HUGE

Hello

Clustering

2018

Agenda.

1. Introduction
2. Purpose.
3. Why and when?
4. Approaches
5. Validation

Who am I?

William Gómez
Web Engineer at HUGE

Ph.D. Student at Universidad de Antioquia

Adjunct professor at Universidad de Antioquia

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Introduction

Artificial intelligence

Study of design of intelligence agents to create machines that can mimic human intelligence.

Soft computing

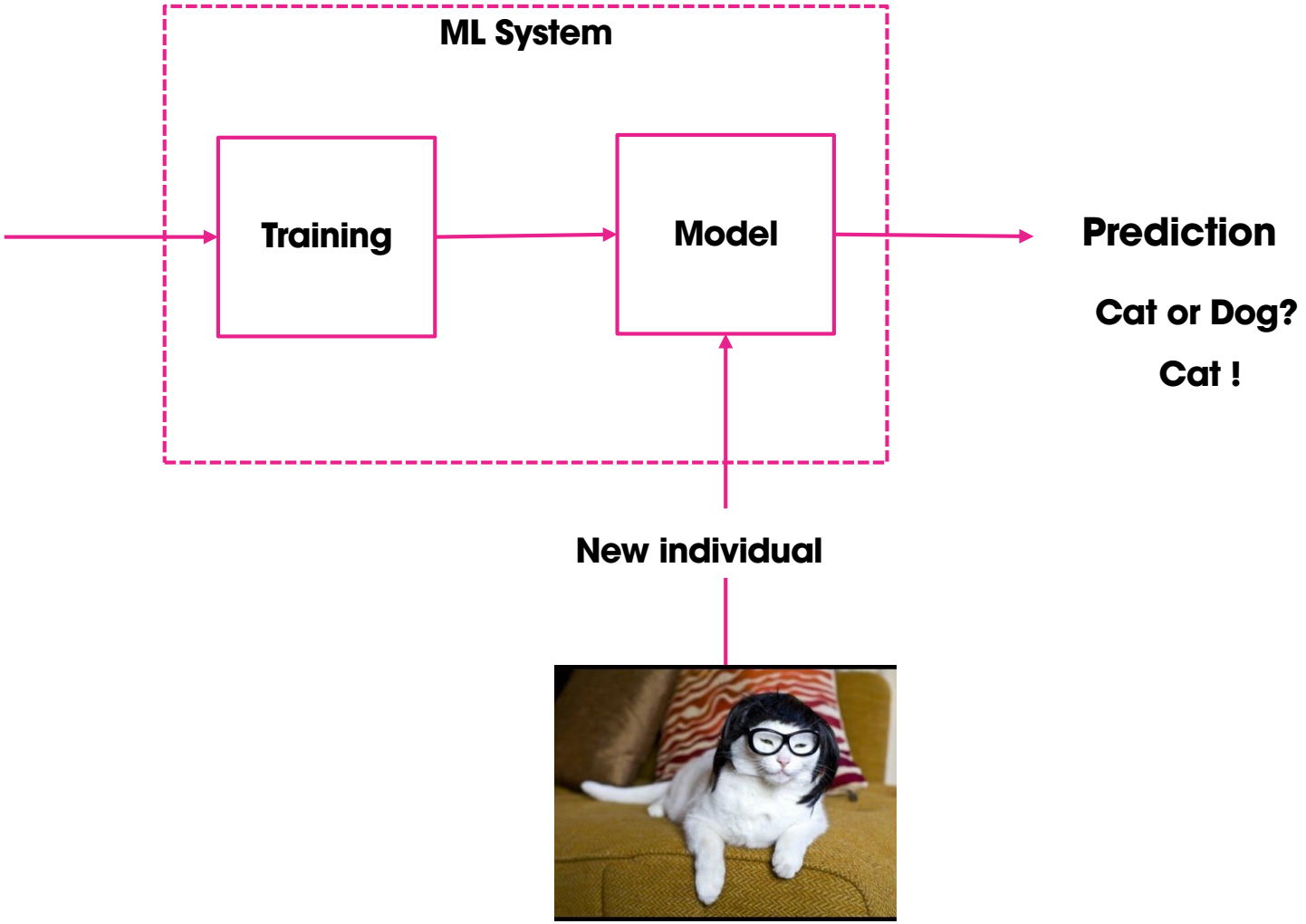
It is a subdiscipline of AI that focuses on heuristics, imperfect solutions to complex problems. Uncertainty.

Machine Learning

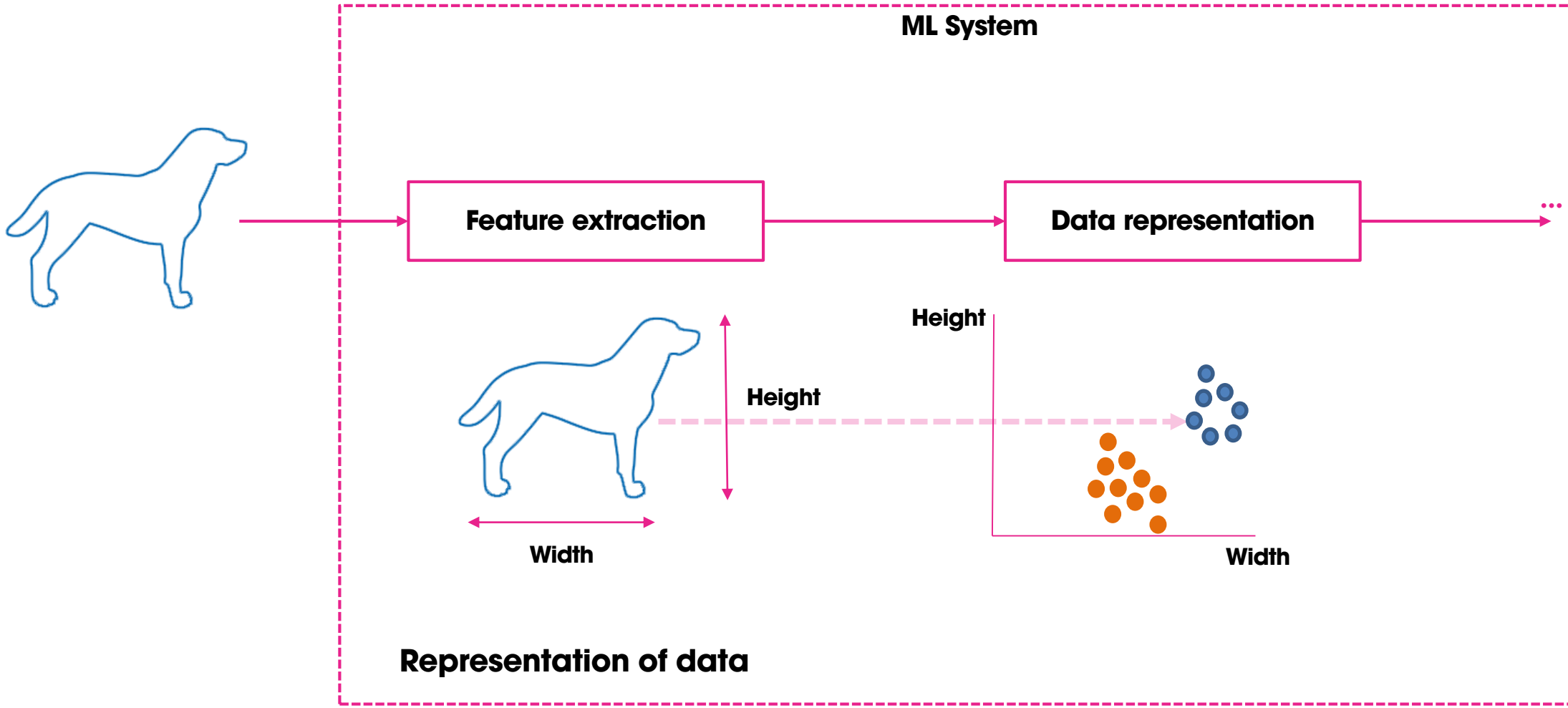
To make the machine learn by itself to solve the problems using a large quantity of data.

So what is ML actually?

Samples used to learn



How can ML be seen?



How can ML be seen?

ML System

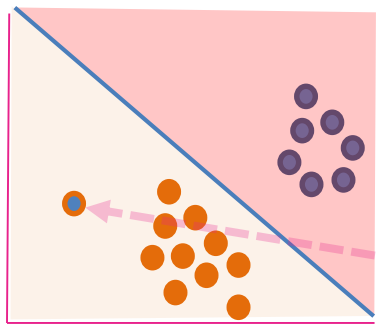
Algorithm (Training)

Model

Prediction

Cat or Dog?

Cat !



New individual

Supervised

There is an expert knowledge that is desired to be reproduced.

