UNSUPERVISED ML

OBJECTIVE

- Discover information from data without labeled examples
- Extract some hidden organisation, patterns, relation between elements
- Extract a (statistical ?) model of the data ?

OBJECTIVE

- Typical objectives:
  - Cluster discovery
  - Anomaly Detection
  - Latent variable discovery / Embedding / dimensionality reduction…

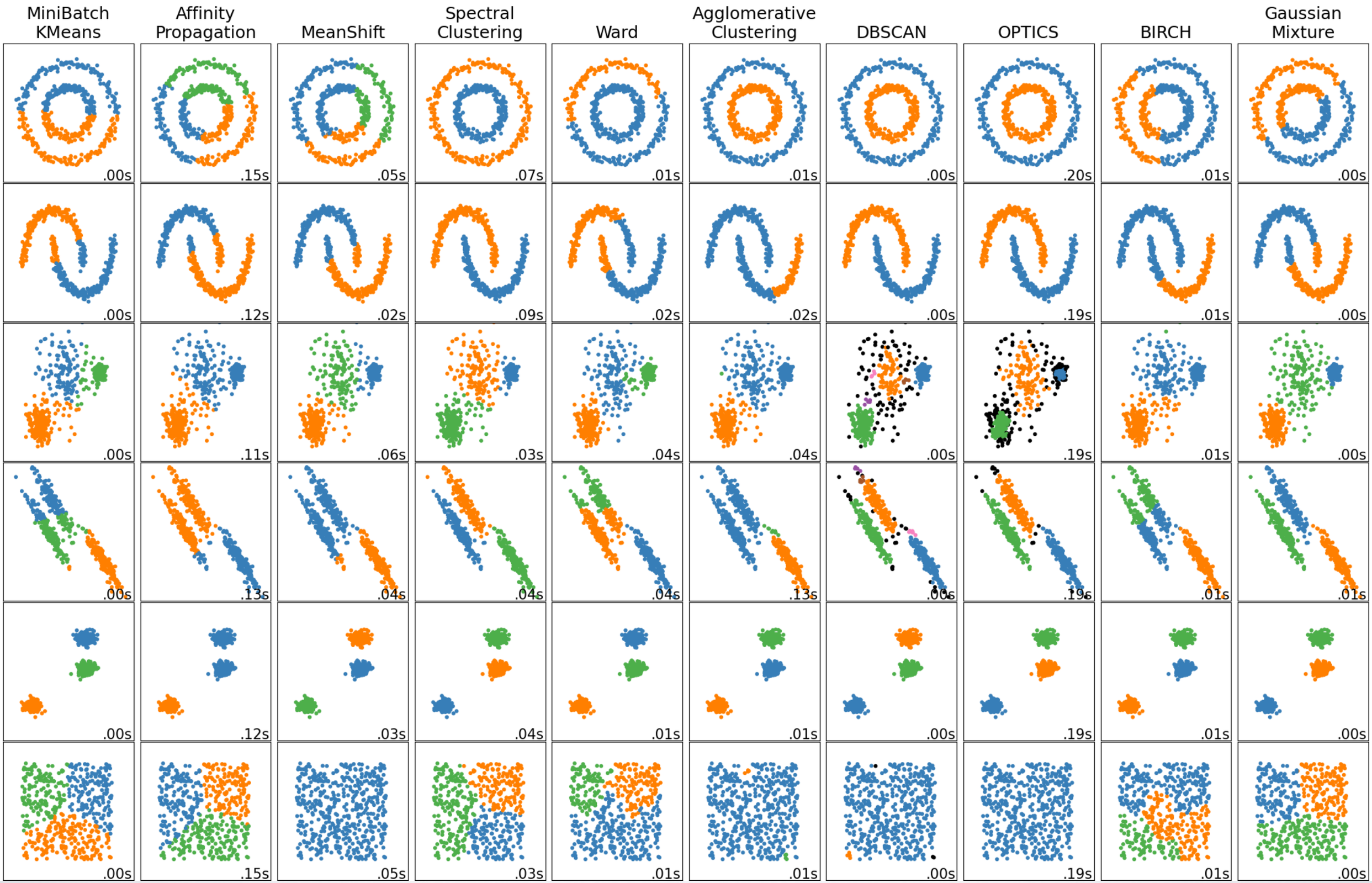
CLUSTERING

CLUSTERING

- The most famous unsupervised ML problem
- 100+ methods exist
  - Most people use "good old" methods: k-means (1967), DBSCAN (1996)
  - They are often "good enough", well implemented, safe, …
- Part of the problem: Clustering is not well defined
  - What is "a good cluster" ?

