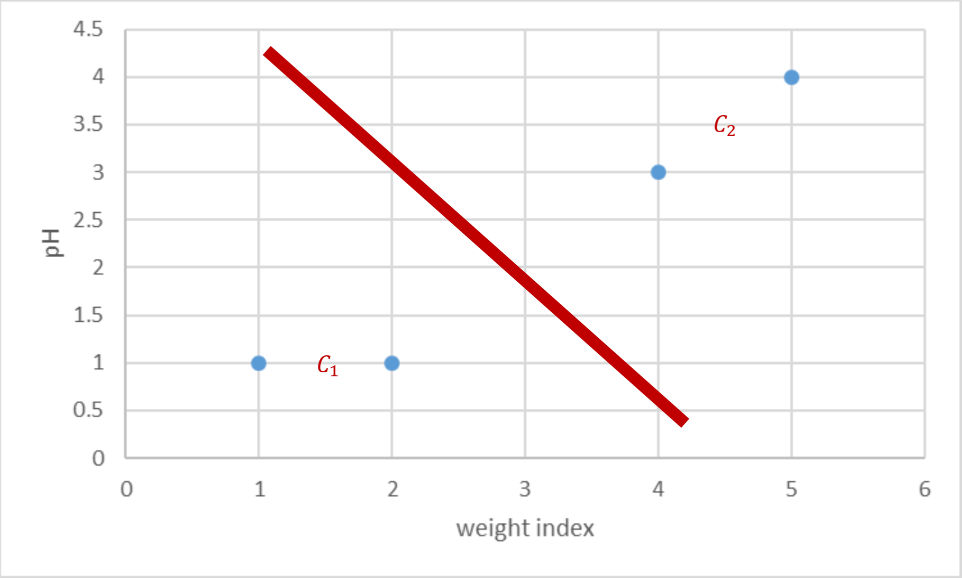
$$\begin{array}{cccc} A & B & C & D \end{array}$$

$$G^2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{array}{l} group\ 1 \\ group\ 2 \end{array}$$

$$G^1 = G^2$$

The object does not move anymore, then k-mean clustering has reached its stability and no more iteration is needed.

An example of K-means clustering



	medicine A	medicine B	medicine C	medicine D
weight index	1	2	4	5
pH	1	1	3	4
Group or Class	1	1	2	2

K-means clustering in Python

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

K-means clustering in Python

```
from sklearn.cluster import KMeans
import numpy as np
X = np.array([[1, 2], [1, 4], [1, 0],
              [10, 2], [10, 4], [10, 0]])
kmeans = KMeans(n_clusters=2, random_state=0).fit(X)
kmeans.labels_
```

Set K = 2 clusters

Set random state = 0

array([1, 1, 1, 0, 0, 0])

```
kmeans.predict([[0, 0], [12, 3]])
```

Predict unlabeled data

array([1, 0])

```
kmeans.cluster_centers_
```

array([[10., 2.], [1., 2.]])

K-means clustering in Python

run kmean2.py

```
print(__doc__)


# Code source: Gaël Varoquaux
# Modified for documentation by Jaques Grobler
# License: BSD 3 clause

import numpy as np
import matplotlib.pyplot as plt
# Though the following import is not directly being used, it is required
# for 3D projection to work
from mpl_toolkits.mplot3d import Axes3D

from sklearn.cluster import KMeans
from sklearn import datasets

np.random.seed(5)

iris = datasets.load_iris()
X = iris.data
y = iris.target

estimators = [('k_means_iris_8', KMeans(n_clusters=8)),
              ('k_means_iris_3', KMeans(n_clusters=3)),
              ('k_means_iris_bad_init', KMeans(n_clusters=3, n_init=1,
                                               init='random'))]
```