Labels

$$f^*\left(\begin{bmatrix}\vec{X}_1\\ \vec{X}_2\\ \vdots\\ \vec{X}_k\end{bmatrix}, \begin{bmatrix}y_1\\ y_2\\ \vdots\\ y_k\end{bmatrix}\right) = \begin{bmatrix}y_1^*\\ y_2^*\\ \vdots\\ y_k^*\end{bmatrix} \qquad \min\left(\begin{bmatrix}y_1^*\\ y_2^*\\ \vdots\\ y_k^*\end{bmatrix} - \begin{bmatrix}y_1\\ y_2\\ \vdots\\ y_k\end{bmatrix}\right)$$

Prediction

Unsupervised

There is no labeling or expected structure of the data.

$$f\begin{bmatrix}\vec{X}_1\\ \vec{X}_2\\ \vdots\\ \vec{X}_k\end{bmatrix} = \begin{bmatrix}y_1\\ y_2\\ \vdots\\ y_k\end{bmatrix}$$

~~Labels~~

Prediction, Hypothesis, Clustering, Patterns

2

Clustering and Purpose

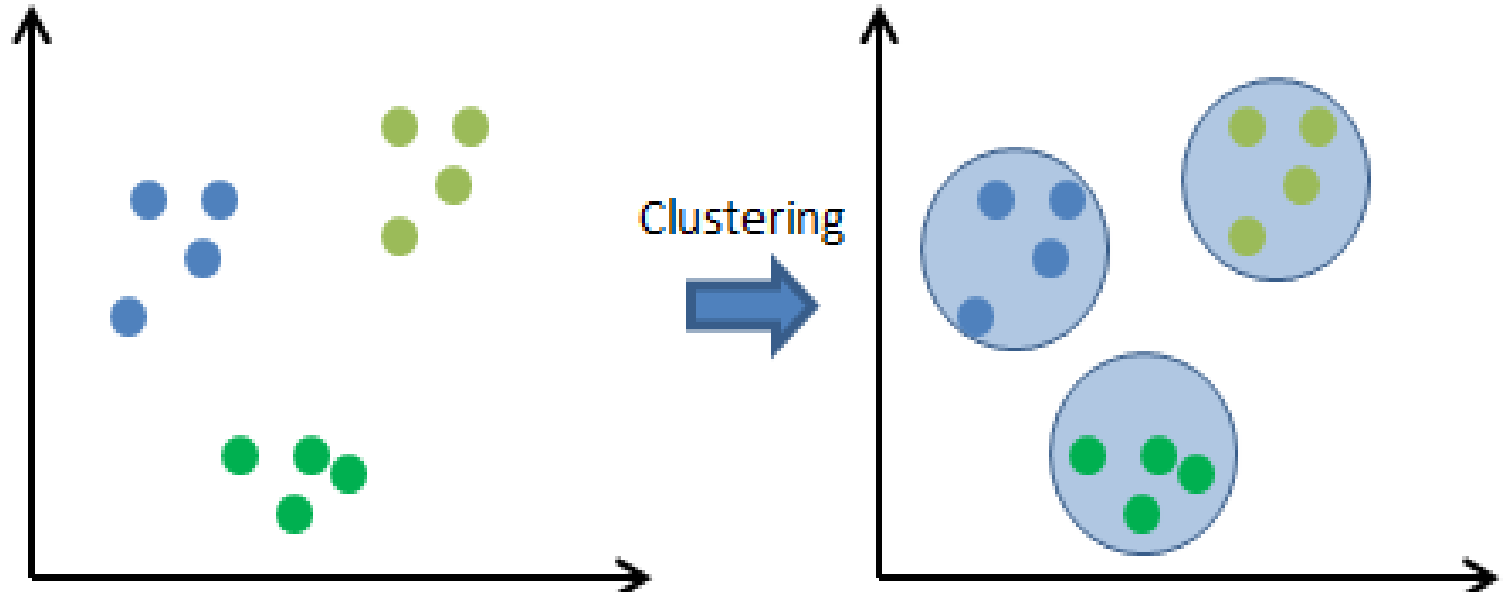
Clustering

Among the unsupervised learning, algorithms are clustering algorithms.

These focus on grouping objects according to their intrinsic characteristics or similarities.

Clustering algorithms aim to find the structure of the data.

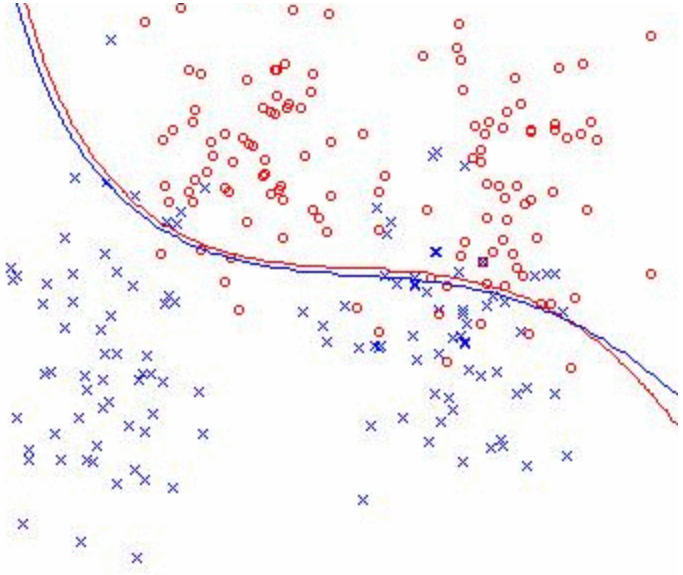
Clustering



Clustering advantages

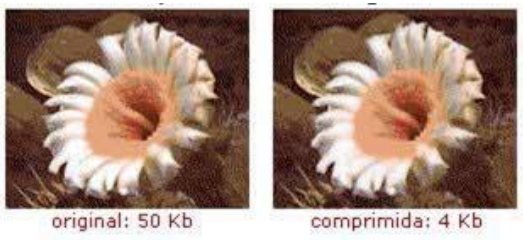
As the elements belonging to a cluster are similar, the prototype of a cluster allows us to make a synthesis of the elements in it.

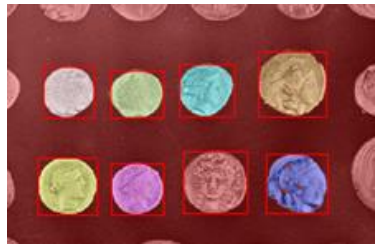
Discovering groups even in predefined classes.

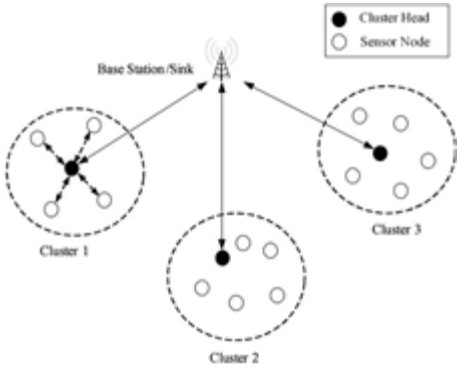


Applications

Data compression.
Image segmentation.
Controllers syntonization.
Grouping of search engine results.
Speaker segmentation.
Multivariate statistics.







3

Why and when?

Why and when?

Data labeling don’t always represents the actual structure of the data.

Why and when?

For example: We can have a dataset with dogs and cats, the labeling tells us that there are only two classes.
However, after applying a clustering algorithm, it is discovered that the cat class is composed of 4 groups of cats.
Not only these insights can be obtained, but also which groups of cats are similar to which group of dogs, and the reasons.

Why and when?

Data labeling is not always possible to be obtained.

Imagine a dataset with 10.000.000.000 records (not very to obtain difficult currently). How much time would require to label this data?

Why and when?

Suppose you have a dictionary of 10000 words (it can be a dictionary of colors, features, keys). It can be reduced using clustering, grouping words and obtaining a representative word of each group.

Yes! You have done data compression.

Why and when?

Semi-supervised approach:

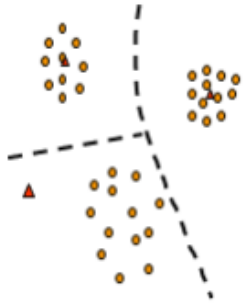
Suppose you have the dataset of Netflix movies. You have the score of only few movies (labeling). How can you assign to the other movies a label? Apply a clustering algorithm to the movies and obtain a label for each of them.