CLUSTERING

- How would you define a good cluster ?
- A good partition in clusters ?


MiniBatch KMeans
Affinity Propagation
MeanShift
Spectral Clustering
Ward
Agglomerative Clustering
DBSCAN
OPTICS
BIRCH
Gaussian Mixture
.00s .15s .05s .07s .01s .01s .00s .20s .01s .00s
.00s .12s .02s .09s .02s .02s .00s .19s .01s .00s
.00s .11s .06s .03s .04s .04s .00s .19s .01s .00s
.00s .13s .04s .04s .04s .13s .00s .19s .01s .01s
.00s .12s .03s .04s .01s .01s .00s .19s .01s .00s
.00s .15s .05s .03s .01s .01s .00s .19s .01s .00s

K-MEANS

- Definition:
  - For a target number of clusters k
  - Find the item assignment minimizing
    - The inter-cluster variance
    - Equivalently => The squared distance from points to their cluster center
    - Equivalently => The squared distance between cluster elements

- This is only one possible objective !
  - Why this one ?
  - Intuitive, good properties…

K-MEANS

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \| \mathbf{x} - \boldsymbol{\mu}_i \|^2 = \arg\min_{\mathbf{S}} \sum_{i=1}^{k} |S_i| \operatorname{Var}(S_i)$$

with

$\mathbf{S}$ a cluster assignment,

x a d dimensional item, and

μ_i the mean of items in cluster $\mathbf{S}_i$.

Note that without fixing k, there is a trivial solution with each item alone in its own cluster.

K-MEANS

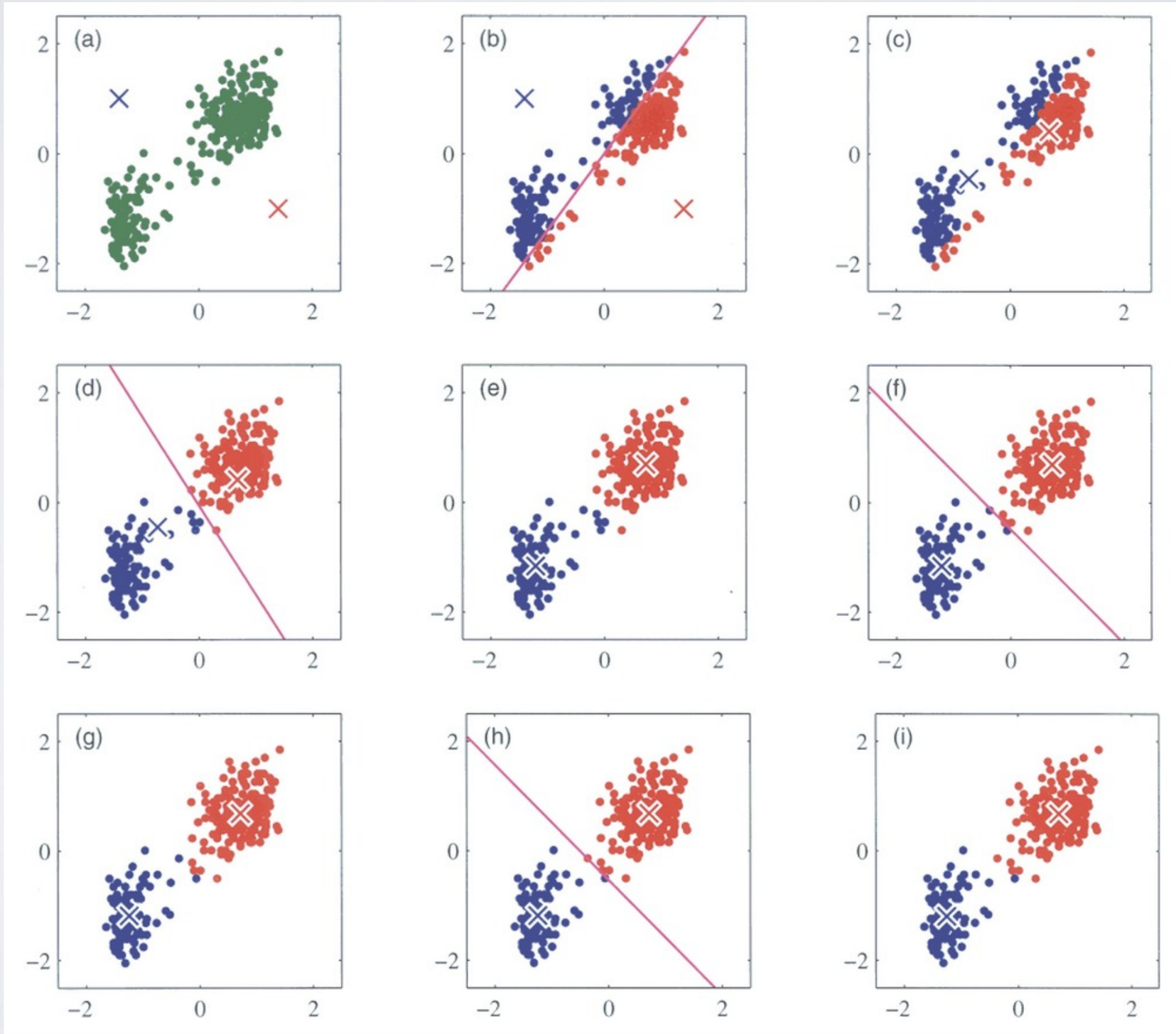
- Discovering the global optimum is NP-hard

