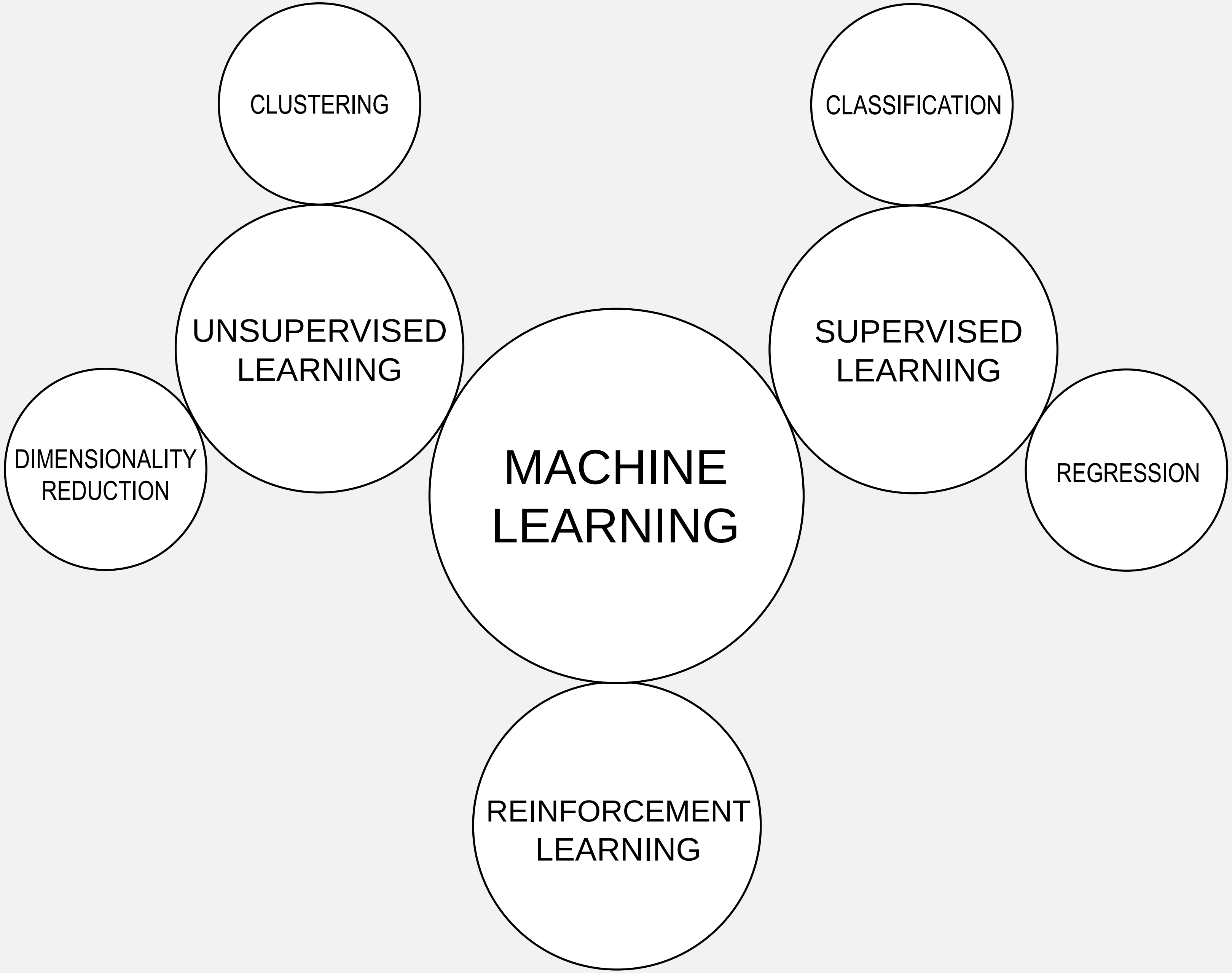
CLUSTERING

Lecture 10

MAL1, 2024


CLUSTERING
CLASSIFICATION
UNSUPERVISED LEARNING
SUPERVISED LEARNING
DIMENSIONALITY REDUCTION
MACHINE LEARNING
REGRESSION
REINFORCEMENT LEARNING

CLUSTERING

CLUSTERING

- What is clustering?
- *k*-means clustering
- Agglomerative clustering
- DBSCAN
- Application

WHAT IS CLUSTERING?

grouping data: unlabeled version of classification

↑

most data
in the world

REVERSE IMAGE SEARCH

I want to know what this bird in my garden is

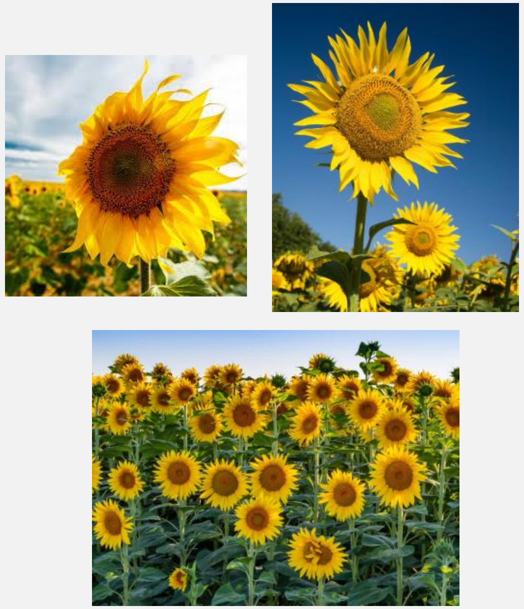
Google Lens

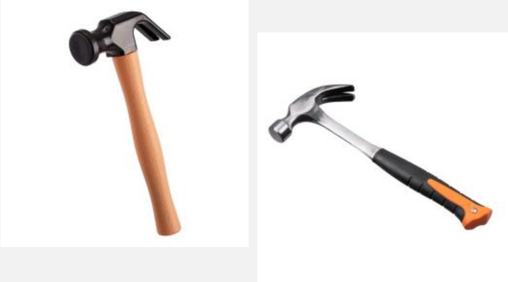
The corresponding websites tell me it's a common linnet

REVERSE IMAGE SEARCH

All the images in the dataset …

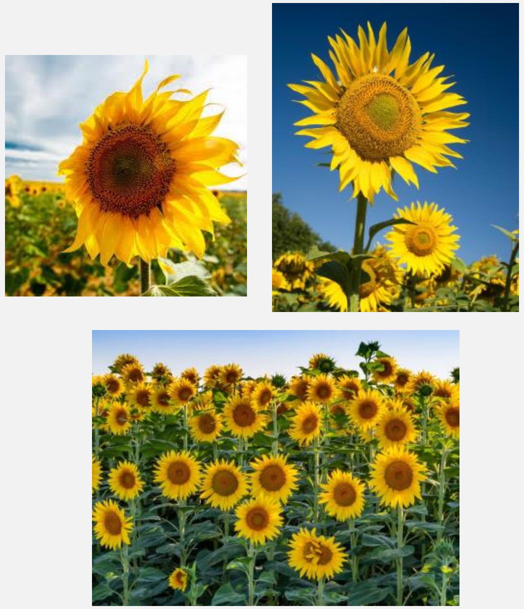
REVERSE IMAGE SEARCH

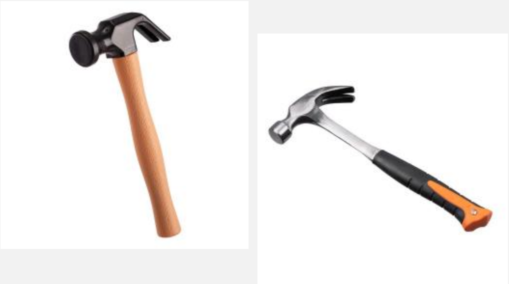




… are **clustered** into groups.

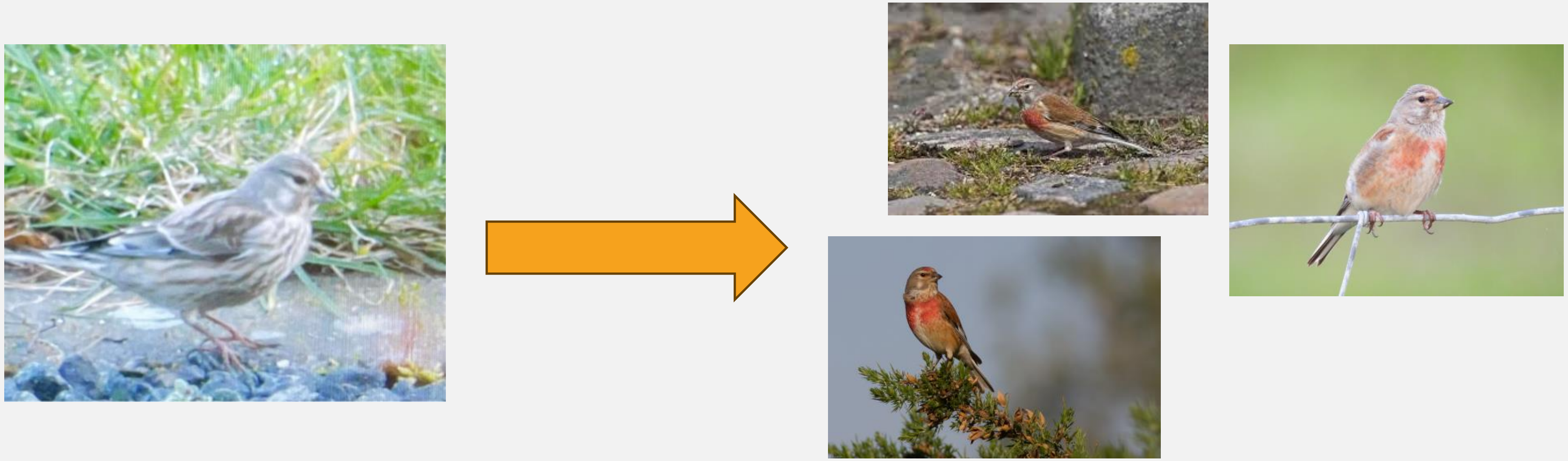
REVERSE IMAGE SEARCH





The image we search with is assigned to a cluster …

REVERSE IMAGE SEARCH



… and the other images in the cluster are returned.

DIFFERENCE FROM CLASSIFICATION?

At no point did we label the images.