4

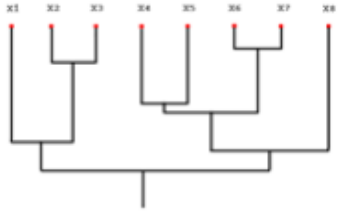
Approaches

Approaches

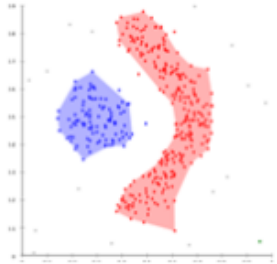
Partitioning-based



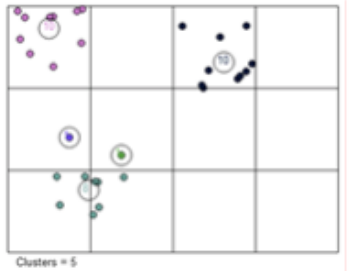
Hierarchical-based



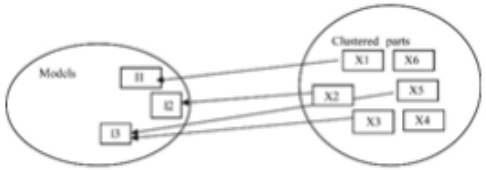
Density-based



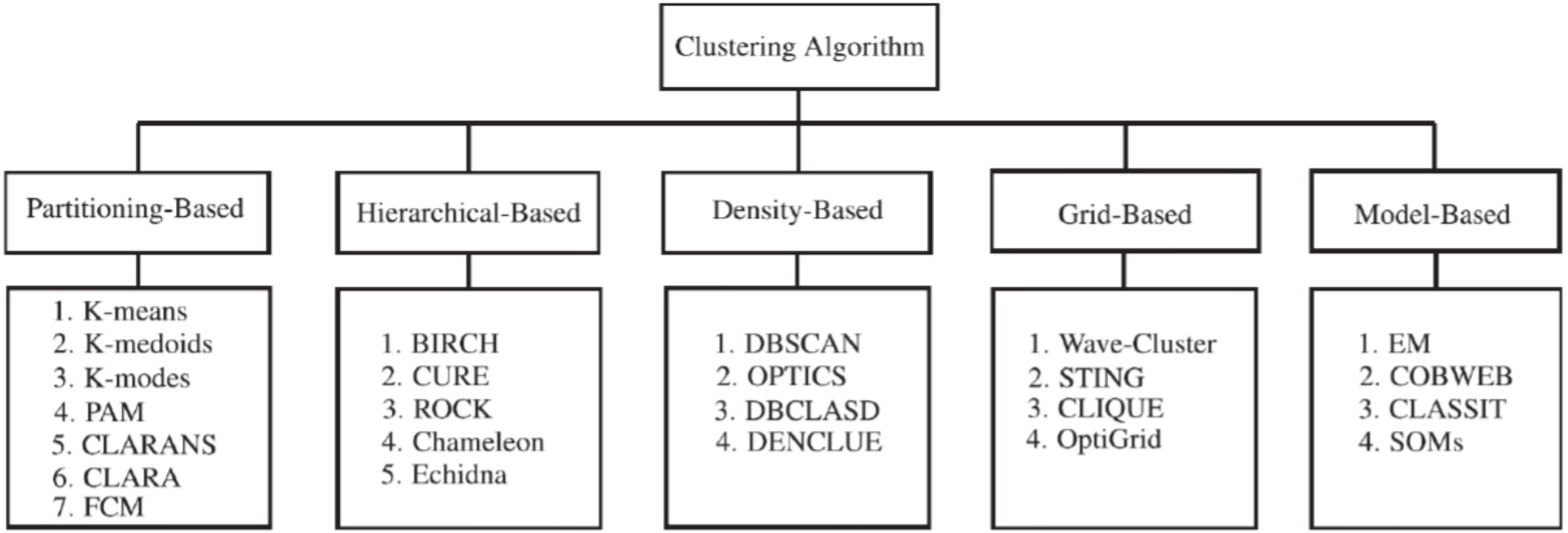
Grid-based



Model-based



Algorithms

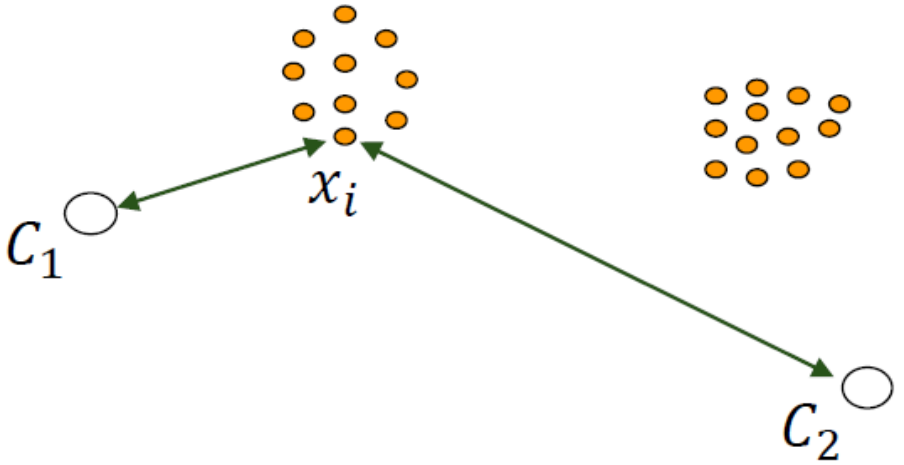

Clustering Algorithm
Partitioning-Based
1. K-means
2. K-medoids
3. K-modes
4. PAM
5. CLARANS
6. CLARA
7. FCM
Hierarchical-Based
1. BIRCH
2. CURE
3. ROCK
4. Chameleon
5. Echidna
Density-Based
1. DBSCAN
2. OPTICS
3. DBCLASD
4. DENCLUE
Grid-Based
1. Wave-Cluster
2. STING
3. CLIQUE
4. OptiGrid
Model-Based
1. EM
2. COBWEB
3. CLASSIT
4. SOMs

K-Means

This algorithm aims to partitioning a set of m objects in k groups/clusters.

Each observation belongs to the nearest cluster.

A similarity metric must to be defined



K-Means: Steps

1. Create k random centroids.

Each centroid is a vector of the shape (1,p).

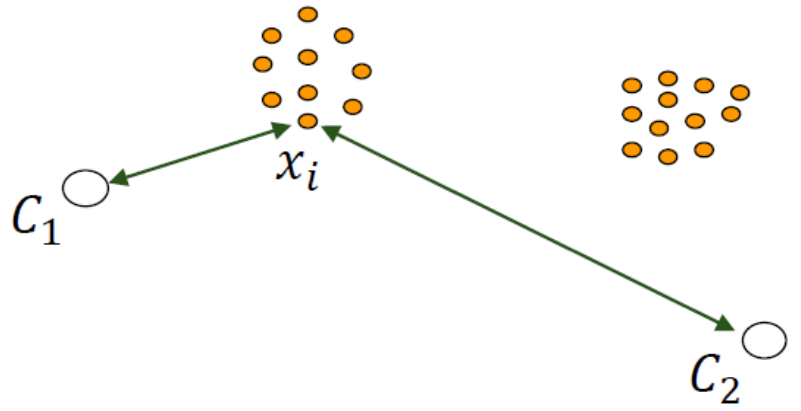
p is the number of descriptors (features)

$$X = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,p} \\ x_{2,1} & x_{1,2} & \cdots & x_{2,p} \\ \vdots & \vdots & & \vdots \\ x_{N,1} & x_{N,2} & \cdots & x_{N,p} \end{bmatrix}$$

$$C_1 = \begin{bmatrix} c_{1,1} & \cdots & c_{1,p} \end{bmatrix}$$
$$\vdots$$
$$C_k = \begin{bmatrix} c_{k,1} & \cdots & c_{k,p} \end{bmatrix}$$

K-Means: Steps

2. Measure the distance of each sample to the cluster centroids.



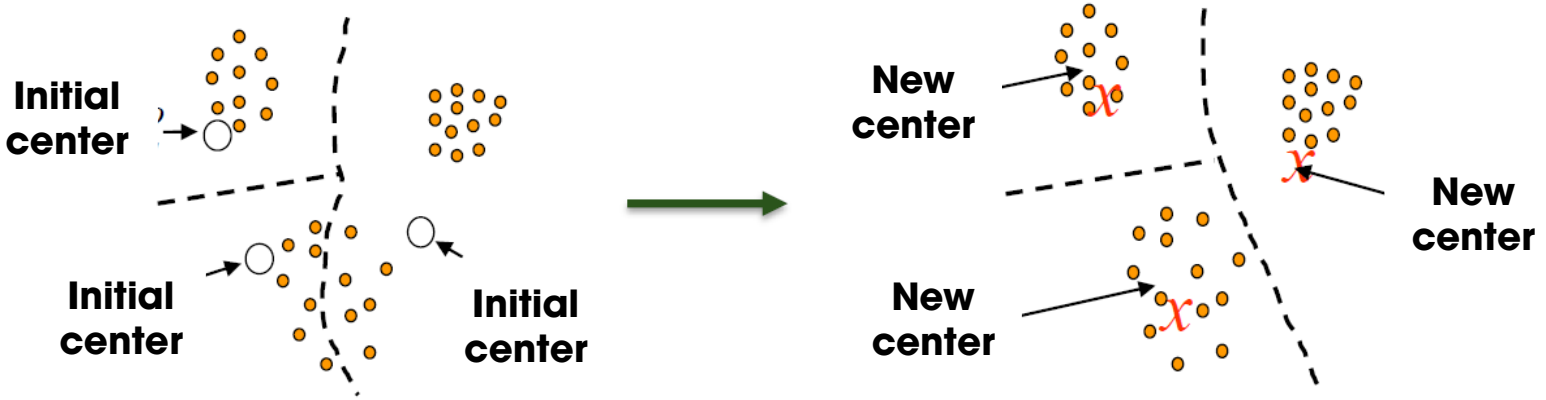
Let's use the Euclidean distance.

$$d_{i,j} = \|x_i - C_j\| = \sqrt{(x_{i,1} - c_{j,1})^2 + \ldots + (x_{i,p} - c_{j,p})^2}$$