- How to find quickly a good solution ?
  - Naive k-means
  - K-means ++ (used in most current implementations)
  - Use optimized data structure (KDtrees…)

NAIVE K-MEANS

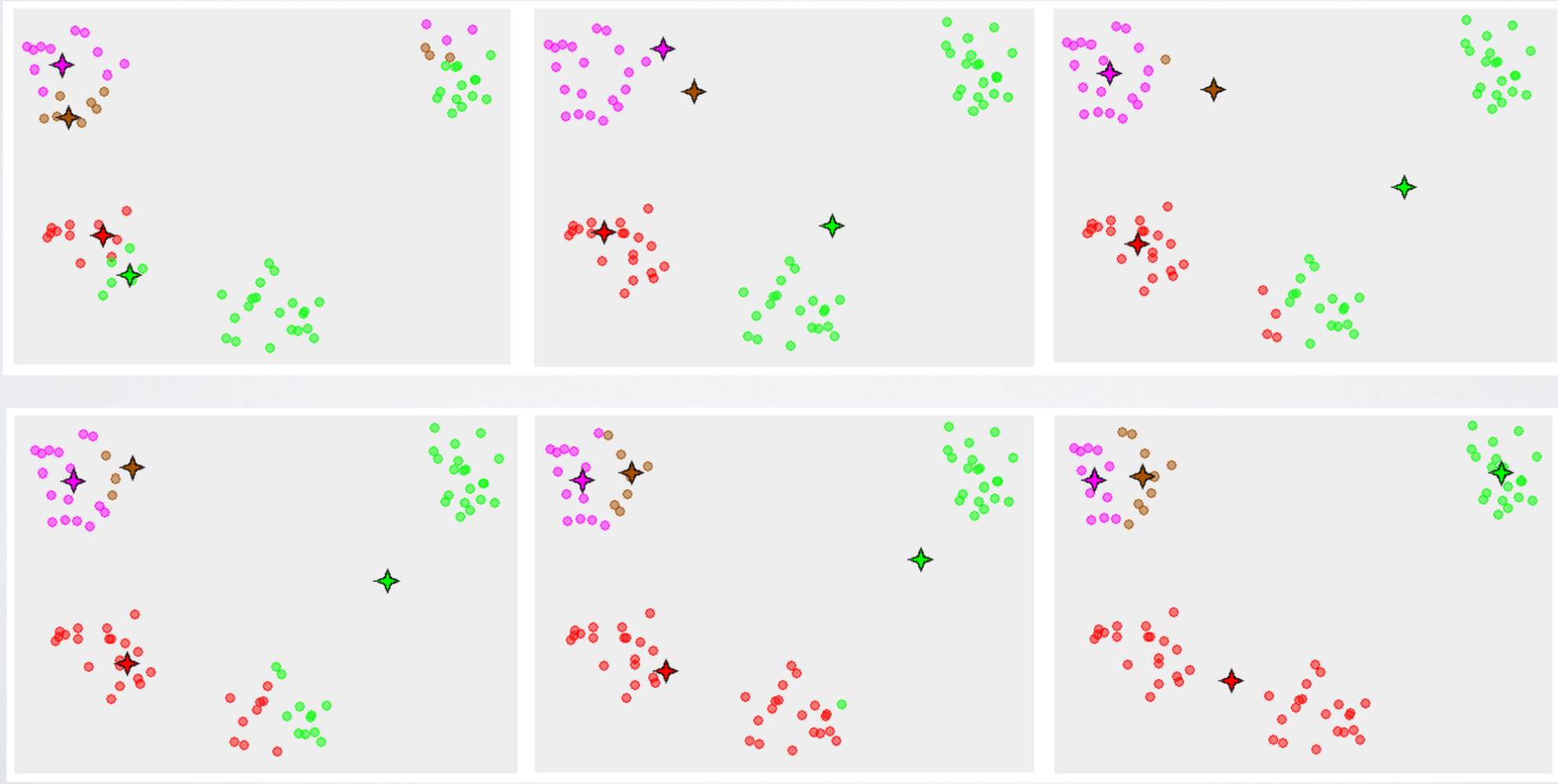
- 1)Assigment: Assign each item to its closest cluster center
- 2) Update: Recompute the center of each cluster as the mean (centroid) of items that compose that cluster
- Start with random centroids