We just saw/figured out that some were similar

measure of similarity

CLUSTERING

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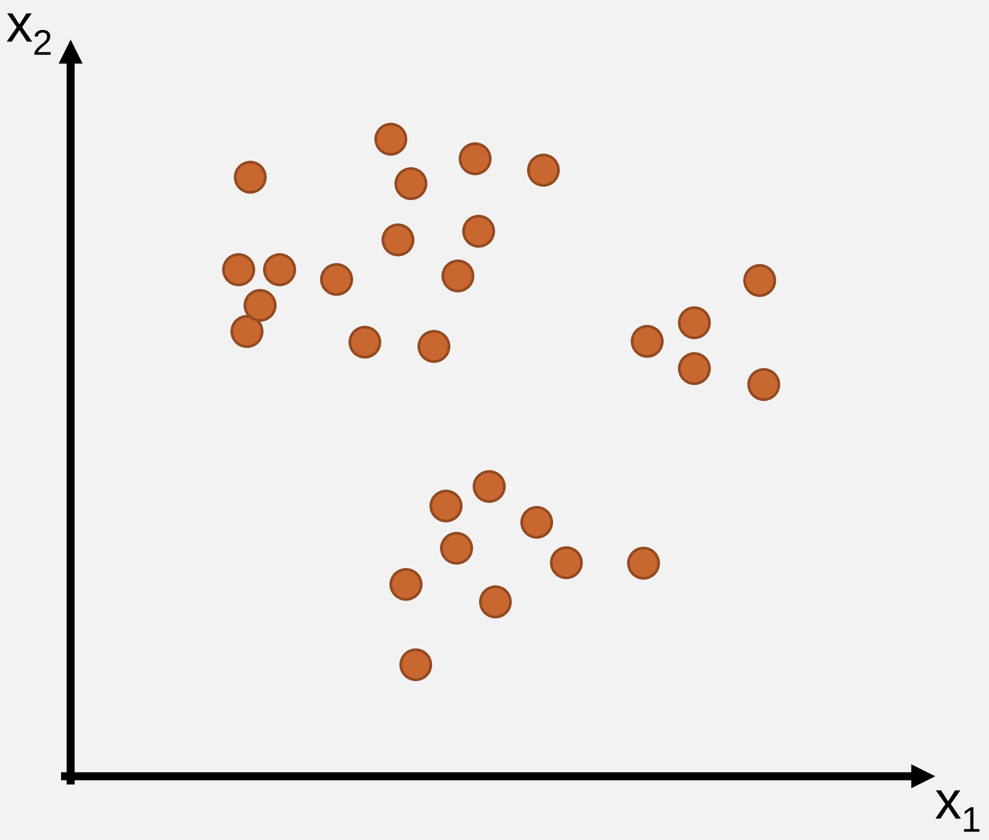
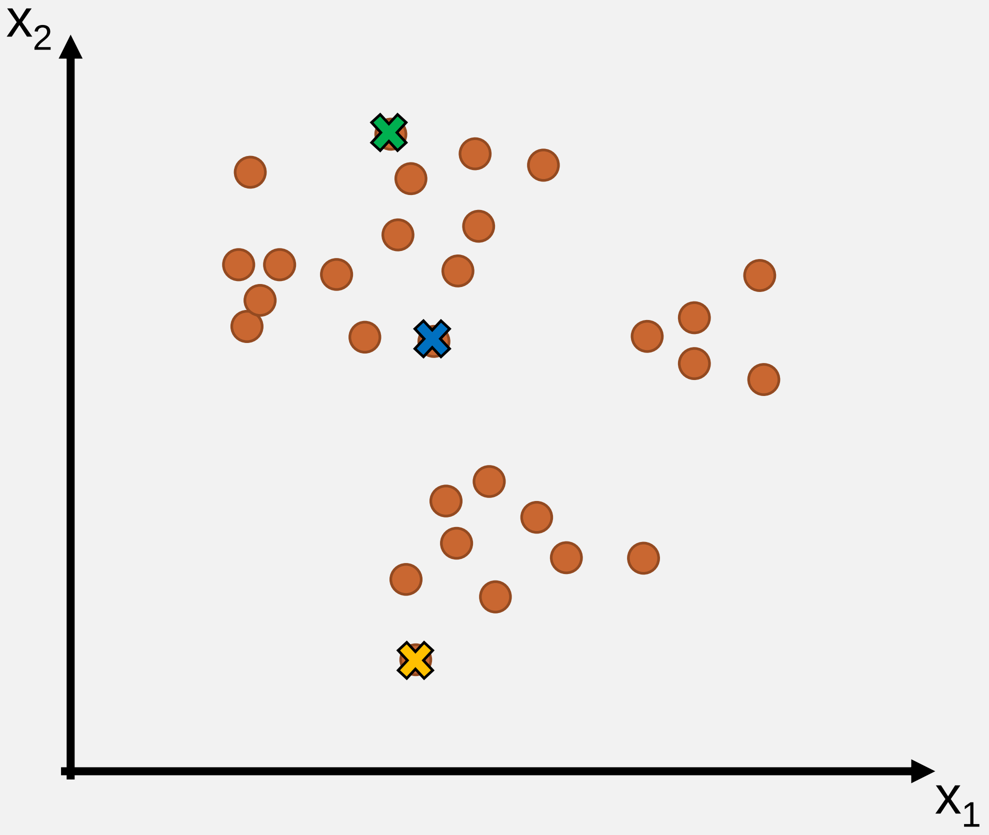
k-MEANS CLUSTERING

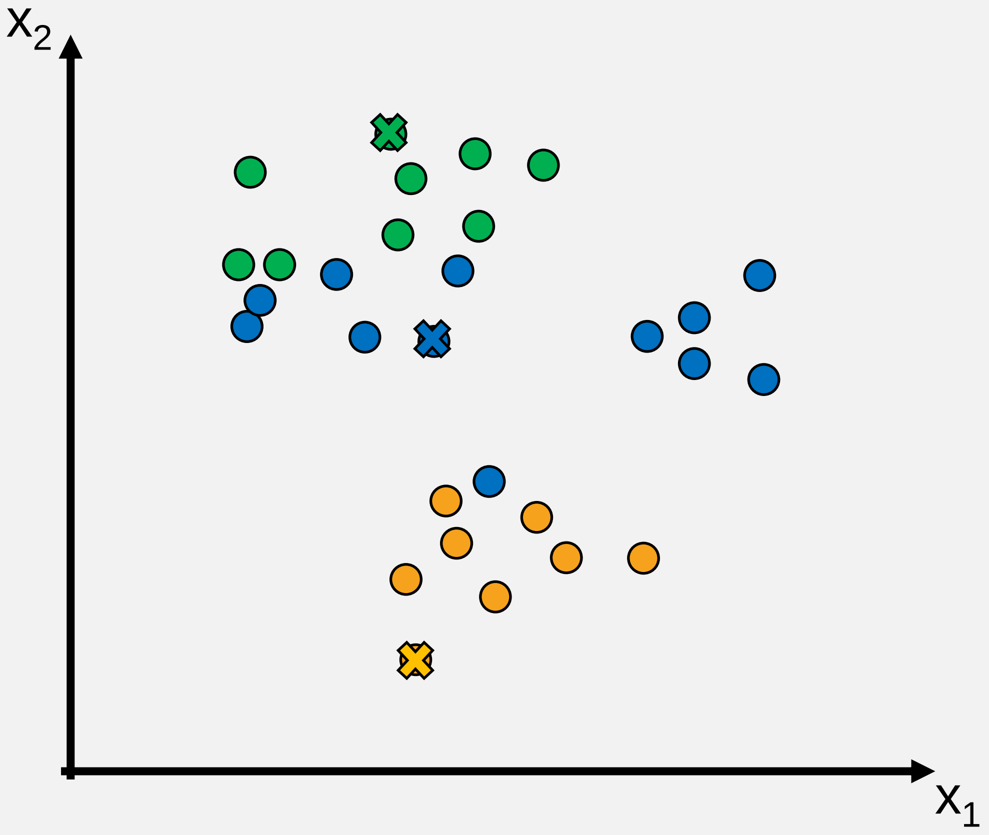


k-MEANS CLUSTERING



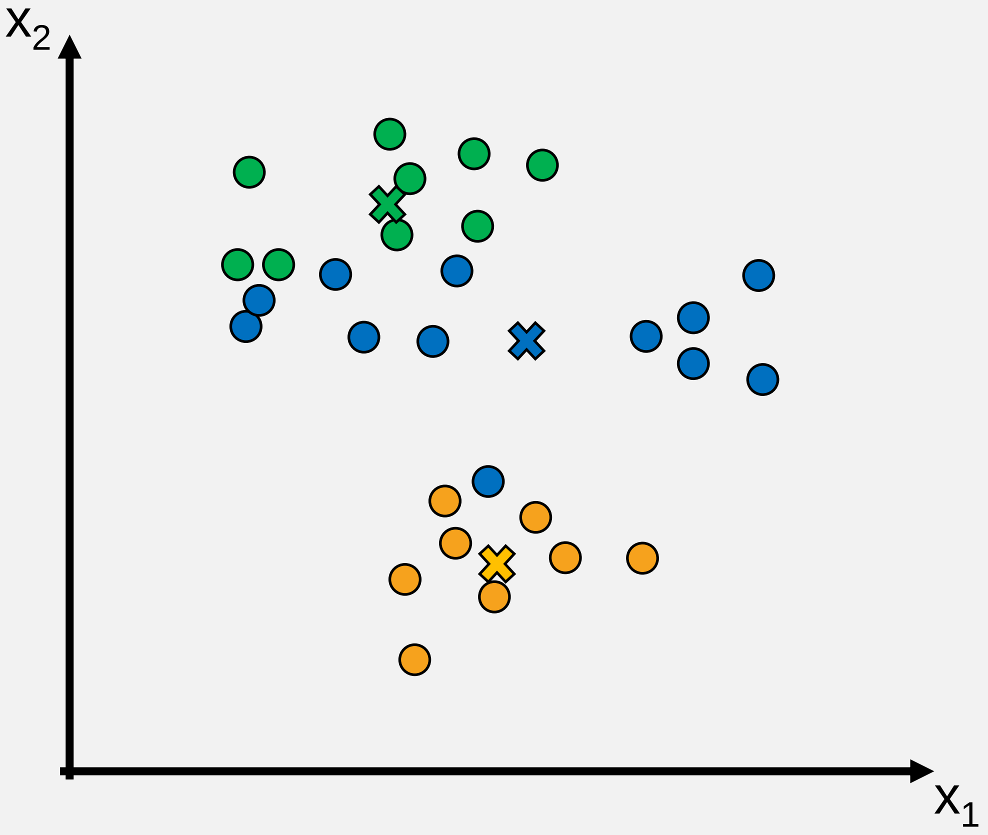
1. Assign k(=3) random points as **centroids**

k-MEANS CLUSTERING



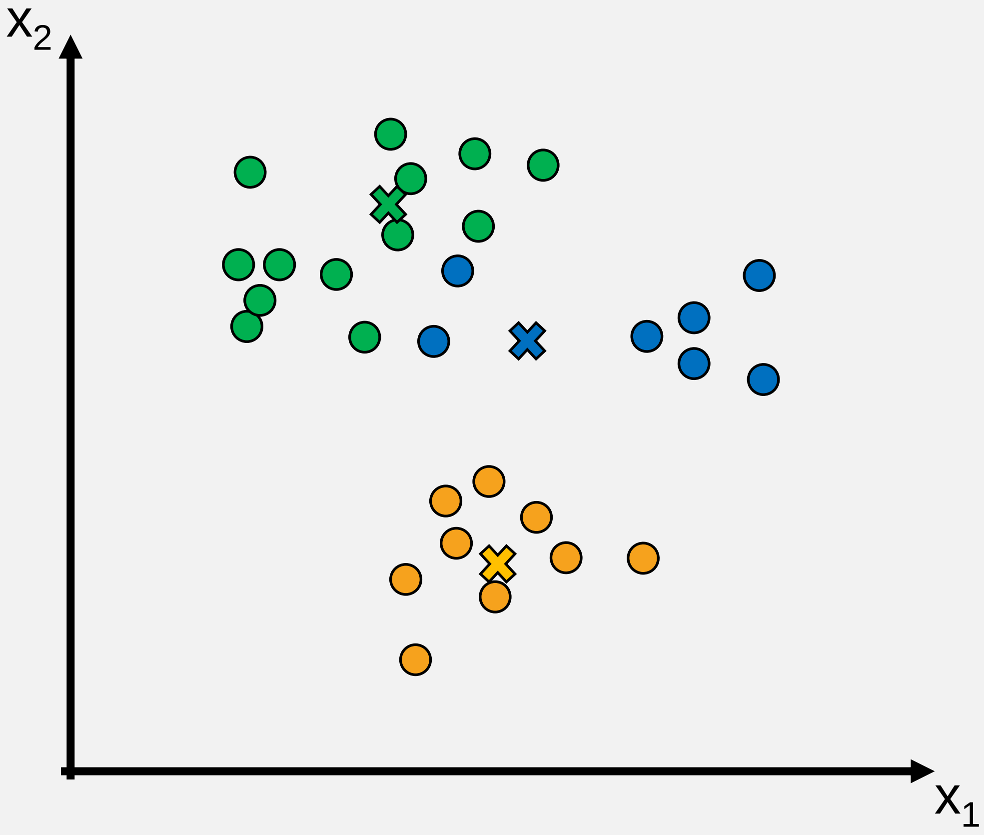
1. Assign k(=3) random points as **centroids**
2. Group the data by their distance to the centroids