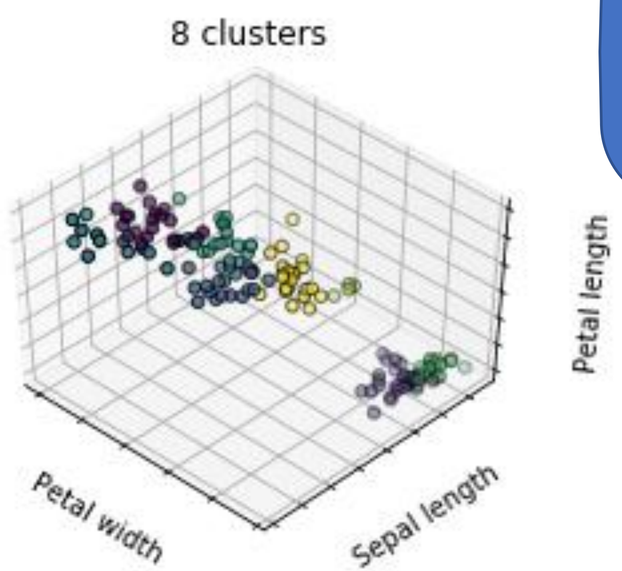
K-means clustering in Python

Set K = 8 clusters:

KMeans(n_clusters=8)

Confusion Matrix

```
[[ 0 28  0  0  0 22  0  0]
 [ 0  0 20  0  3  0  4 23]
 [22  0  0 12 15  0  0  1]
 [ 0  0  0  0  0  0  0  0]
 [ 0  0  0  0  0  0  0  0]
 [ 0  0  0  0  0  0  0  0]
 [ 0  0  0  0  0  0  0  0]
 [ 0  0  0  0  0  0  0  0]]
```



K-means clustering in Python

Set K = 3 clusters:

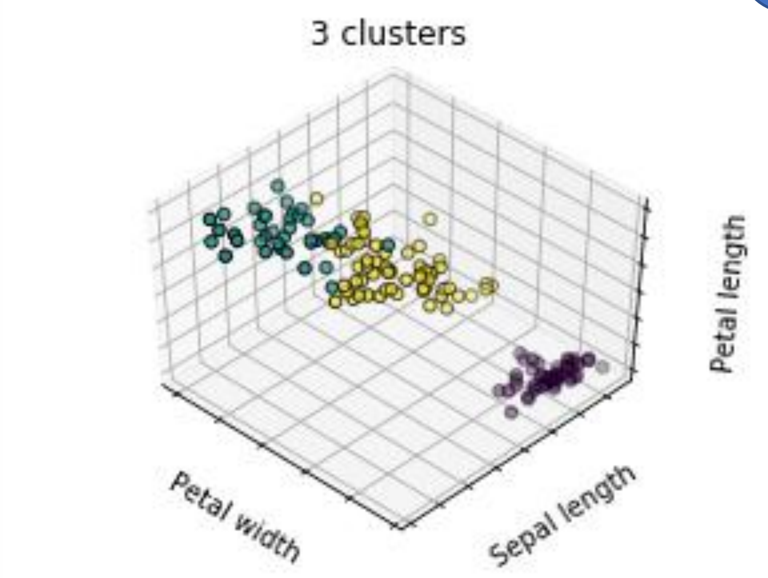
KMeans(n_clusters=3)

Confusion Matrix

[[50 0 0]

[0 2 48]

[0 36 14]]



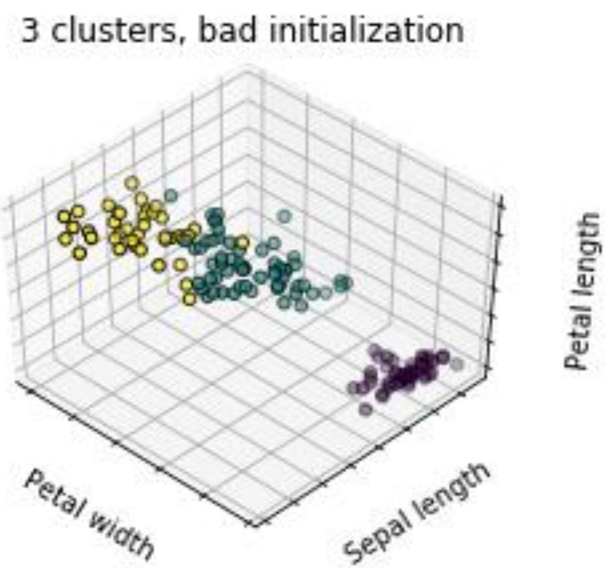
K-means clustering in Python

Set K = 3 clusters with bad initialization

KMeans(n_clusters=3, n_init=5, init='random')

A Bad initialization is on the classification process:
By setting n_init to only 5 (default is 10), the amount of times that the algorithm will be run with different centroid's initialization is reduced.