NAIVE K-MEANS



NAIVE K-MEANS

- Known limit: convergence to poor local minimum if poor initial centroids



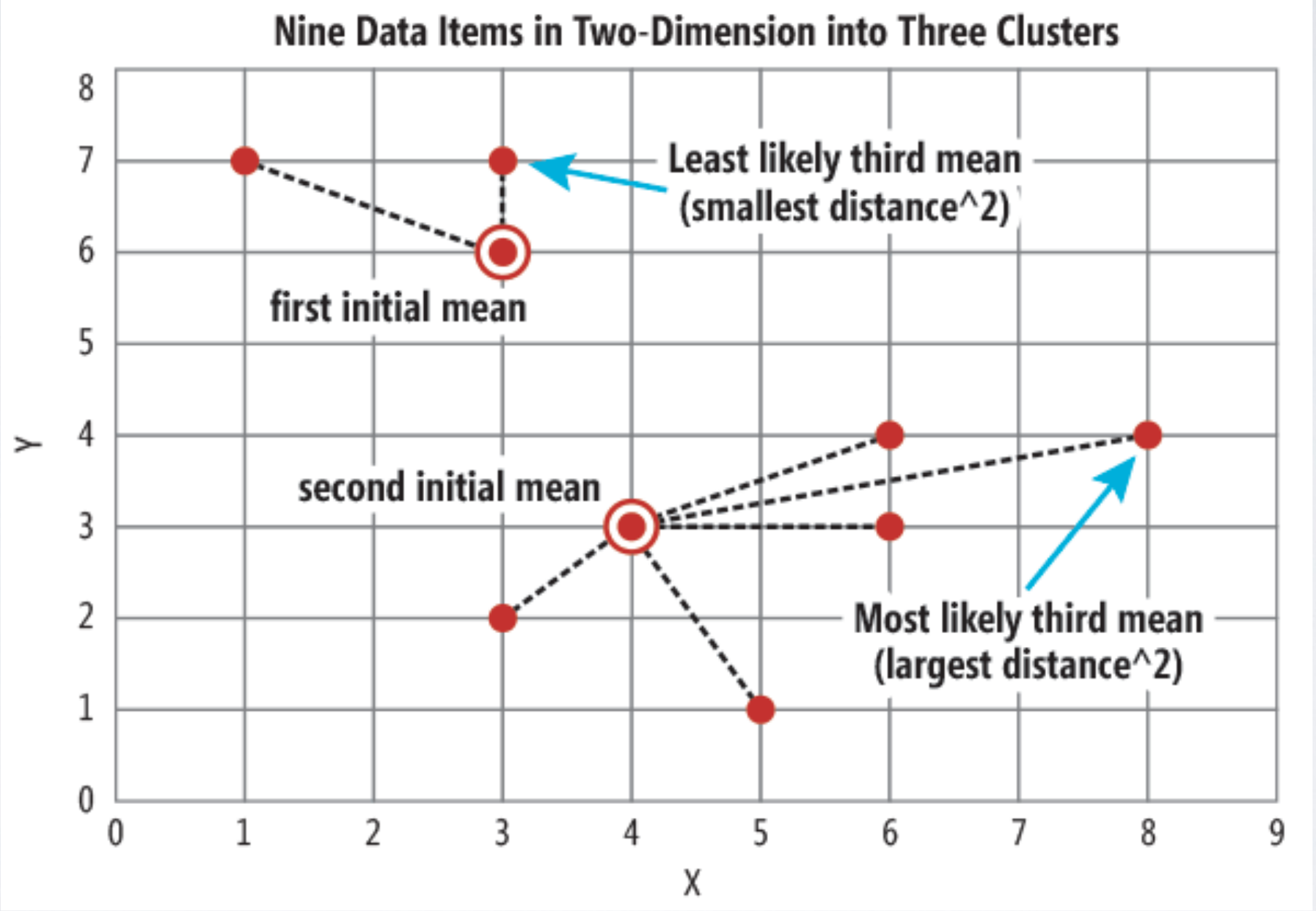
K-MEANS++

- Several variants to choose wisely the initial centroids
- K-means++ is proven to improve the results, statistically
  - Not always, but improves more often than deteriorate the results.

K-MEANS++

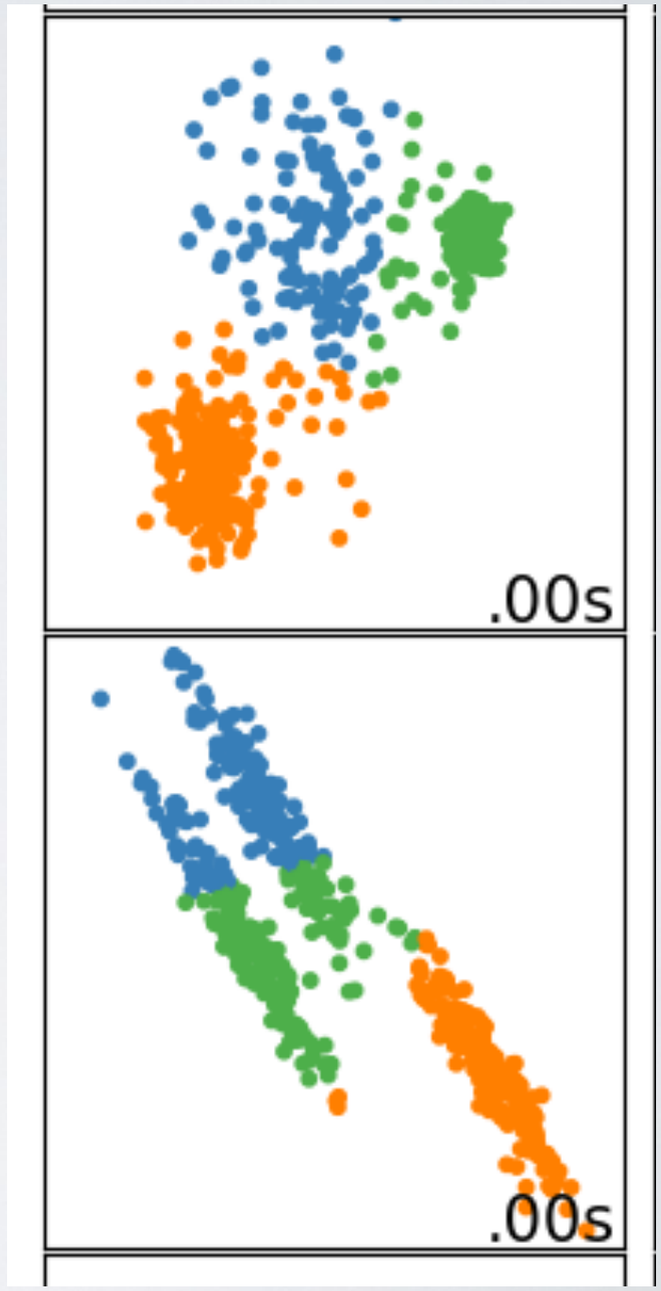
1. Choose one center uniformly at random among the data points.
2. For each data point x not chosen yet, compute $D(x)$, the distance between x and the nearest center that has already been chosen.
3. Choose one new data point at random as a new center, using a weighted probability distribution where a point x is chosen with probability proportional to $D(x)^2$.
4. Repeat Steps 2 and 3 until k centers have been chosen.