k-MEANS CLUSTERING



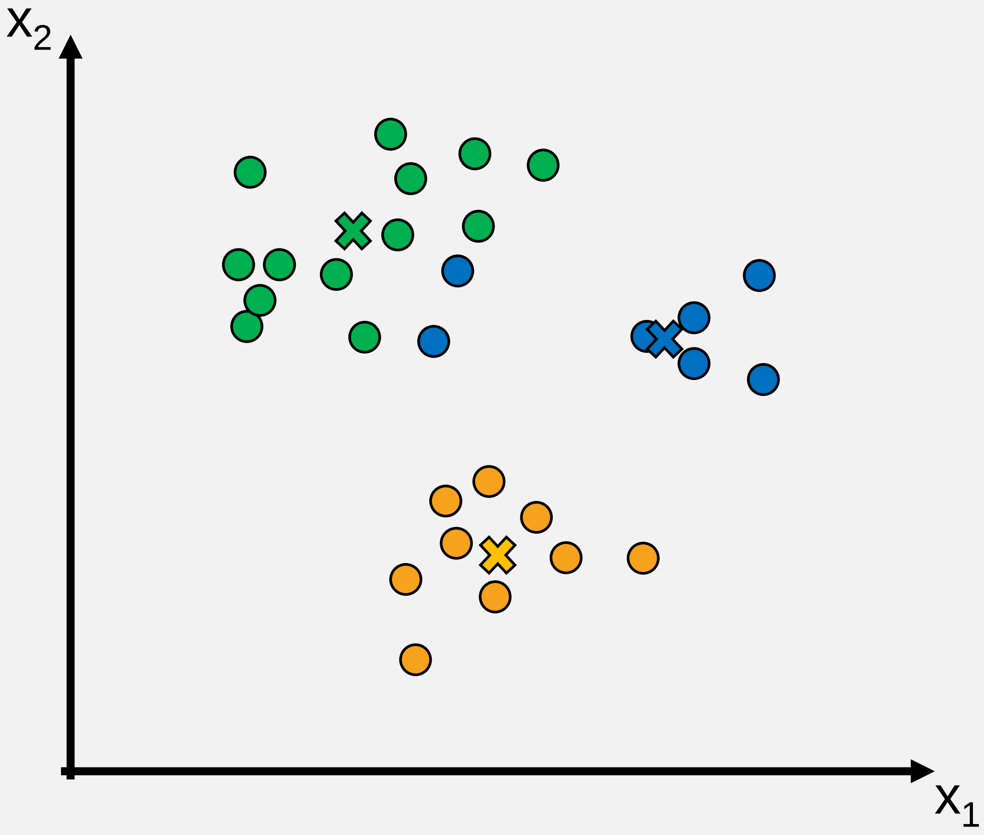
1. Assign k(=3) random points as **centroids**
2. Group the data by their distance to the centroids
3. Move the centroids to the cluster centers

k-MEANS CLUSTERING



1. Assign k(=3) random points as **centroids**
2. Group the data by their distance to the centroids
3. Move the centroids to the cluster centers
4. Regroup the data

k-MEANS CLUSTERING



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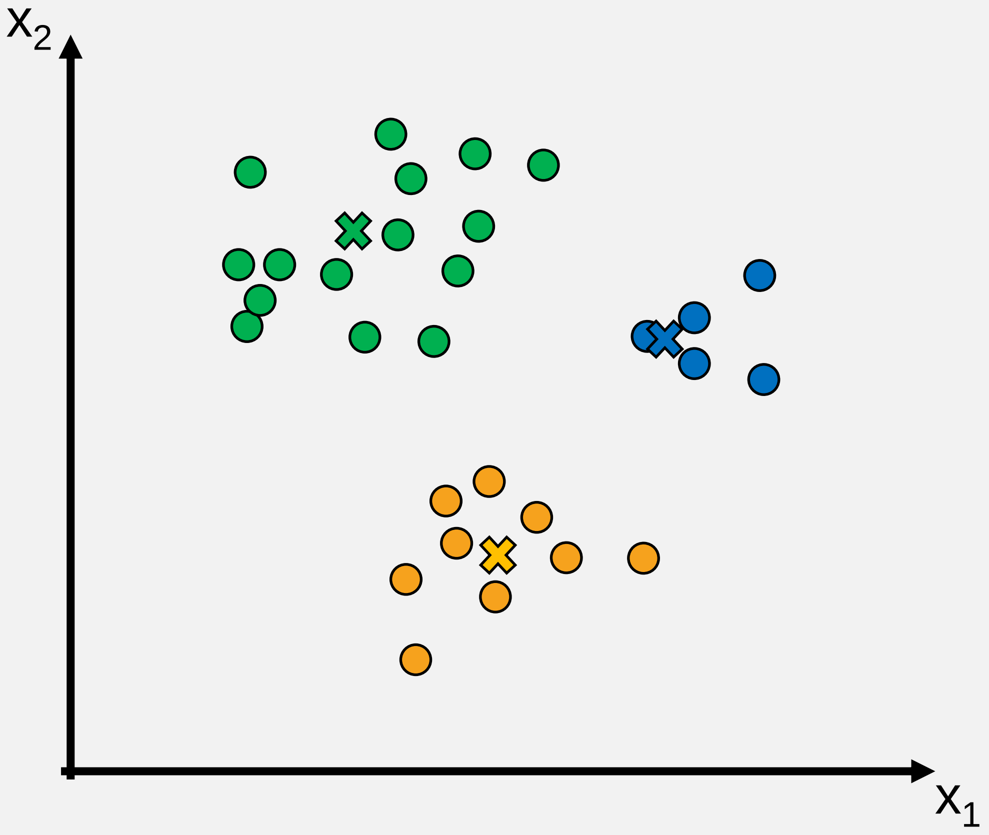
4. Regroup the data
5. Repeat 3-4 until nothing changes

k-MEANS CLUSTERING



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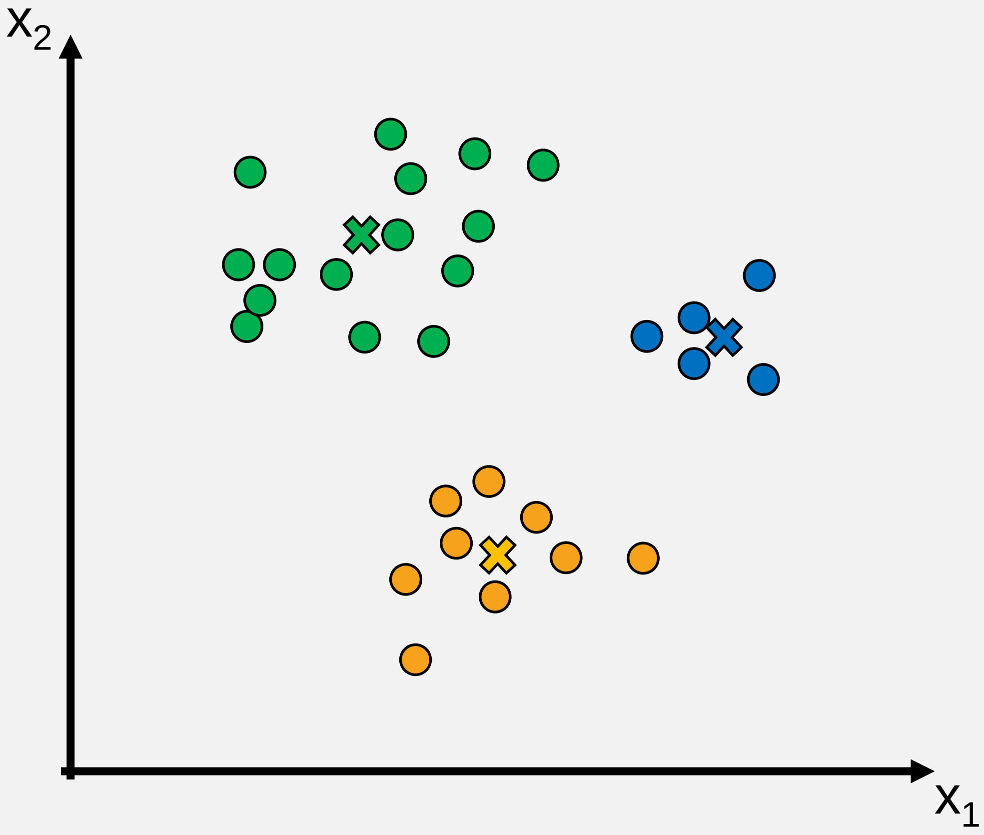