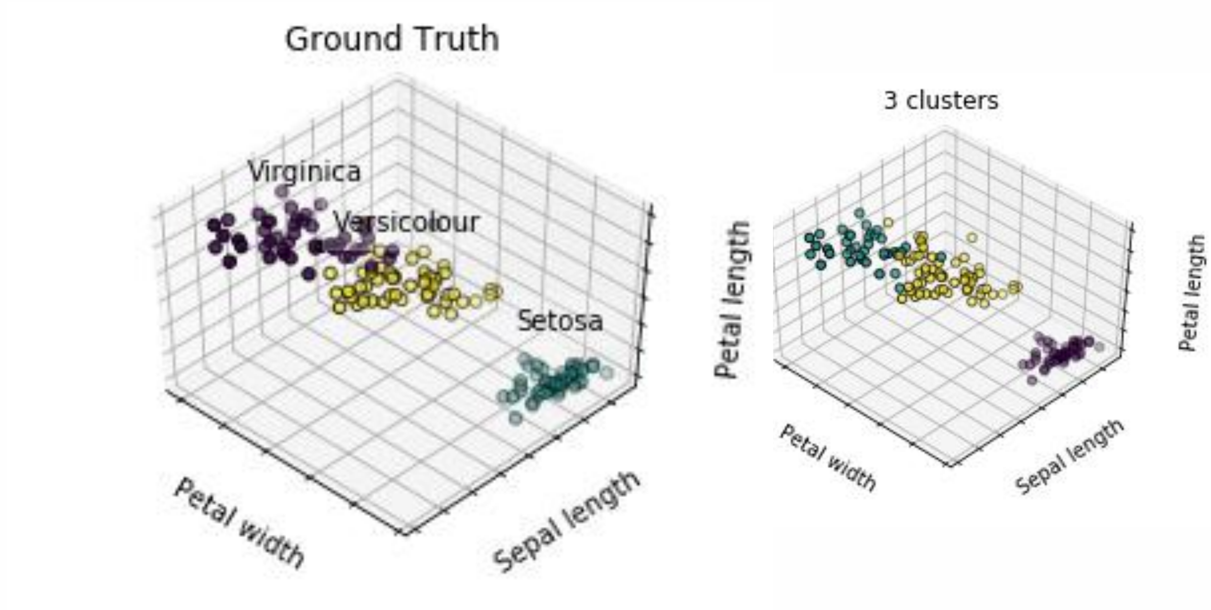
Note: Run only 5 times and select the best on



Confusion Matrix
[[0 0 50]
[2 48 0]
[36 14 0]]

K-means clustering in Python

The comparison between K-Means clustering at K = 3 and the Ground Truth (Real labeled data)



Introduction of "K" estimation techniques

a) Applied a Hierarchical Clustering

b) Applied an elbow plot

Hierarchical Clustering in Python

1. Compute distance between every pairs of point/cluster
   - Distance between point is just using the distance function
   - Compute distance between point X to cluster A may involve many choices (such as the min/max/average distance between the point X and points in the cluster A
   - Compute distance between cluster A and the other from cluster B and then pick either min/max/average of these pairs
2. Combine the two closet point/cluster into a cluster, Go back to 1) until only one big cluster remains

https://docs.scipy.org/doc/scipy/reference/generated/scipy.cluster.hierarchy.linkage.html

Hierarchical Clustering in Python

```
from sklearn import datasets
from scipy.cluster.hierarchy import dendrogram, linkage
from matplotlib import pyplot as plt
iris = datasets.load_iris()
X = iris.data

linked = linkage(X, 'single')
labelList = range(150)
plt.figure(figsize=(10, 7))
dendrogram(linked,
           orientation='top',
           labels=labelList,
           distance_sort='descending',
           show_leaf_counts=True)
plt.show()
```