K-MEANS++


Nine Data Items in Two-Dimension into Three Clusters
Least likely third mean
(smallest distance^2)
first initial mean
second initial mean
Most likely third mean
(largest distance^2)
Y
X
0
1
2
3
4
5
6
7
8
9

WEAKNESSES

- We can identify some clear weaknesses:
  - K-means has a tendency to search for clusters of equal sizes (minimize **overall** cluster variance)
  - Clusters tend to be **circular**, since all directions are worth the same.



NORMALIZATION

- Very important point: k-means is based on **euclidean distance**.
  - We minimize the inter-cluster euclidean distance between points
  - We could adapt the method to other distances

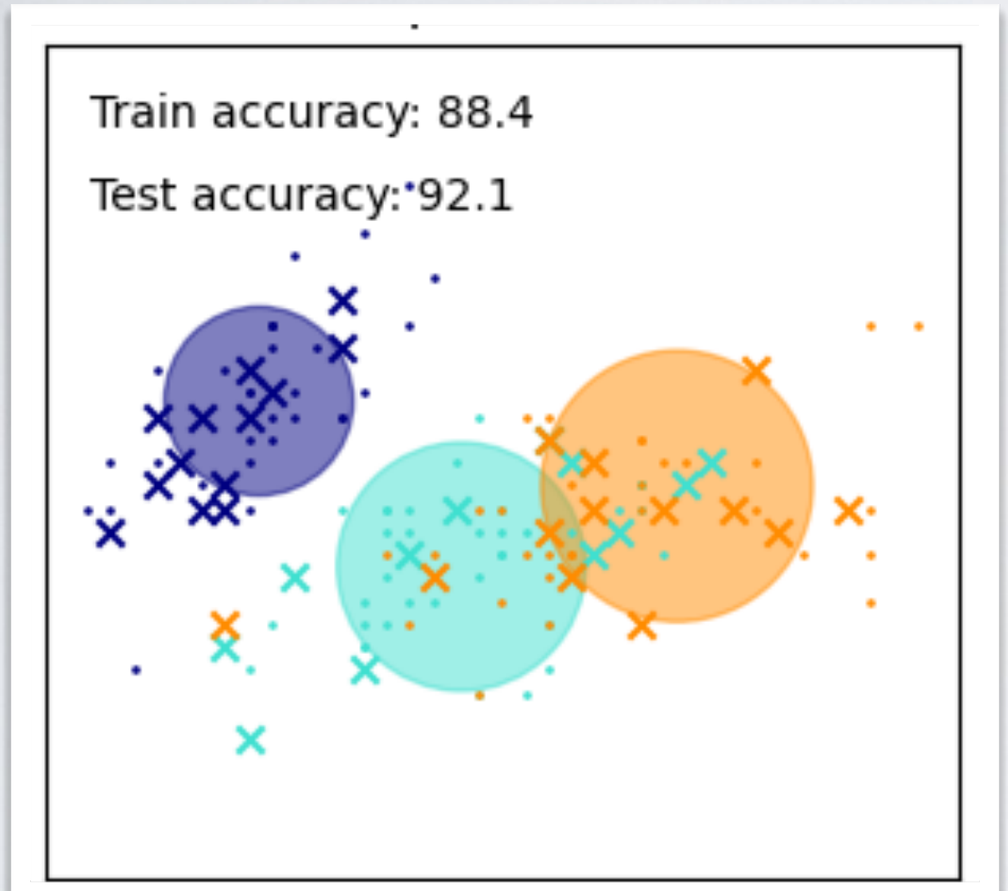
- Data need to be **normalized/standardized**
  - Clustering based on age in years and revenue in $. The "distance" in $ will dominate
  - Remember: normalization/standardization are not fixing magically problems (outliers..)
    - You need to **think**: is 1 unit in one dimension *worth* 1 unit in other dimensions ?