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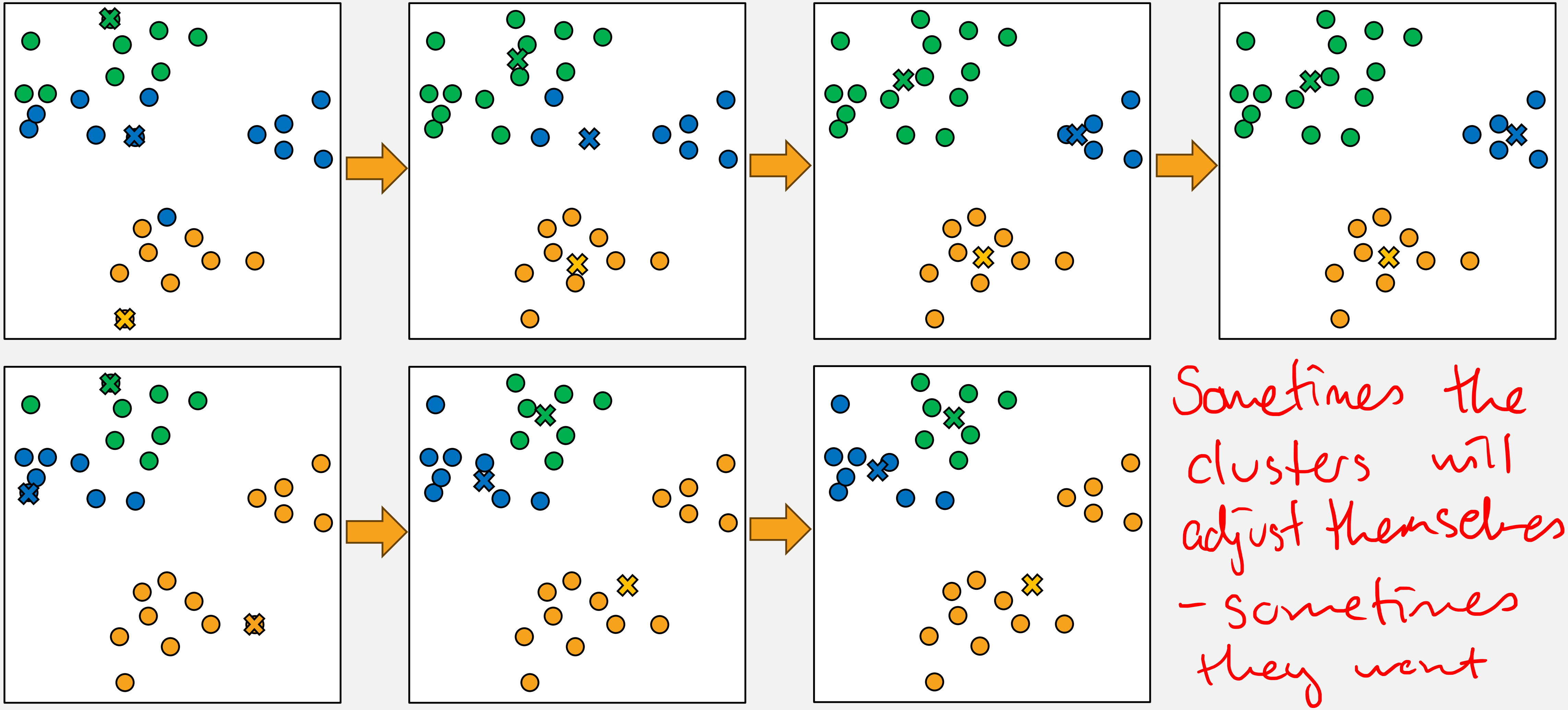
A FEW THINGS WE HAVE TO DEAL WITH

The value of k

The initial centroids

THE INITIAL CENTROIDS



Sometimes the clusters will adjust themselves - sometimes they won't

THE INITIAL CENTROIDS

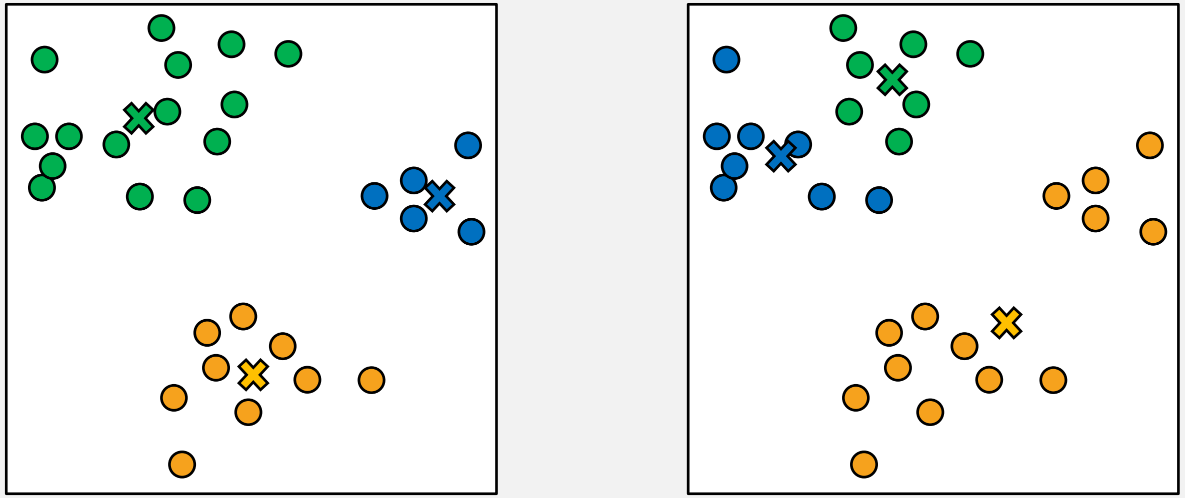
Solution 1: Try different, randomized initializations and compare the **costs** of the final clusterings

data points

$$C = \sum_i ||x_i - \mu(x_i)||^2$$

associated centroid

pick the one with the lowest cost



C = 171.4

C = 241.3

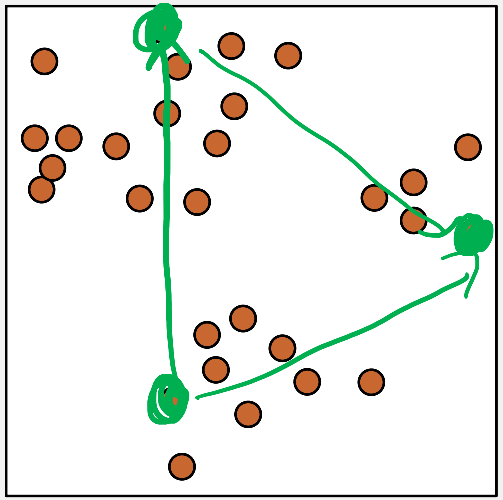
THE INITIAL CENTROIDS

Solution 2: Choose the initial centroids based on the distance to the previous ones

Choose the point furthest away

⇒ likely to select different points from different cluster :)

and outliers :(

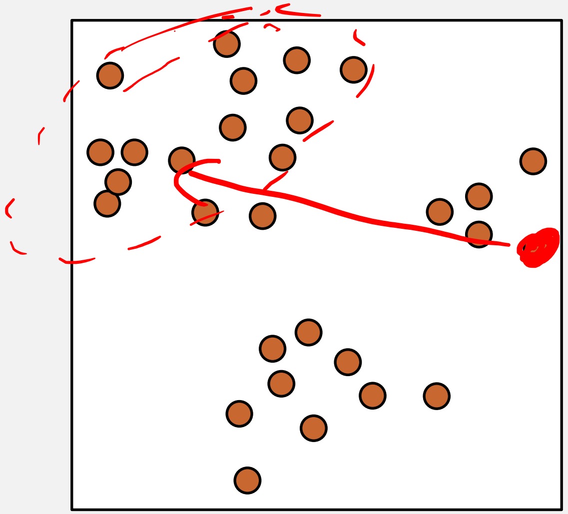


THE INITIAL CENTROIDS

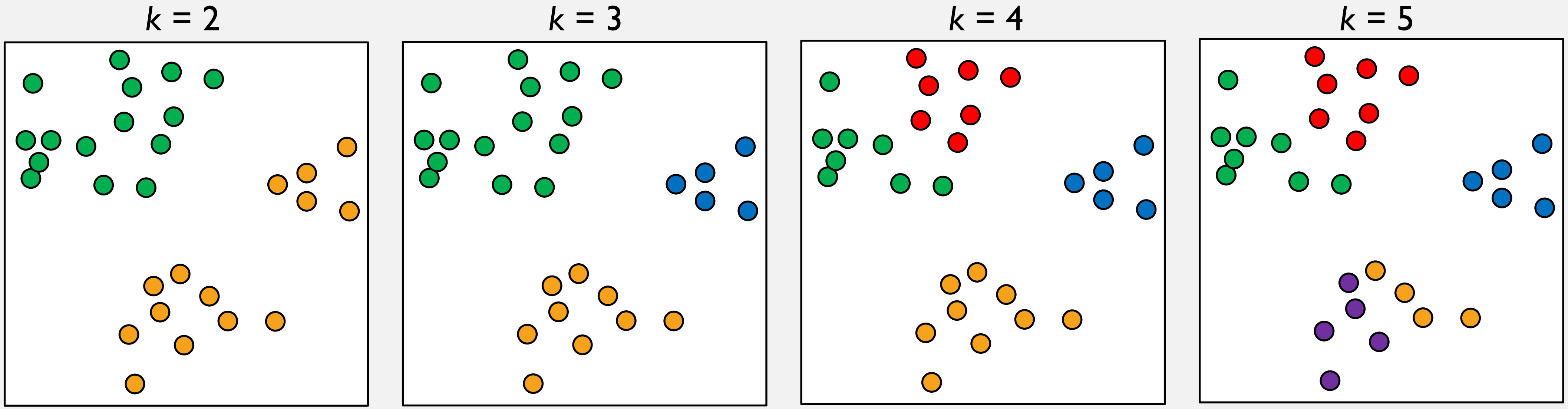
Solution 3: Choose "far away but random" points ("k-means++")

assign a distance-based probability

of picking next point



THE NUMBER OF CLUSTERS (k)

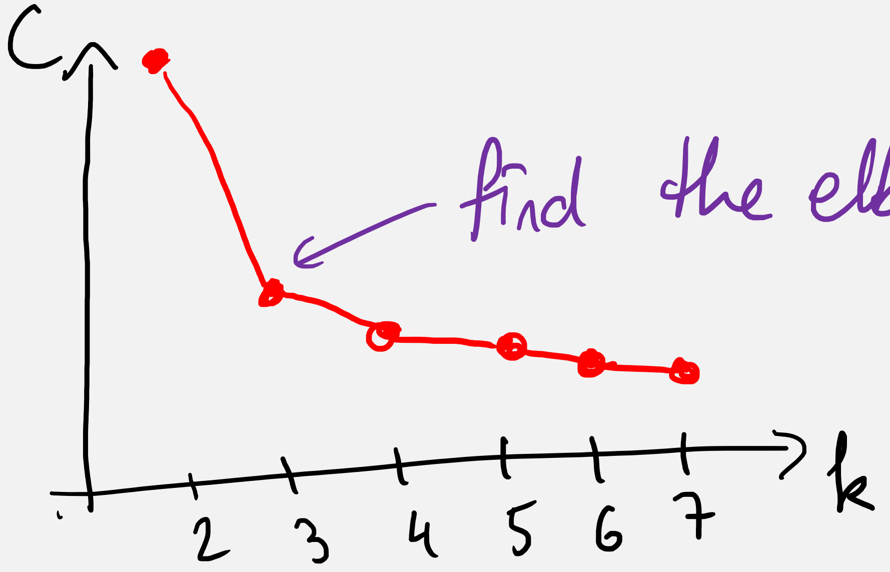


THE NUMBER OF CLUSTERS (k)

The easy way: You already know it (domain knowledge)