Single assign to cluster (one centroid)

labeling all 150 points

Figure size 10 * 7

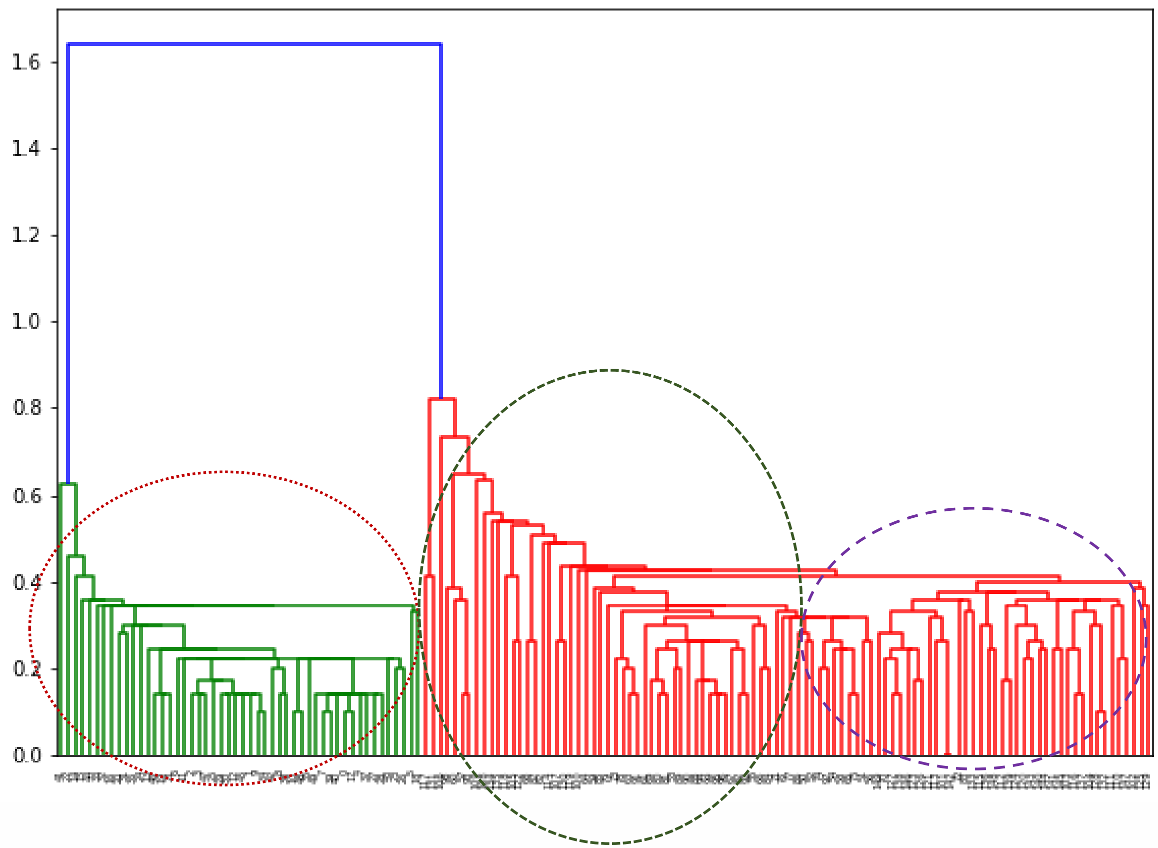
Plots the root at the top, and plot descendent links going downwards

The child with the maximum distance between its direct descendents is plotted first