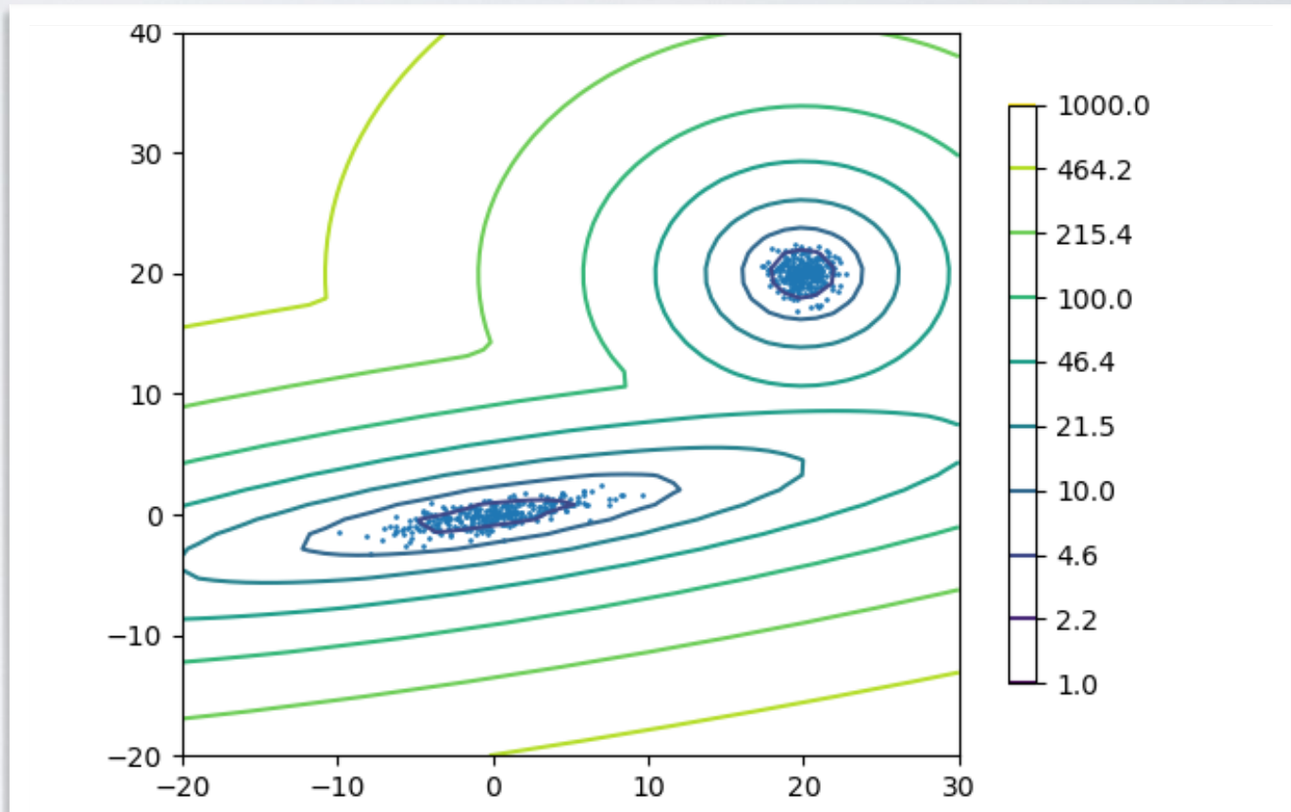
GAUSSIAN MIXTURES

GAUSSIAN MIXTURES

- Generalize k-means concept:
  - Clusters are sets of points that are close in euclidean space
  - Different clusters tend to be far appart
- Translate it statistically:
  - Each cluster can be described using a normal distribution centered on its centroid, with the probability of observing points decreasing with the distance to the centroid.