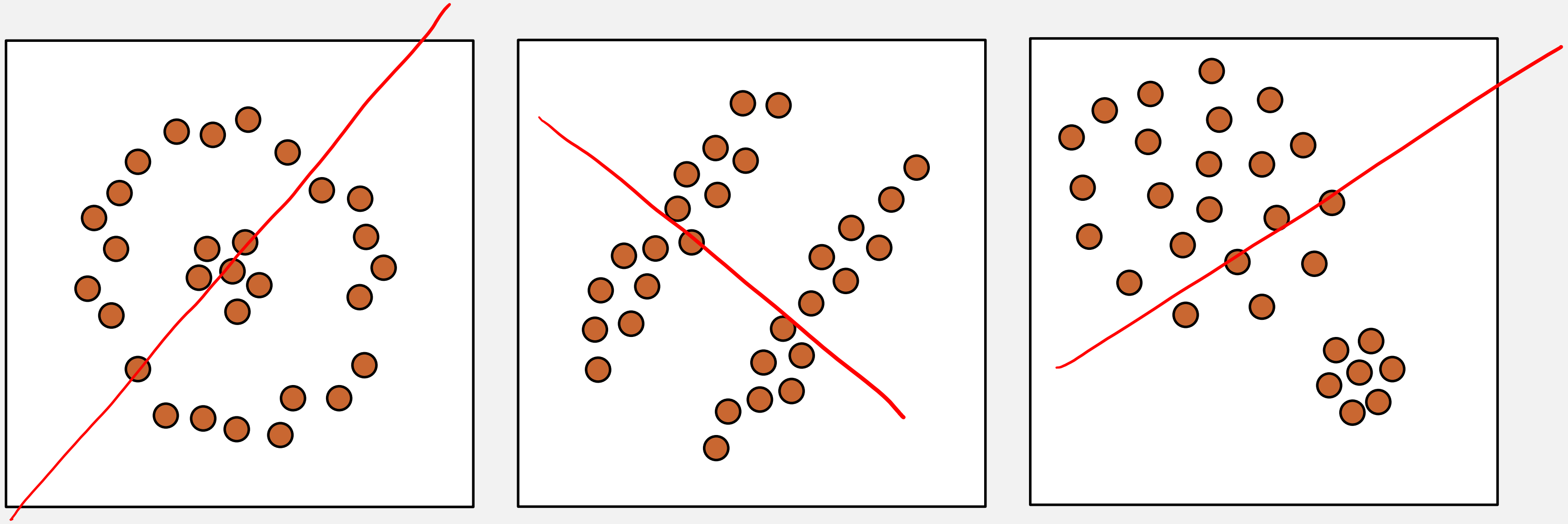
The hard way: "The elbow method"

cost function $\rightarrow$ $C = \sum_i ||x_i - \mu(x_i)||^2$ always decreases with k



find the elbow: new clusters don't contribute a lot

WHERE *k*-MEANS FAILS



CODE EXAMPLE

Jupyter Notebook **Clustering methods**

CLUSTERING

- What is clustering?
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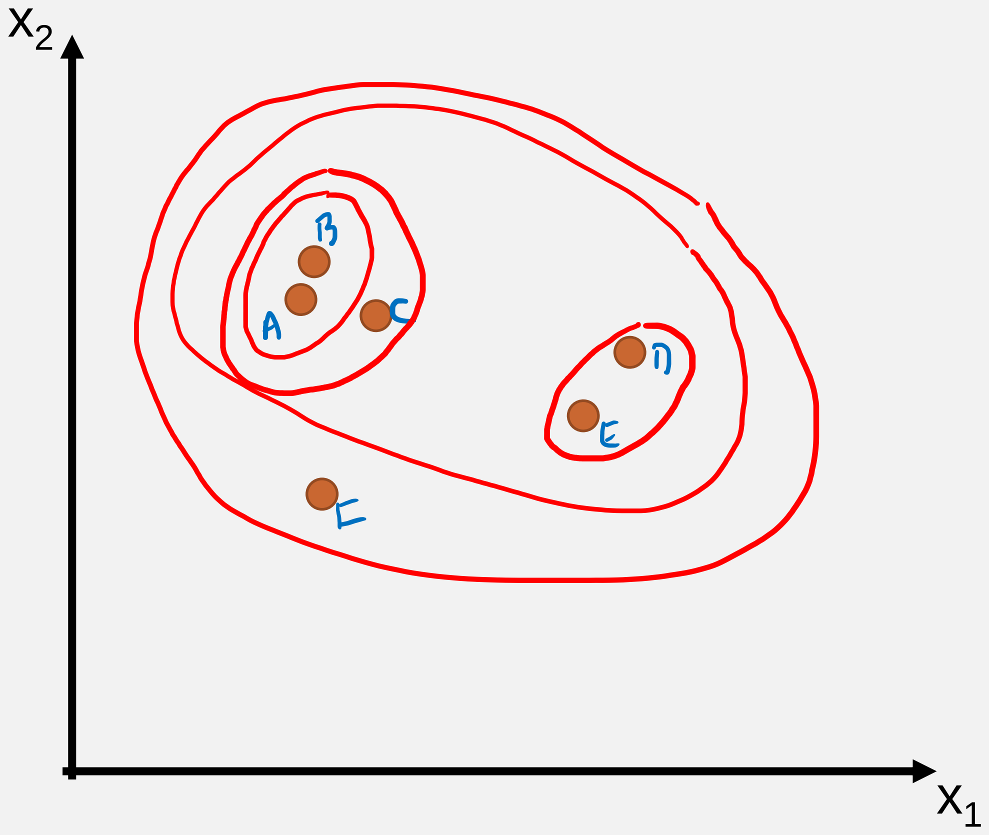
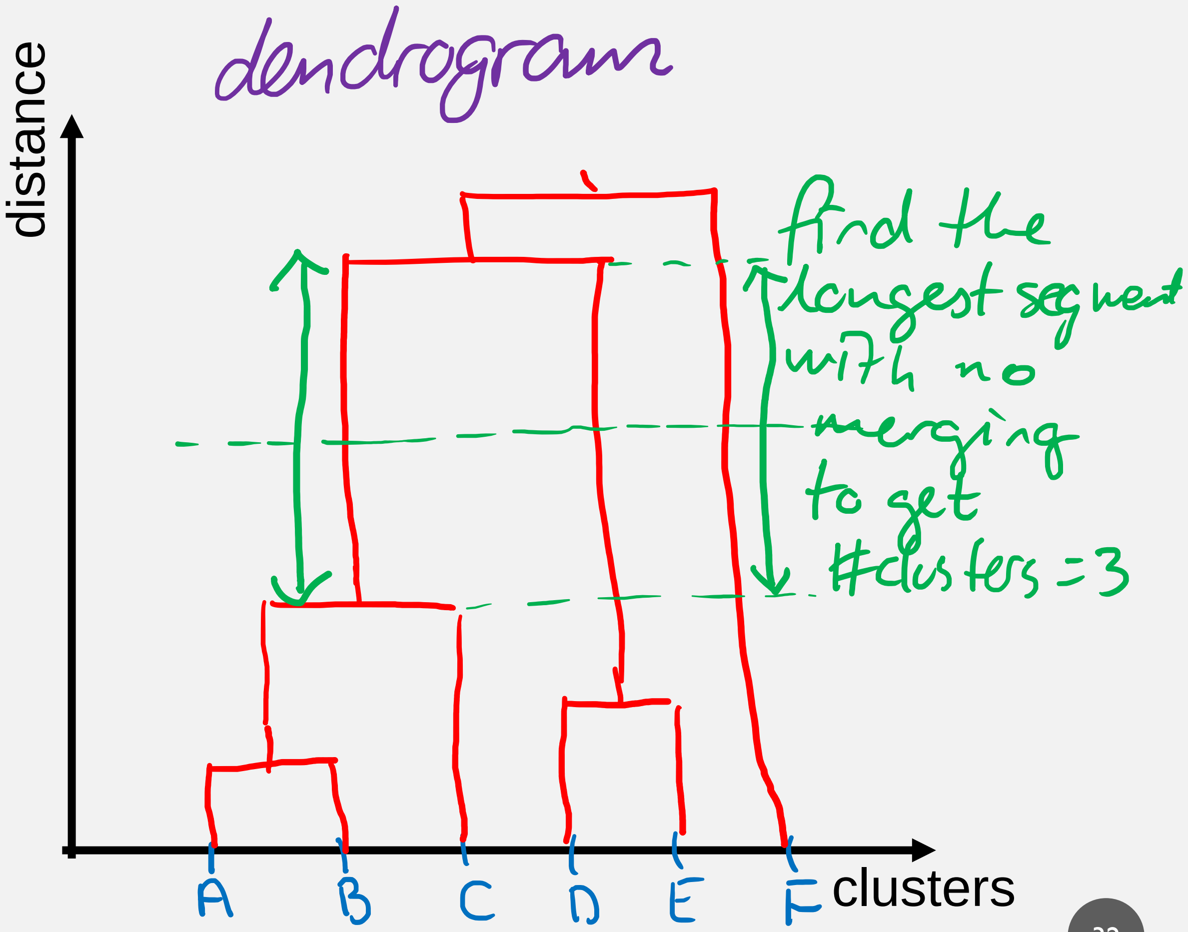
AGGLOMERATIVE CLUSTERING

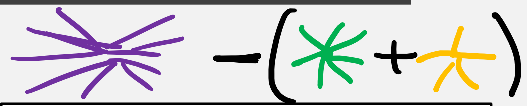
let each point be its own cluster
while there are more than 1 cluster:
    merge the two closest clusters

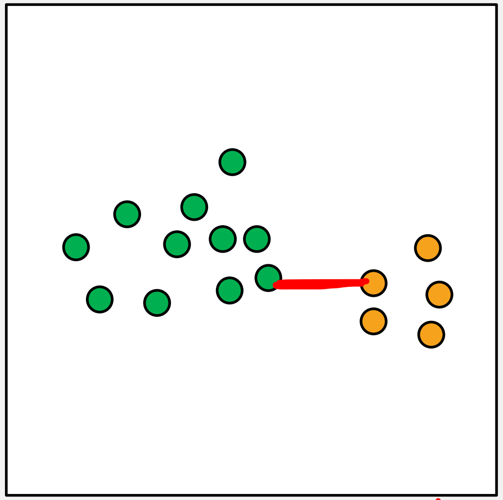
AGGLOMERATIVE CLUSTERING



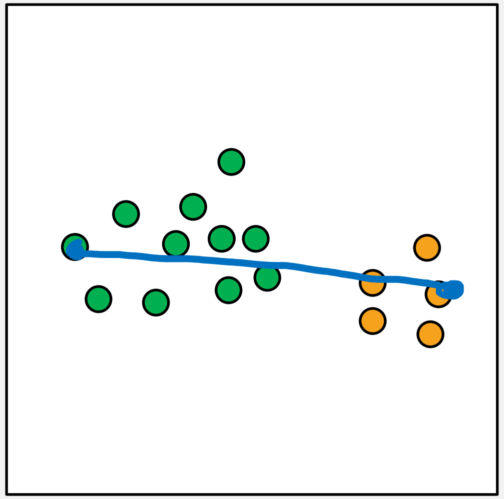


THE DISTANCE BETWEEN CLUSTERS

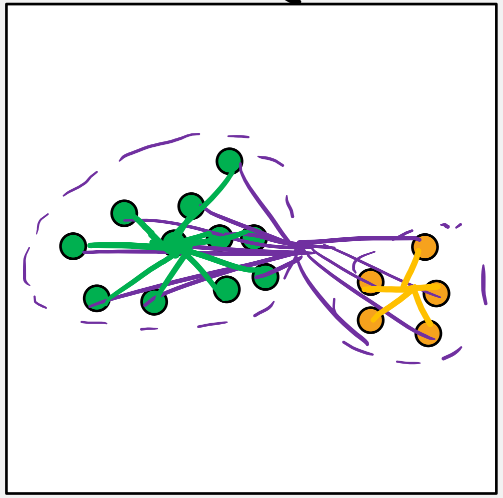




"single link"
(min distance)
→ sensitive to outliers/noise



"complete link"
(max distance)
→ may break large clusters



"Ward's method"
(change in cost function)
→ difficulty with different sizes/weird shapes

several others...