K-Means: Steps

3. Recompute the centroids using the mean of the samples assigned to that cluster.

$$C_j = \frac{1}{n_j} \sum_{x_i \in C_j} x_i$$



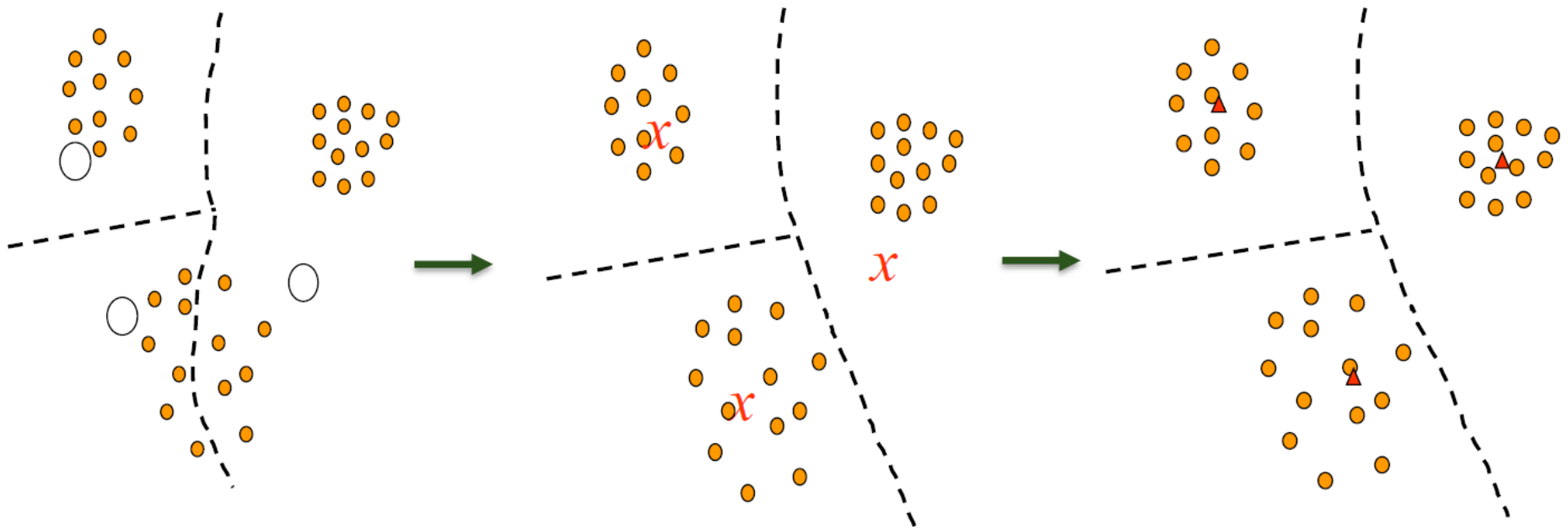
K-Means: Steps

3. Check if the stopping rule is achieved.

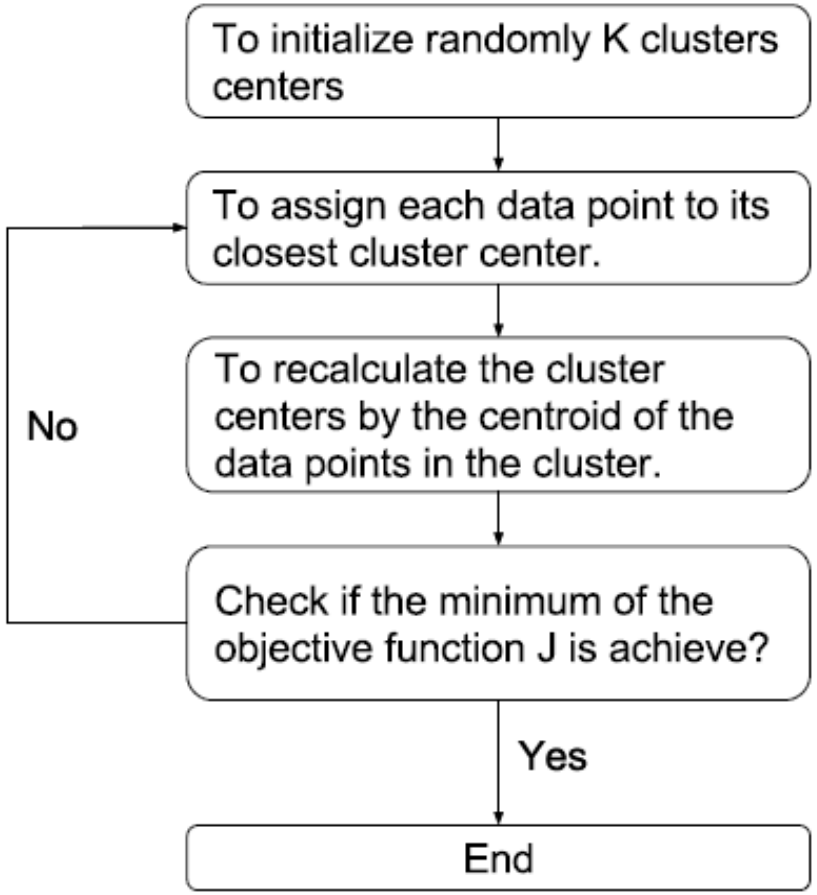
$$S = \sum_{j} \sum_{x_i \in C_j} \|x_i - C_j\|$$

If S stops decreasing.

K-Means: Graphically



K-Means: Flow and Python




```
Clusters = np.random.rand(nclusters, data.shape[1])
```

```
for m in range(iterations):
 for i in range(data.shape[0]):
  distances =
    np.linalg.norm(Clusters - data[i,:], axis = 1)
  assign[i] = np.argmin(distances)
```

```
for j in range(nclusters):
  ind = assign == j
  Clusters[j, :] = np.mean(data[ind, :], axis = 0)
```

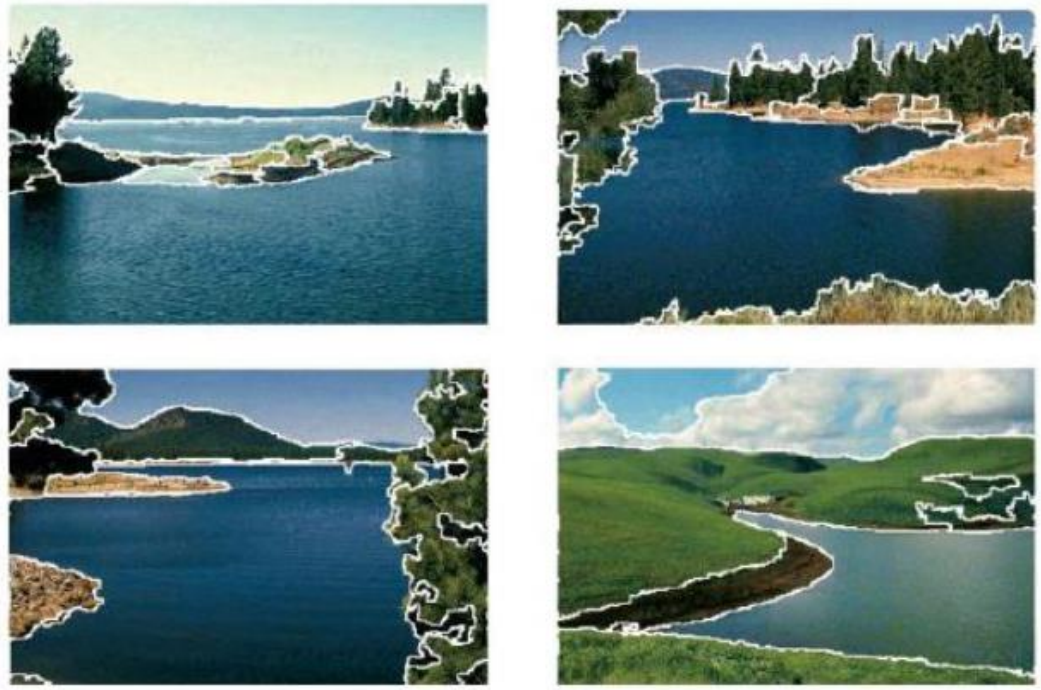
```
for j in range(nclusters):
  ind = assign == j
  distances =
    np.linalg.norm(Clusters[j, :] - data[ind,:], axis = 1)
  J += np.sum(distances)

  if (abs(J - Jprev) < 0.01):
     return assign, Clusters
```

K-Means: Image segmentation example

Segmentation:

Divide the image in regions/sequences with coherent properties

Let's do Color Segmentation.