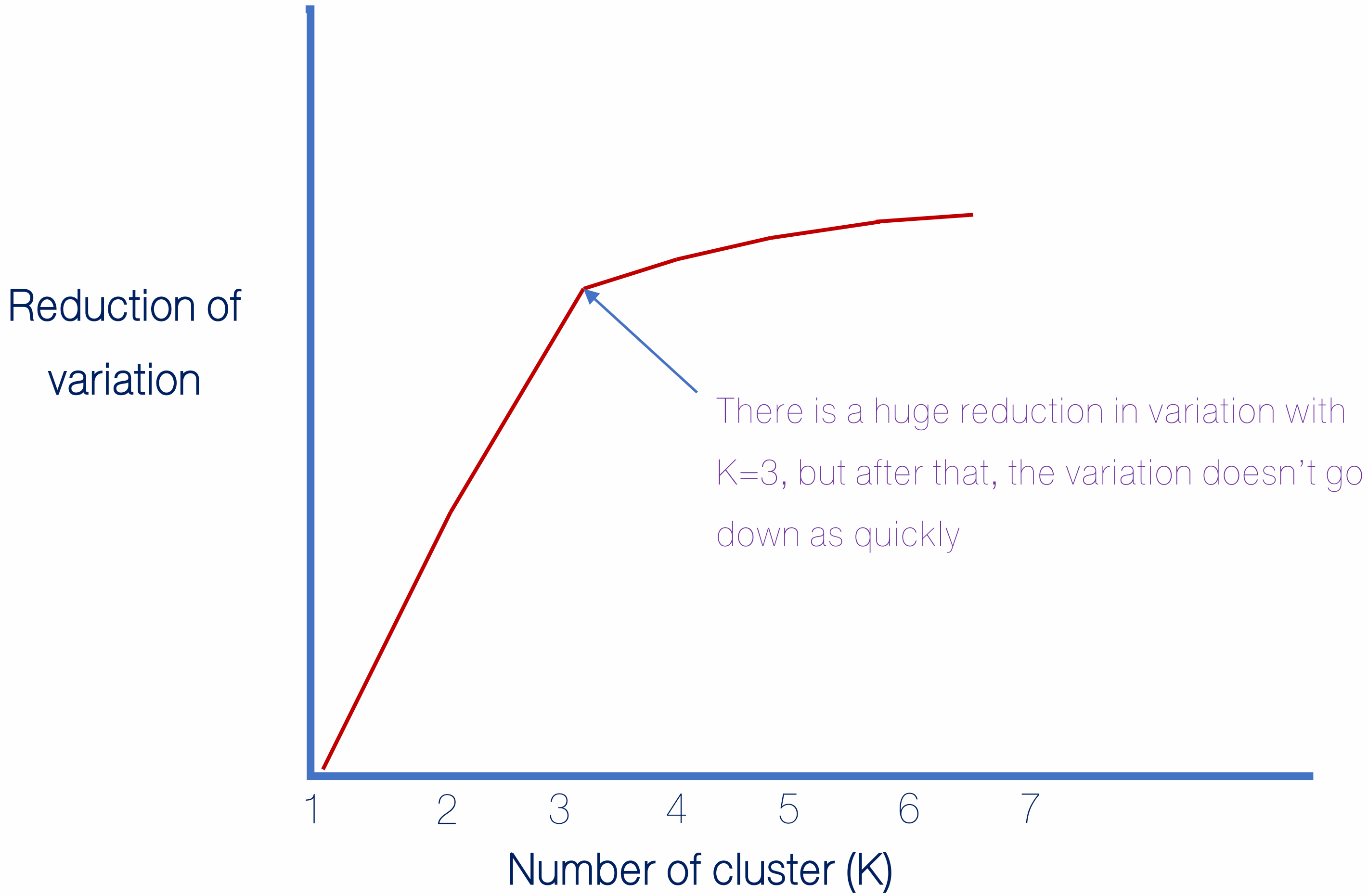
leaf nodes representing k>1 original observation are labeled with the number of observations they contain in parentheses.

Estimate a value of K by using a hierarchical clustering

Three big hierarchies



Pick up "K" by finding the elbow in the plot



Assignment:

Due date: November 21, 2022 (10 points)

Find (by manual and show calculation steps) the appropriate centroids by using a K-means clustering with Euclidean distance (K = 2)

Samples	S1	S2	S3	S4	S5	S6
Feature #1	1	2	1	5	4	5
Feature #2	1	1	3	2	3	4

Samples	STU#1	STU#2	STU#3	STU#4	STU#5	STU#6
C1	(1,1)	(2,1)	(5,2)	(5,2)	(4,3)	(2,1)
C2	(1,3)	(1,3)	(4,3)	(5,4)	(4,4)	(5,2)