CODE EXAMPLE

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DBSCAN

density-based spatial clustering of applications with noise

$\Rightarrow$ partition points into dense regions separated by not so dense regions

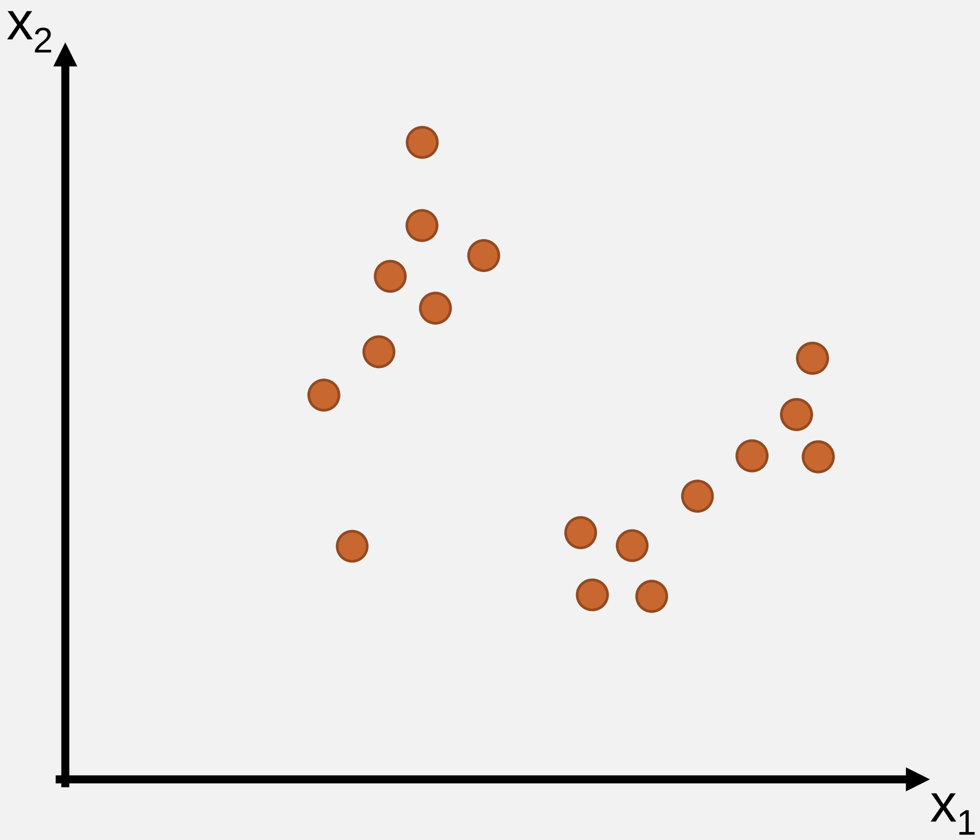
- How do we measure density?

  = number of points in a circle of radius ε

- What is a dense region?

  = density of at least n points

DBSCAN



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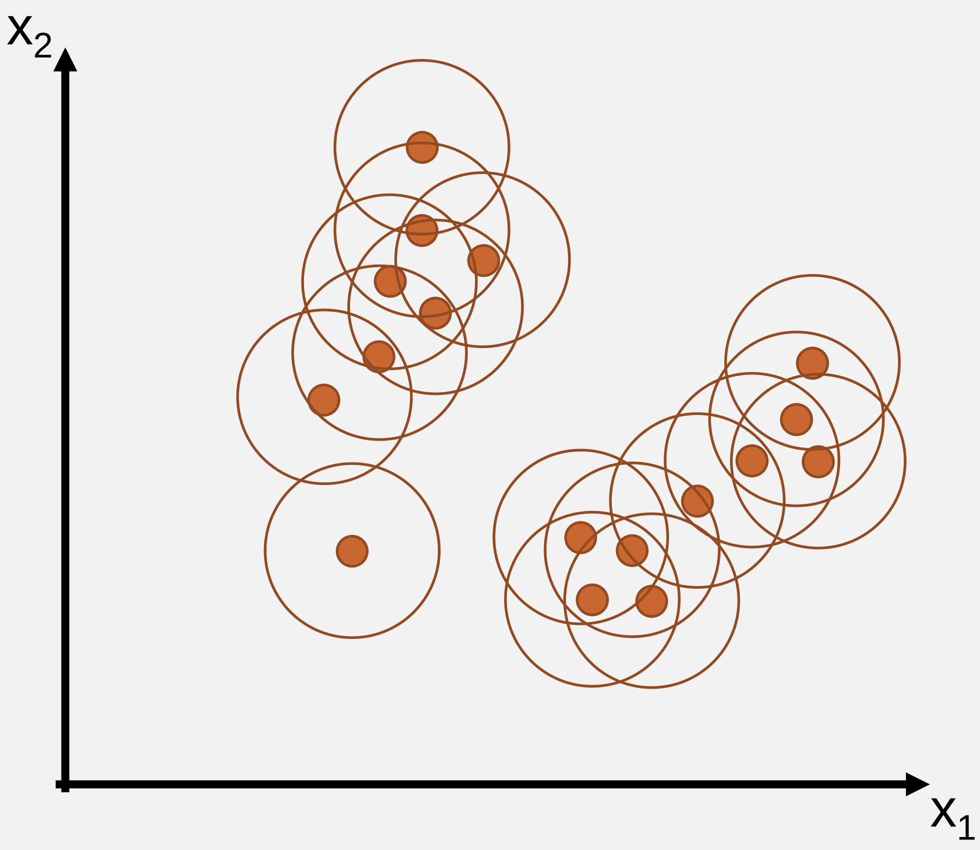
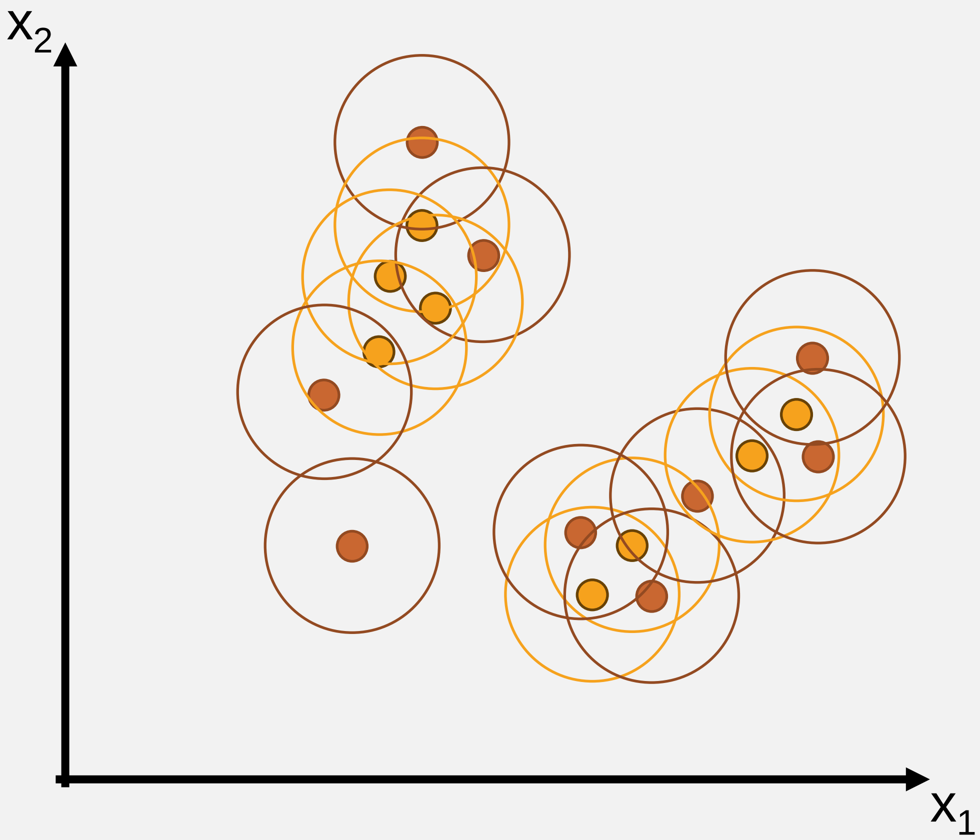


1. Draw a circle of radius ε around every point. This region is the ε-neighbourhood.

DBSCAN



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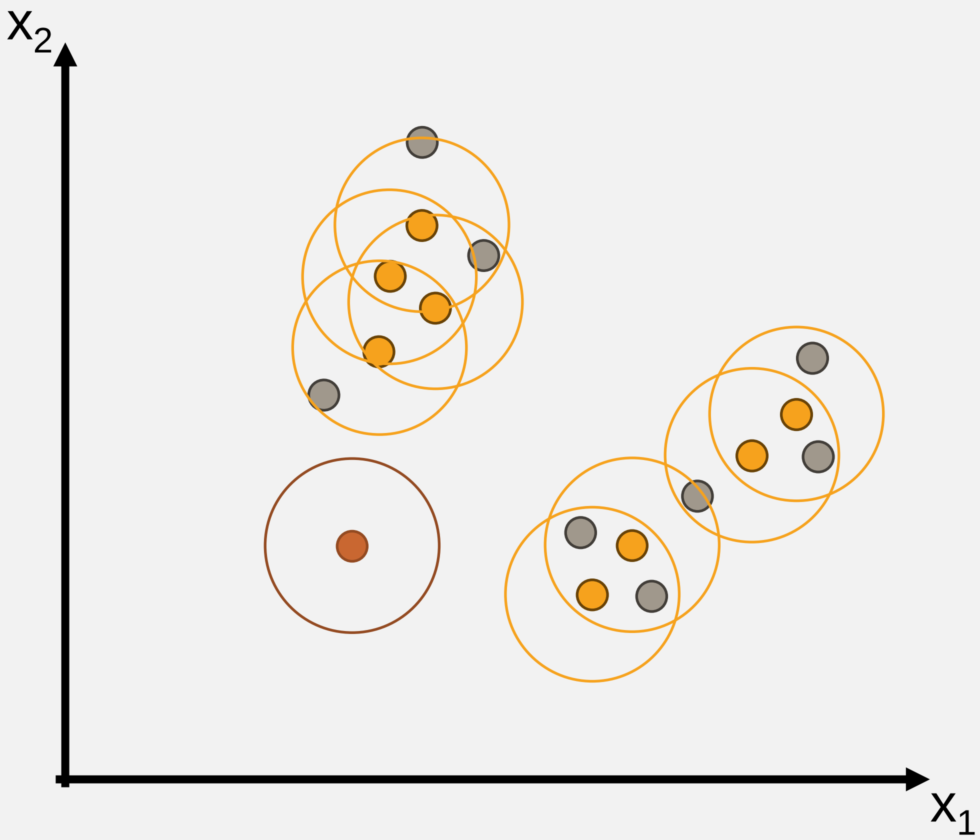
DBSCAN