K-Means: Image segmentation example

Segmentation:

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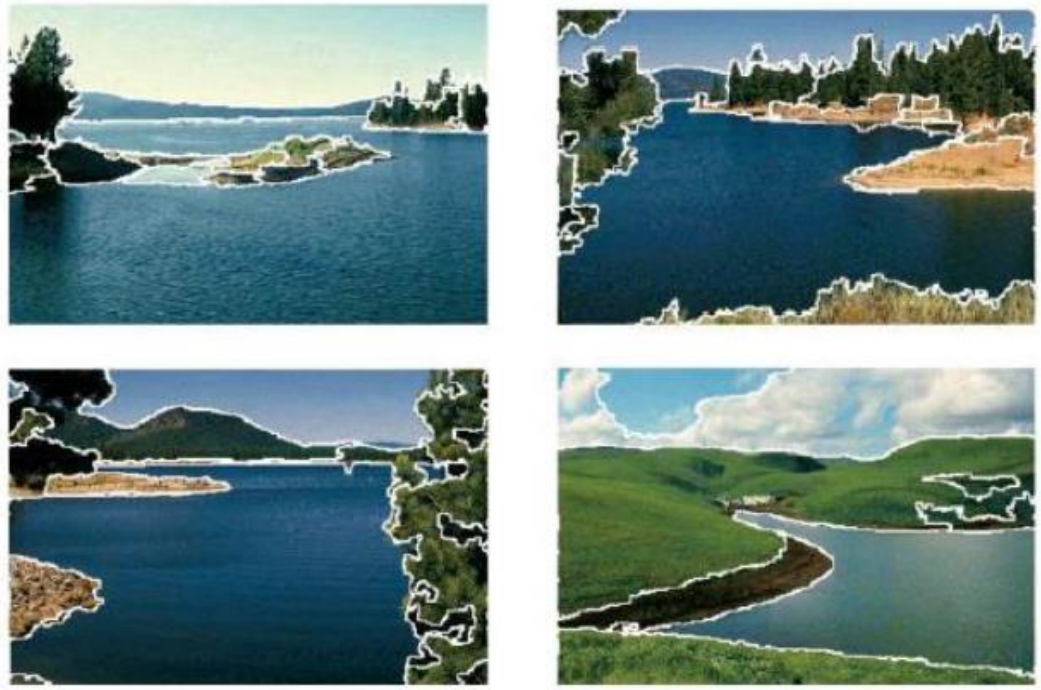
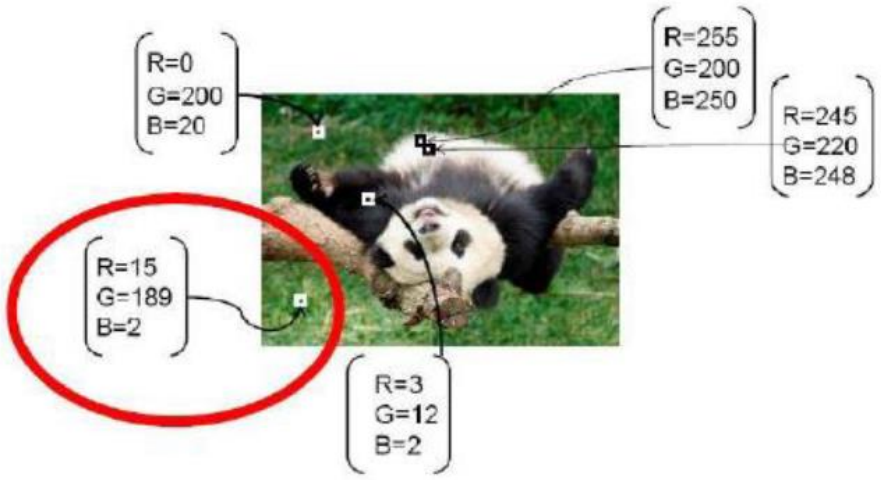
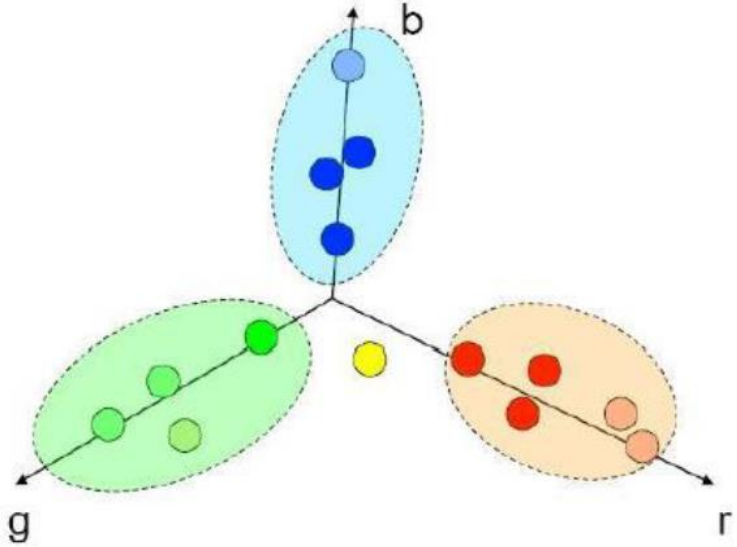


K-Means: Image segmentation example

Each pixel becomes a sample of three values (Red, Green, Blue).



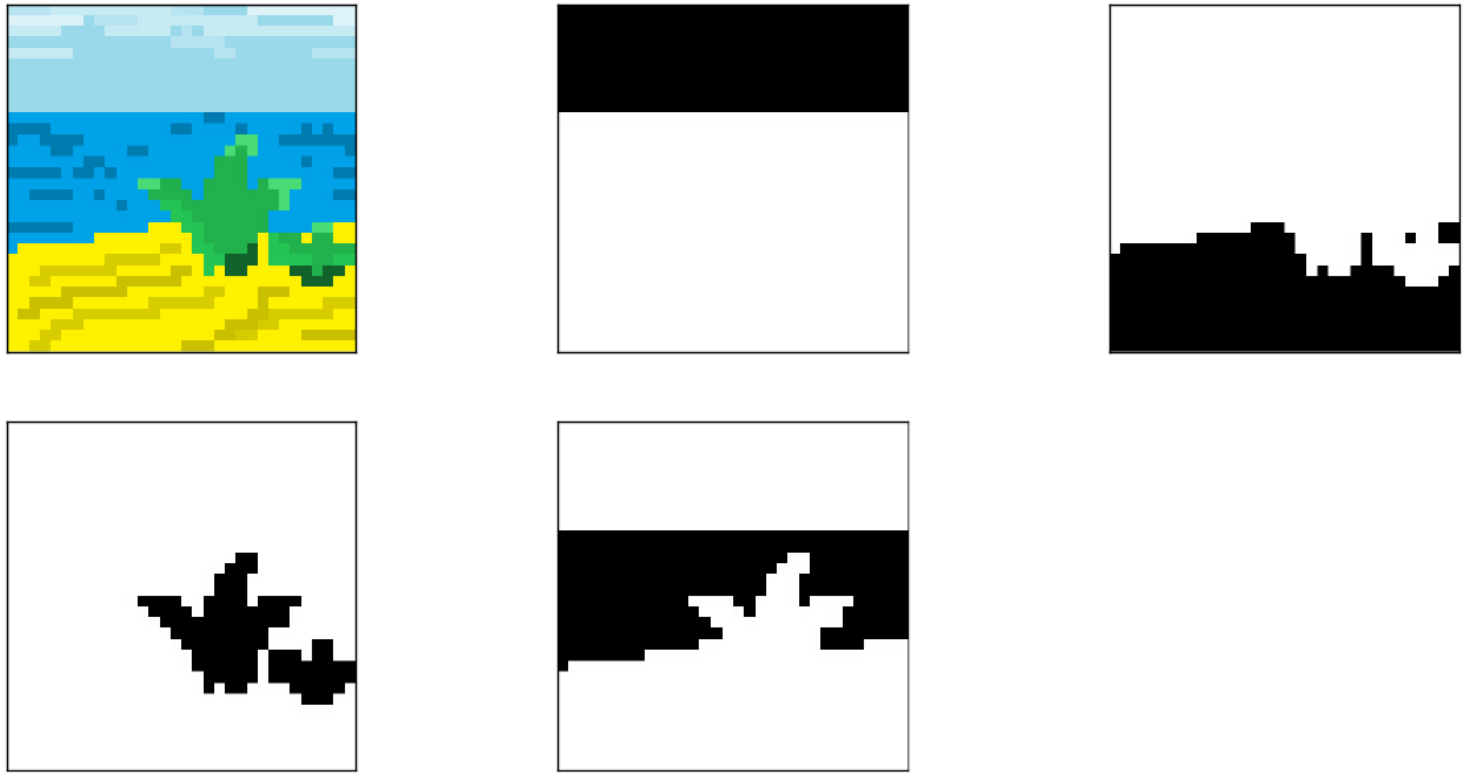


K-Means: Image segmentation example

To group regions also is important to add pixel's position information.

$$X = \begin{bmatrix} p_1 & R_1 & G_1 & B_1 \\ p_2 & R_2 & G_2 & B_2 \\ \vdots & \vdots & \vdots & \vdots \\ p_N & R_N & G_N & B_N \end{bmatrix}$$

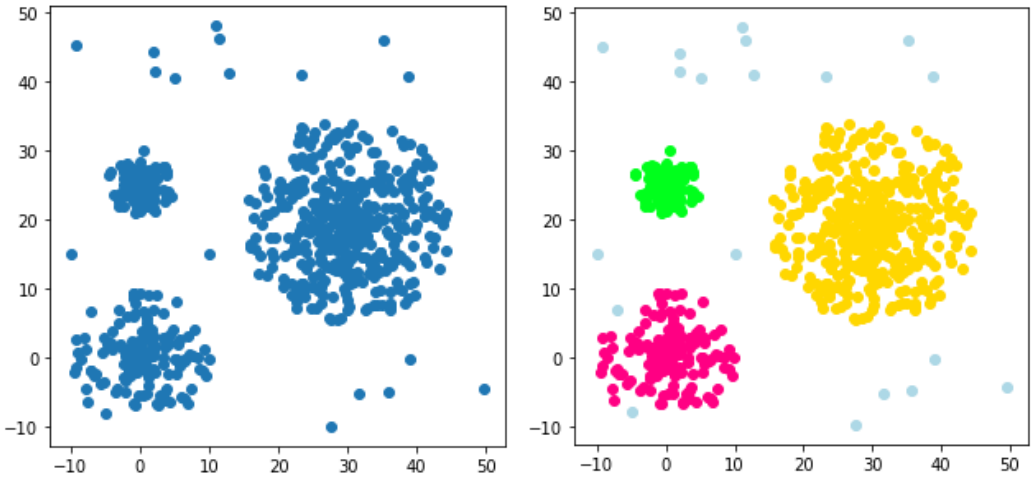
K-Means: Image segmentation example



DBSCAN

This algorithm estimates the density around each sample.

The idea is create clusters once the density around a group of points exceeds an threshold.

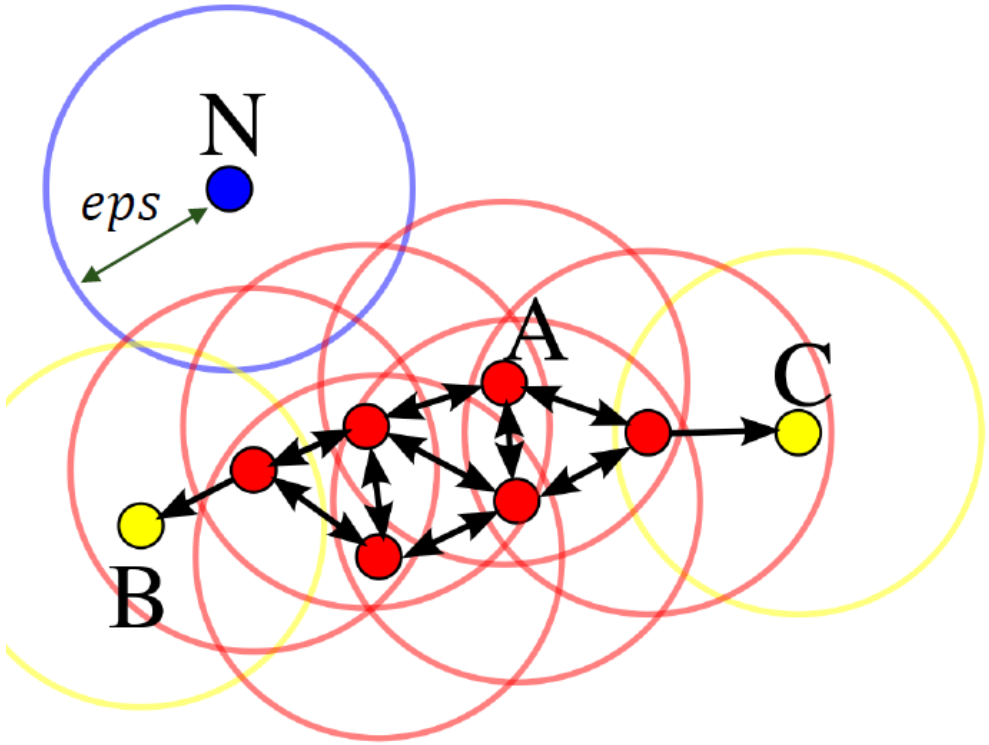


DBSCAN: Point classification

1. Nuclear points (A)
2. Boundary points (B, C)
3. Noisy points (N)

Two parameters:

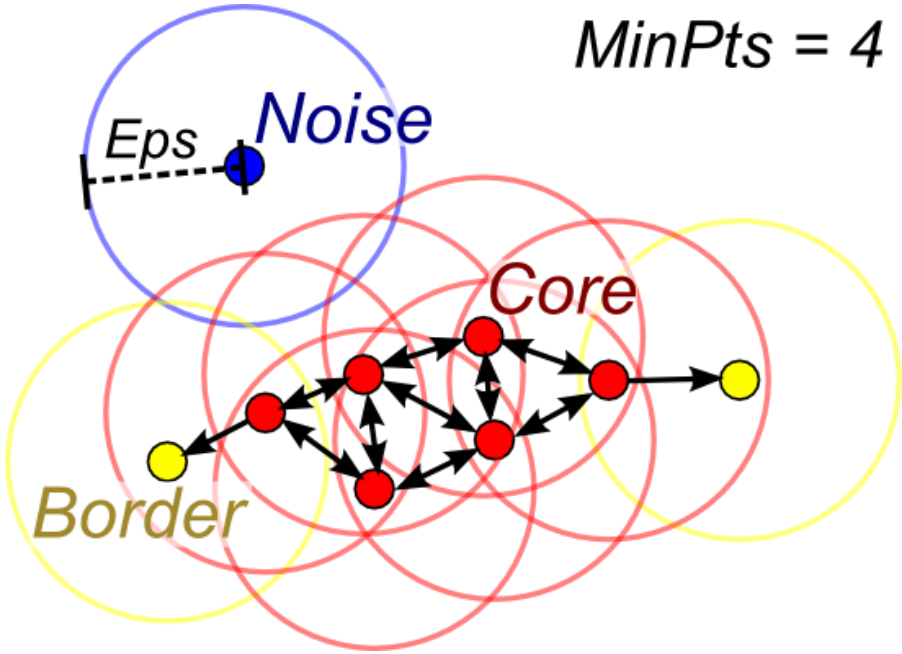
- eps: analysis radius.
- MinPts: Min number of points in the analysis radius.



DBSCAN: Steps

1. Select a random sample.

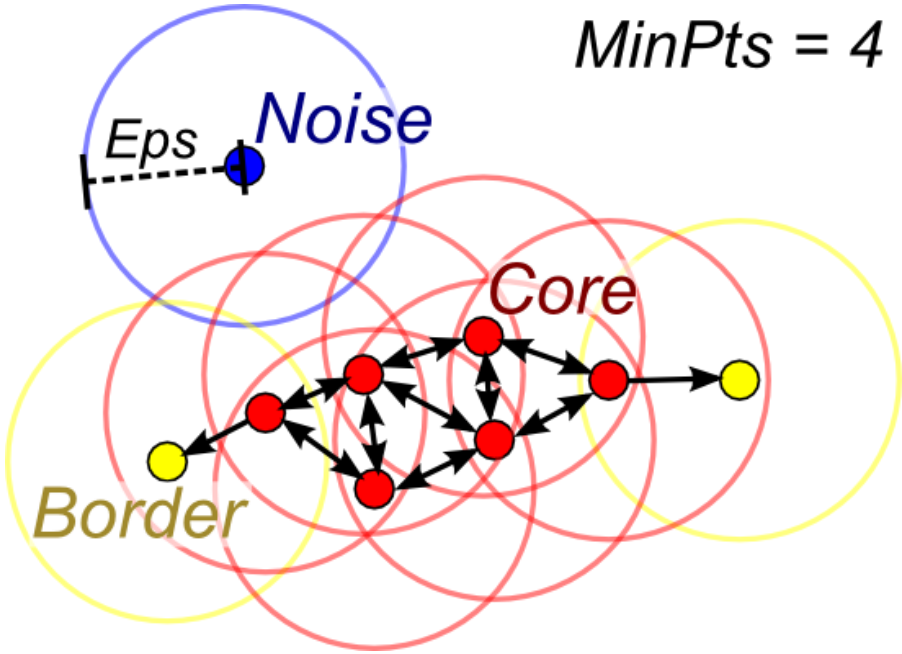
2. Checks if in the analysis radius (eps) there are more or equal number of points (MinPts).



DBSCAN: Steps

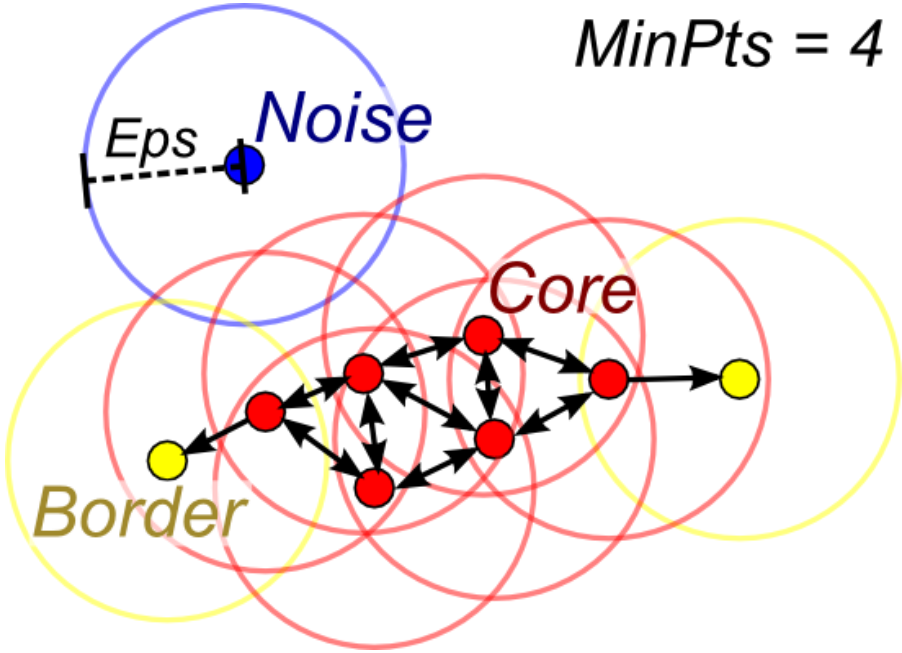
3. If the condition is fulfill a new cluster is created from this random point.