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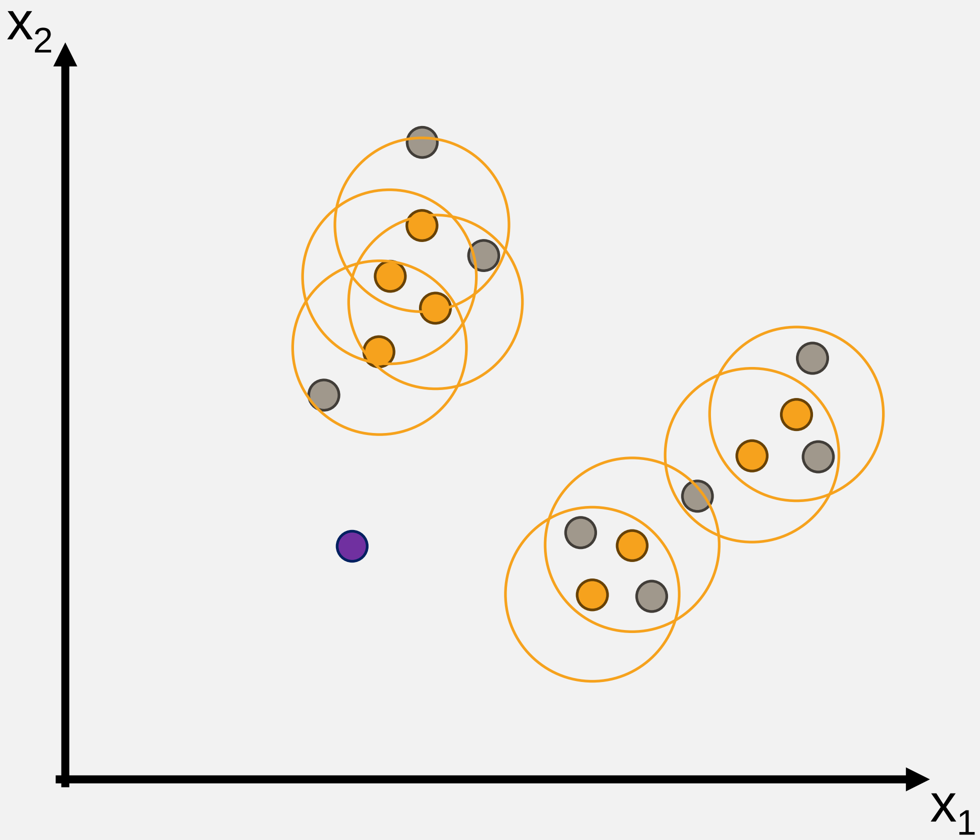
DBSCAN



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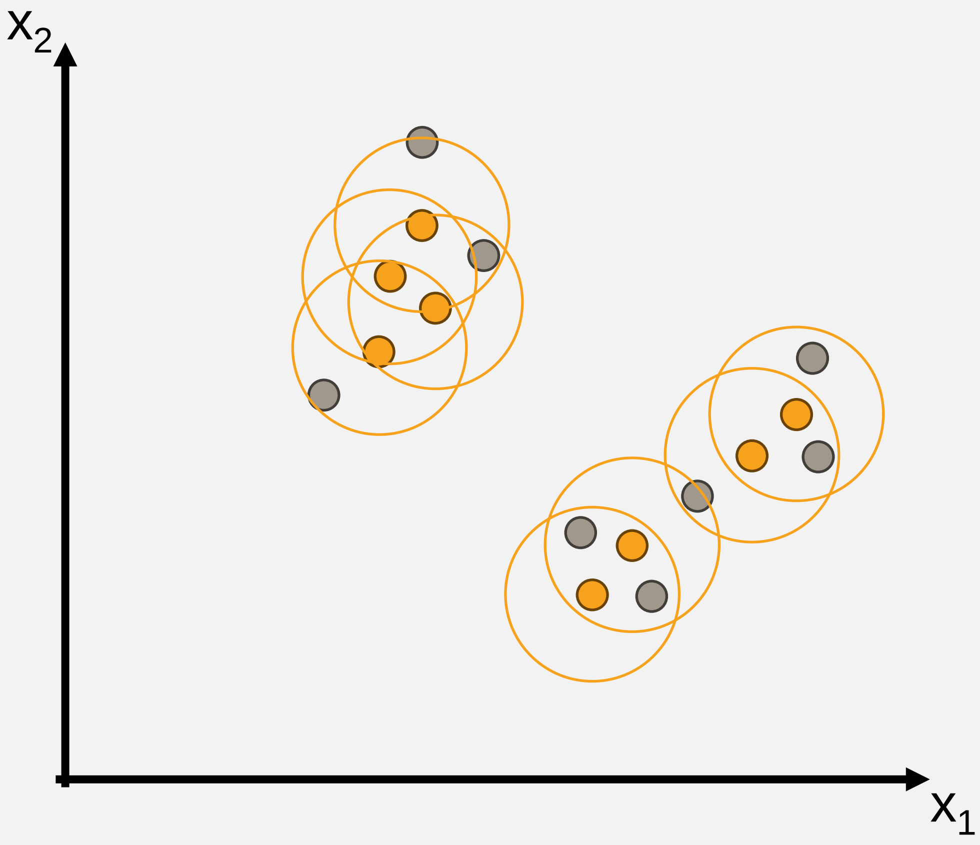
DBSCAN



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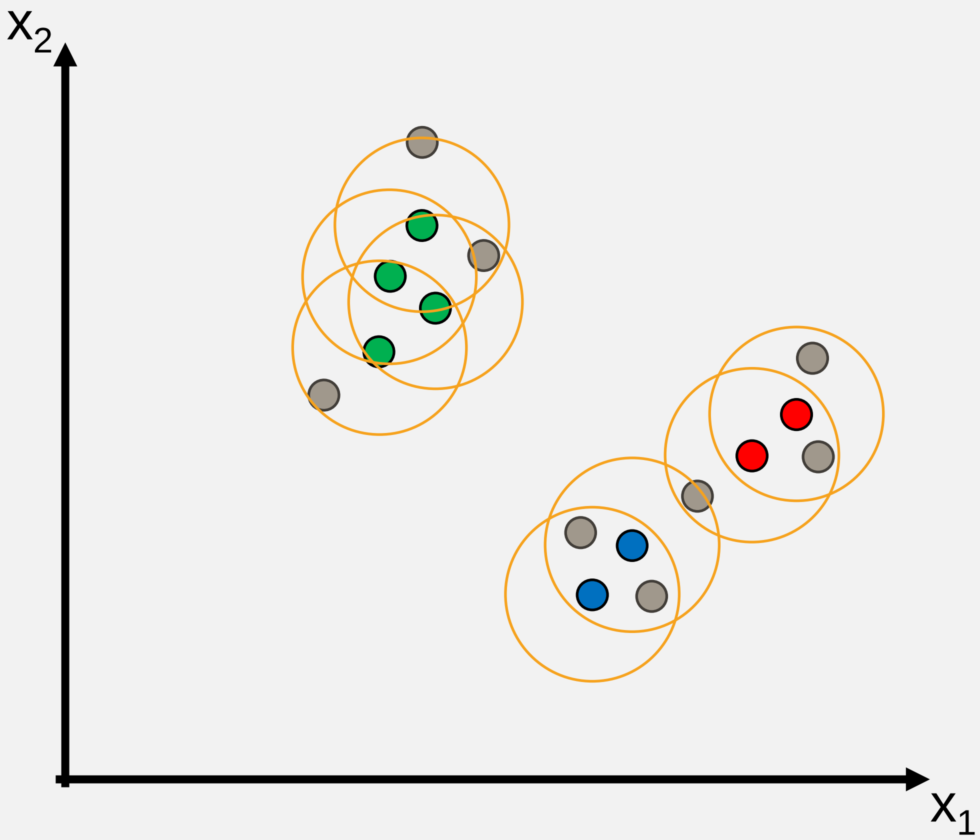
5. Get rid of **noise** points.

DBSCAN



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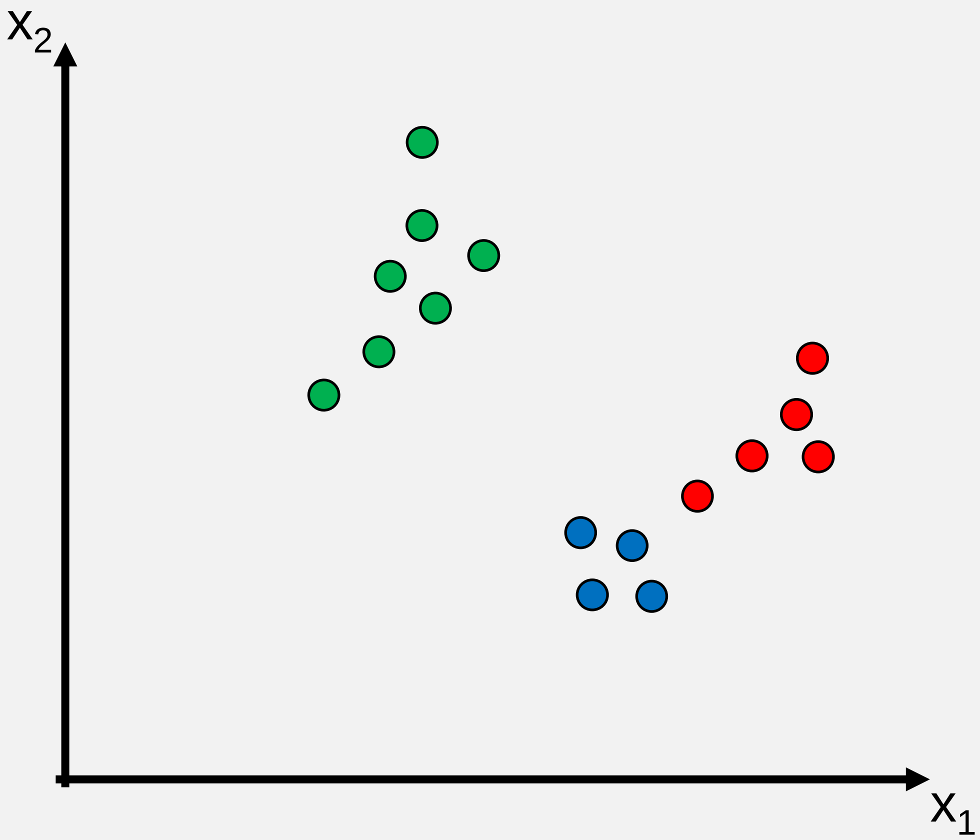
4. Otherwise, it is a **noise** point.
5. Get rid of **noise** points.
6. All **core** points reachable through each other's ε-neighbourhoods belong to the same cluster.

DBSCAN



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5. Get rid of **noise** points.
6. All **core** points reachable through each other's ε-neighbourhoods belong to the same cluster.
7. All **border** points are assigned to the cluster of closest core point.