4. Check iteratively the points in the analysis radius.

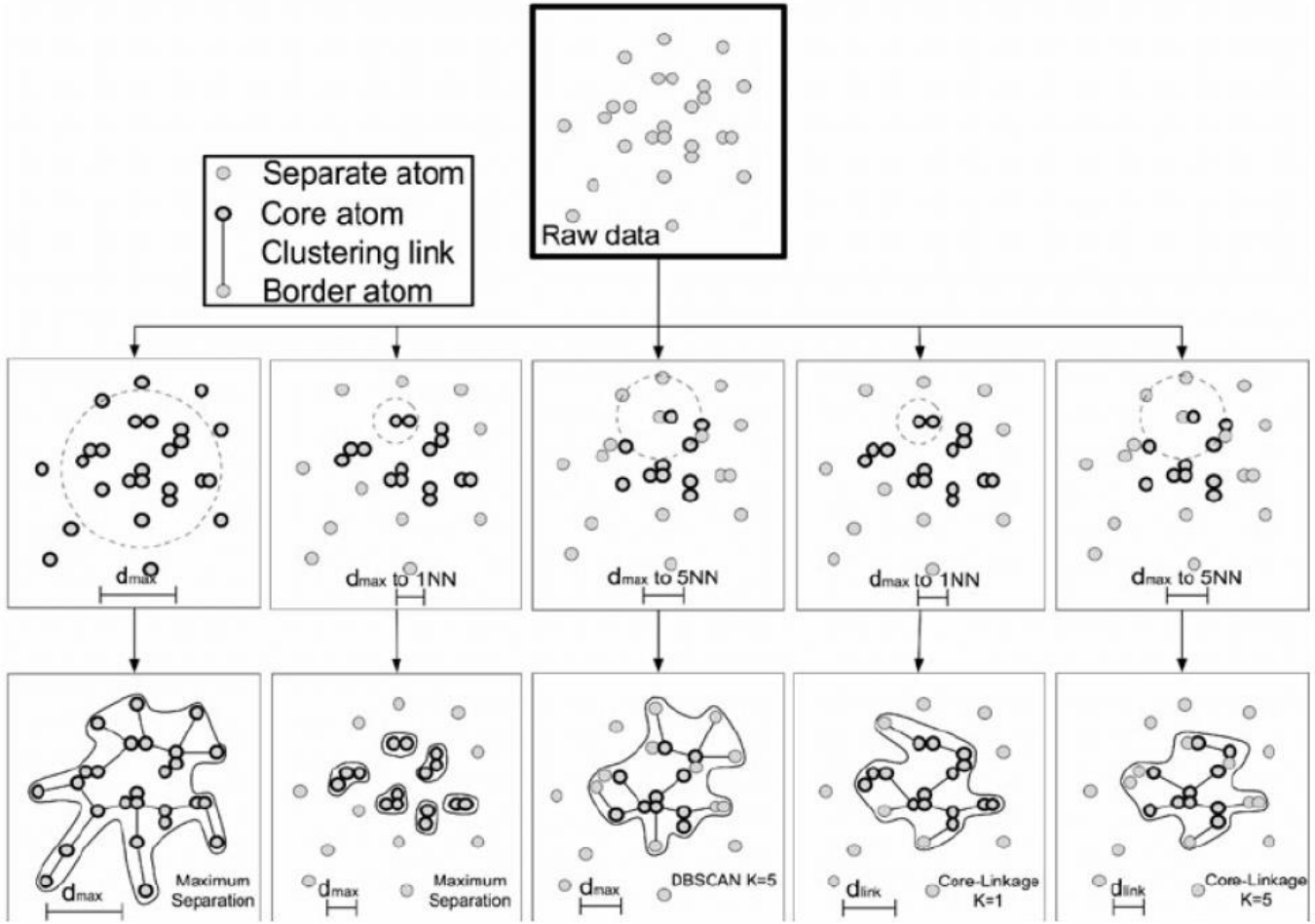


DBSCAN: Steps

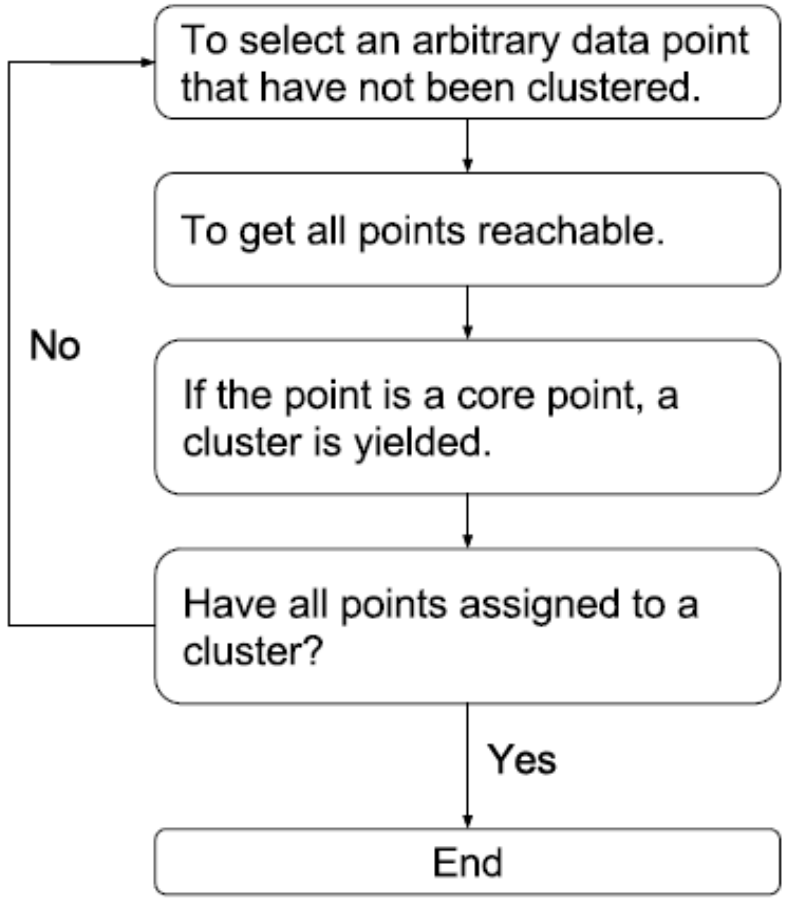
5. The new cluster is prolongated until no more points can be added to it.



DBSCAN: Graphically



DBSCAN: Flow and Python




```
while (len(clusteredPoints) != len(allPoints)):
 noClusteredPoints = np.setdiff1d(allPoints, clusteredPoints)
 index = np.random.choice(noClusteredPoints)
```

```
clusterIndices = np.array([index])
clusterIndices, alreadyChecked =
  self.CheckNeighbors(index, clusterIndices, alreadyChecked)
```

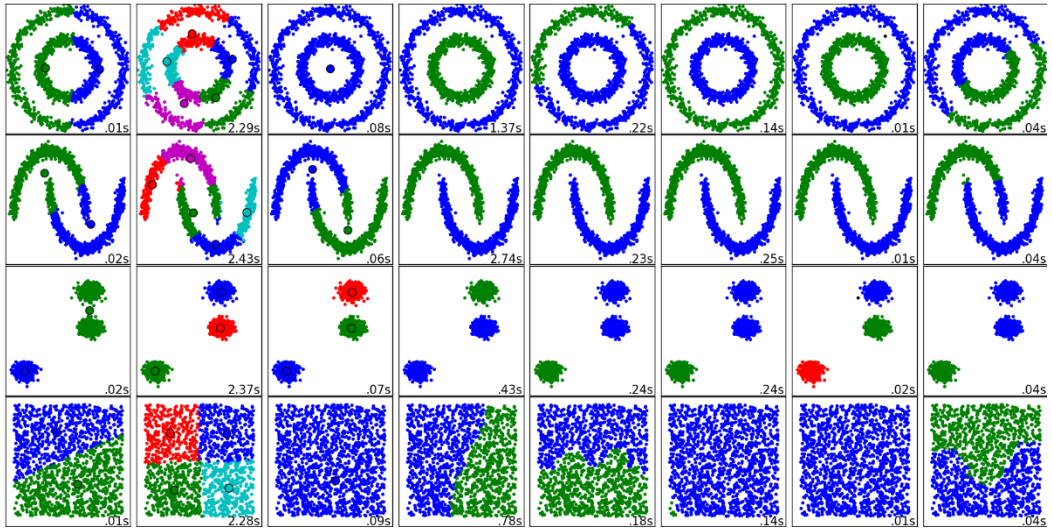
```
if (len(clusterIndices) >= self.minPts): #Nuclear Points
  self.assign[clusterIndices] = self.nclusters
  self.nclusters = self.nclusters + 1
else:
  self.assign[index] = -1 #Outlier, Noisy Point
```