DETERMINING ε AND n

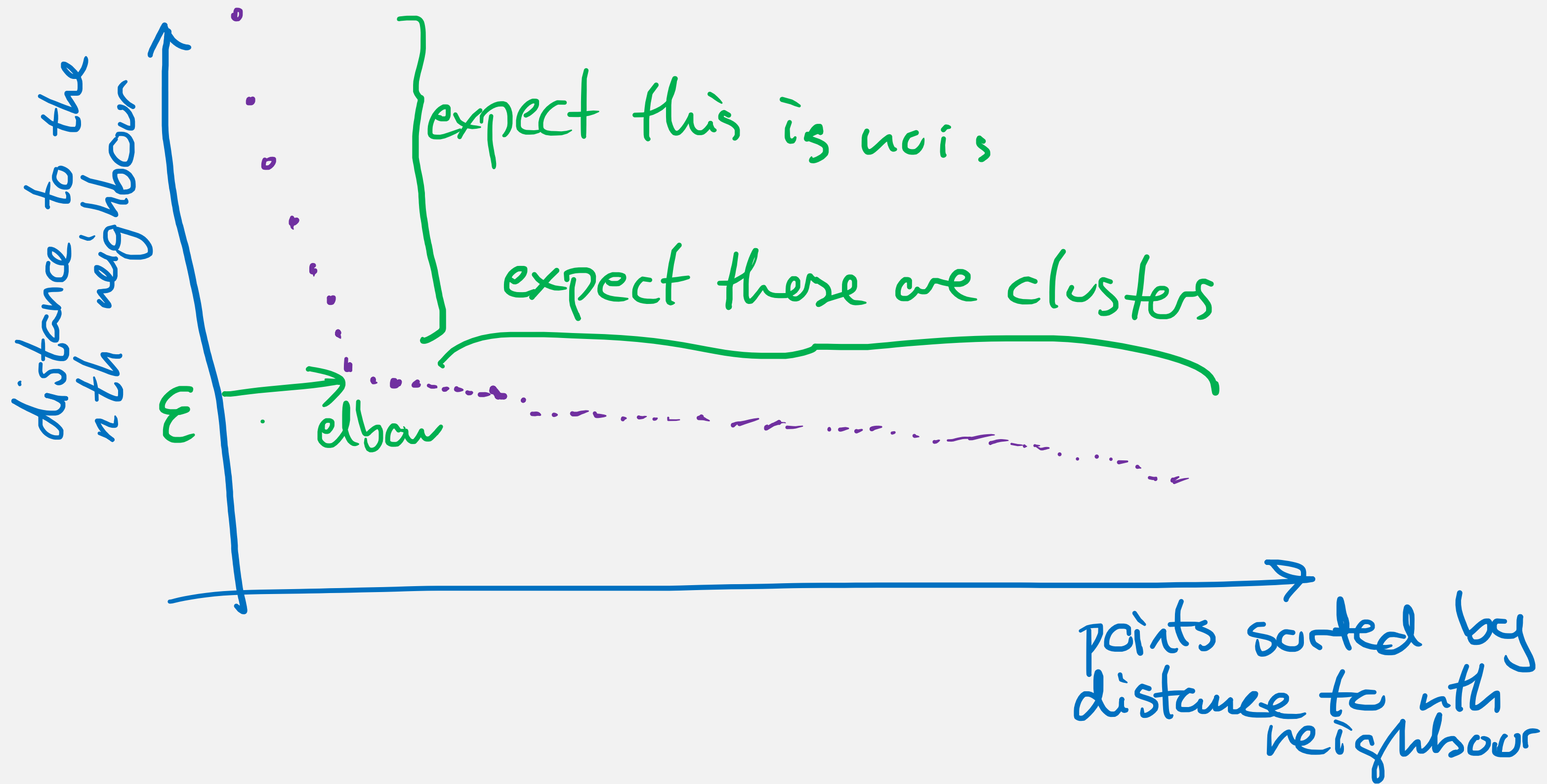
(recommendations ....)

n (=minPts) = $2 \times d$

→ dimensionality

→ 2D data ⇒ $n=4$

ε

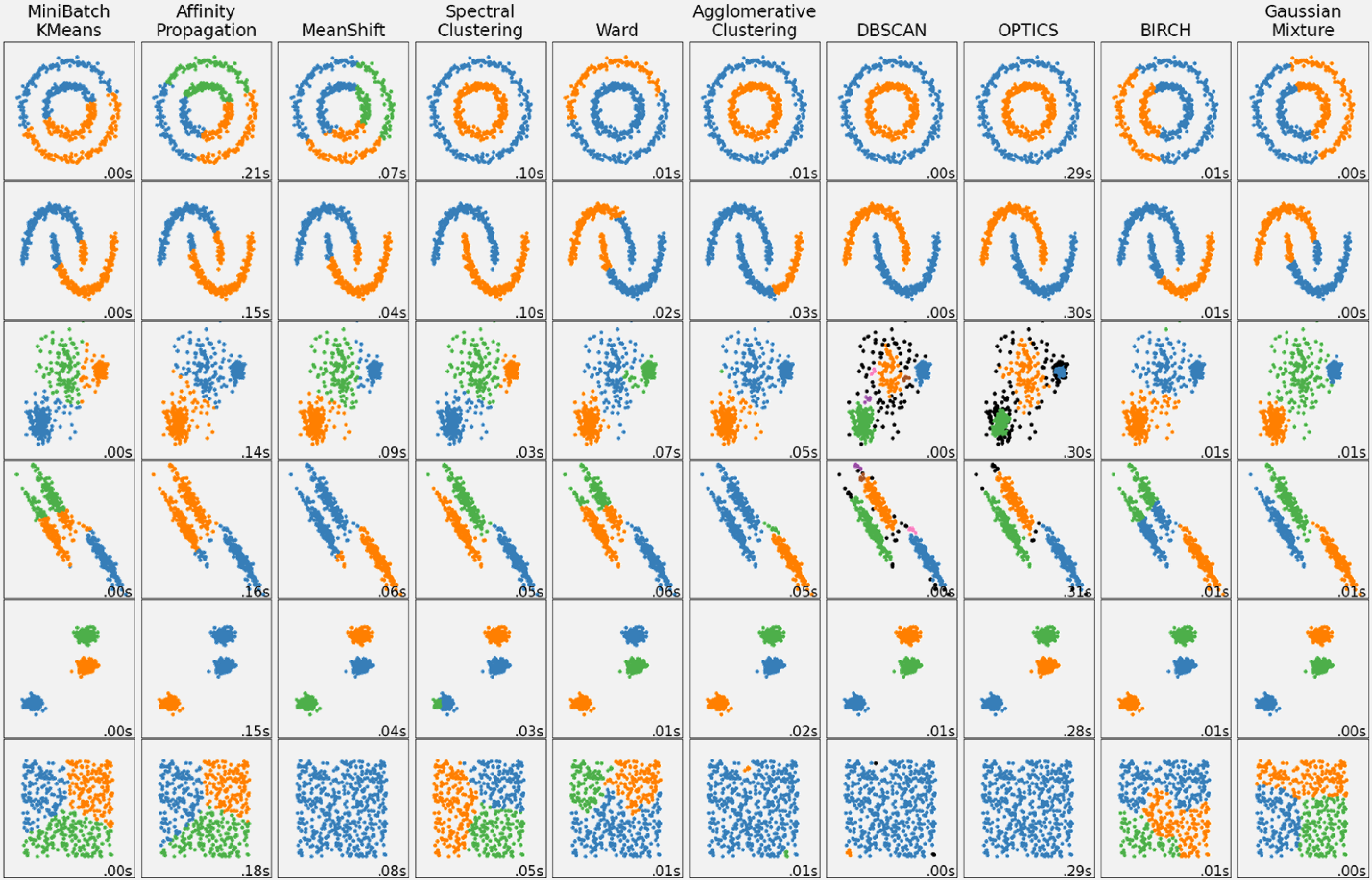


CODE EXAMPLE

Jupyter Notebook **Clustering methods**

COMPARING THE MODELS

	Pros	**Cons**
***k*-means clustering**	Efficient	Can't handle noise/outliers Can't handle weird shapes Initialization User must provide k
Agglomerative clustering	No a priori knowledge of #clusters needed	Dendrograms can be ambiguous Computationally heavy Each distance metric has its own problems
DBSCAN	Weird shapes Handles outliers No a priori knowledge of #clusters needed	Trouble with different densities



http://scikit-learn.org/stable/modules/clustering.html

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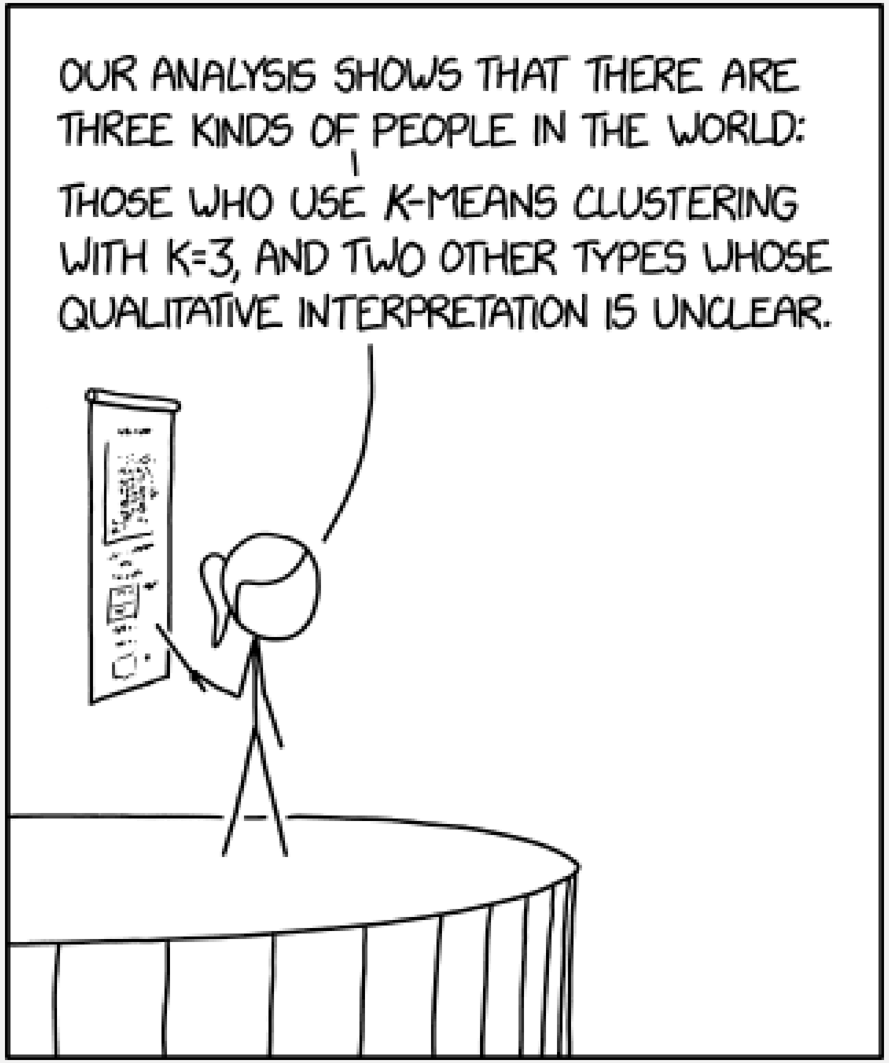
APPLICATION: IMAGE SEGMENTATION

Jupyter Notebook **Image segmentation**


OUR ANALYSIS SHOWS THAT THERE ARE THREE KINDS OF PEOPLE IN THE WORLD:
THOSE WHO USE K-MEANS CLUSTERING WITH K=3, AND TWO OTHER TYPES WHOSE QUALITATIVE INTERPRETATION IS UNCLEAR.