5

Validation

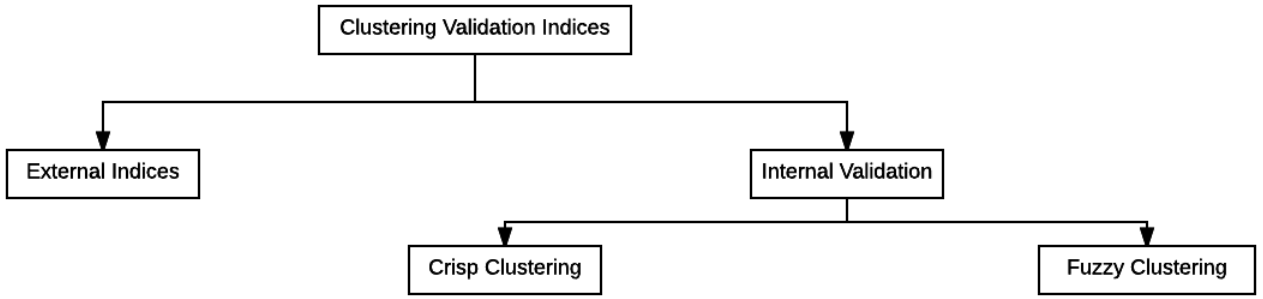
Validation problem

As there is no expected structure of the data, the evaluation of the quality of the data partitions becomes into a complicated task.



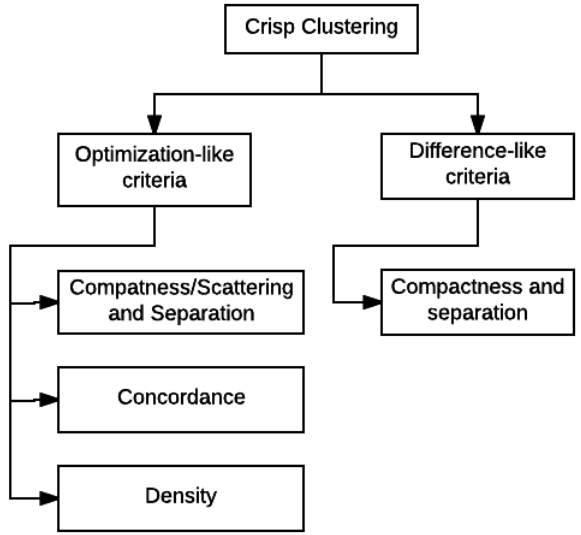
Validation indices

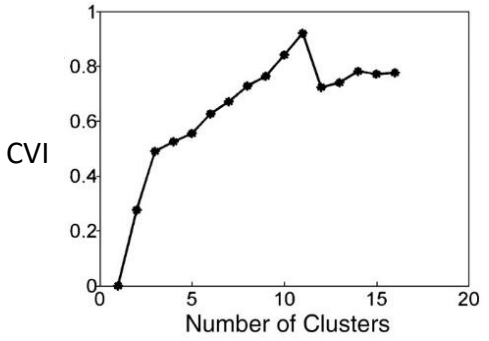
Validation indices are classified in two types: external criteria and internal criteria.

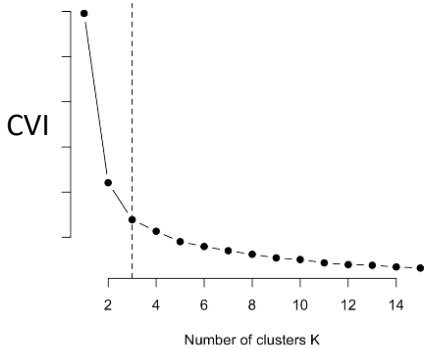


Validation indices

Several studies have compared clustering validation indices (CVIs) used in crisp clustering. None of these studies has been conclusive.







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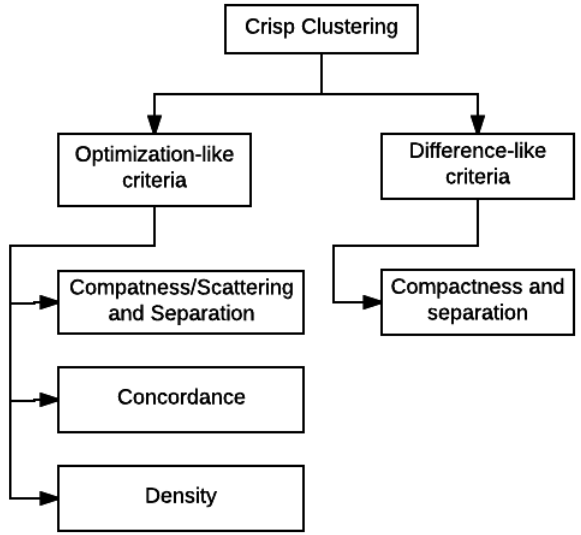
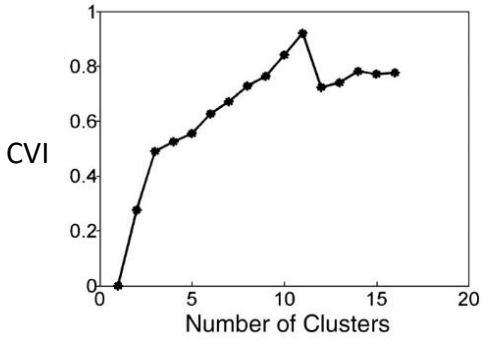
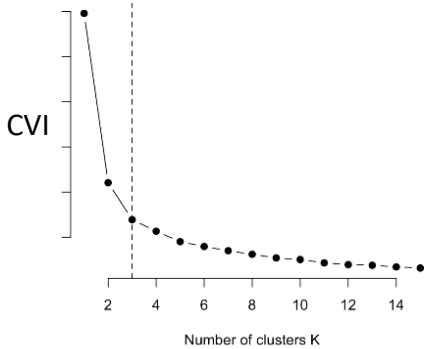
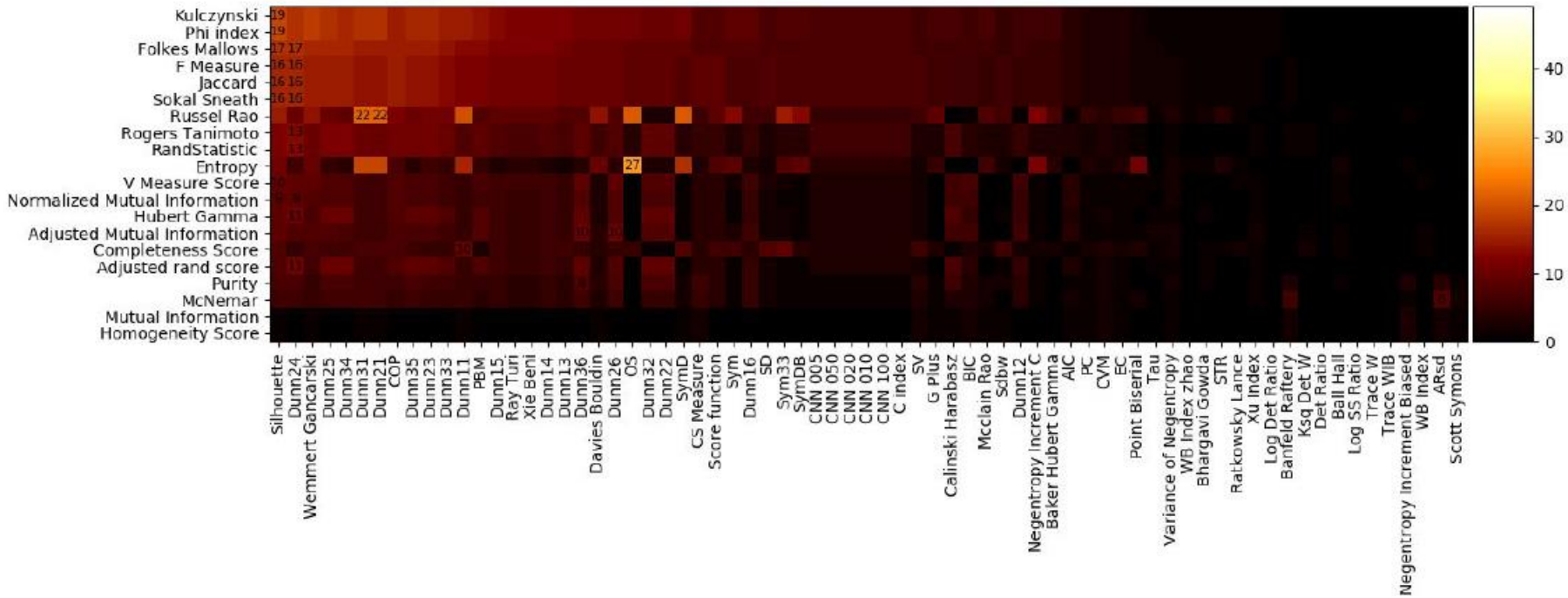






Work in progress

Validation library: 49 Datasets, 20 external indices and 72 external indices



Work in progress

Validation library:

https://github.com/williamegomez/Clustering-Validation-Indices