GAUSSIAN MIXTURES





GAUSSIAN MIXTURES

- We define a **generative model** for k clusters
  - Each cluster corresponds to a gaussian distribution, defined by a center and a *variance*, or *covariance matrix*
  - The problem to solve is to find the parameters Θ (centers, variances) that maximize the likelihood of the corresponding model to generate the observed items X
  - More formally, we are searching for: $\arg\max_{\Theta} p(X \mid \Theta)$

K-MEANS EQUIVALENCE

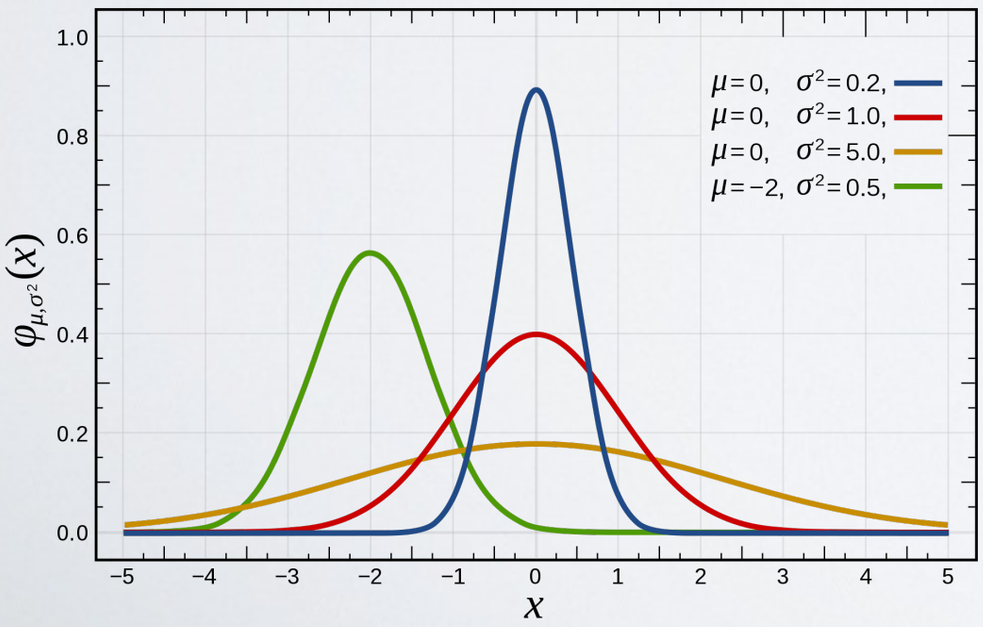
$$\begin{bmatrix} \mathrm{Var}(x_1) & \cdots\cdots & \mathrm{Cov}(x_n,x_1) \\ \vdots & \cdot & \vdots \\ \vdots & \cdot & \vdots \\ \mathrm{Cov}(x_n,x_1) & \cdots\cdots & \mathrm{Var}(x_n) \end{bmatrix}$$

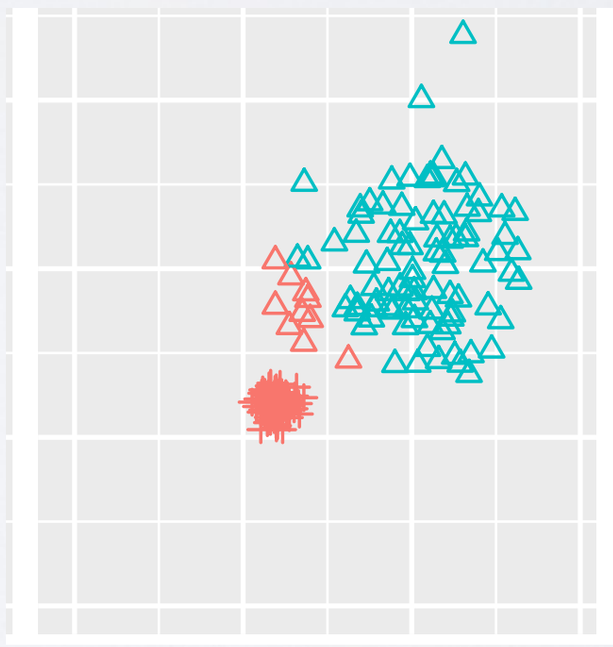
- If we assume that:
  - The gaussian distributions are defined only by their variance, not by complete covariance matrices
    - Similar in all directions, "spherical"
  - The variance value is the same for all gaussian distributions
    - Spheres of the same "size"
  - The probability for each item to be generated by each of the gaussian distribution is identical

- Then it can be shown that the objective is equivalent to the k-means objective !
  - We can relax some of those constraints to get better results

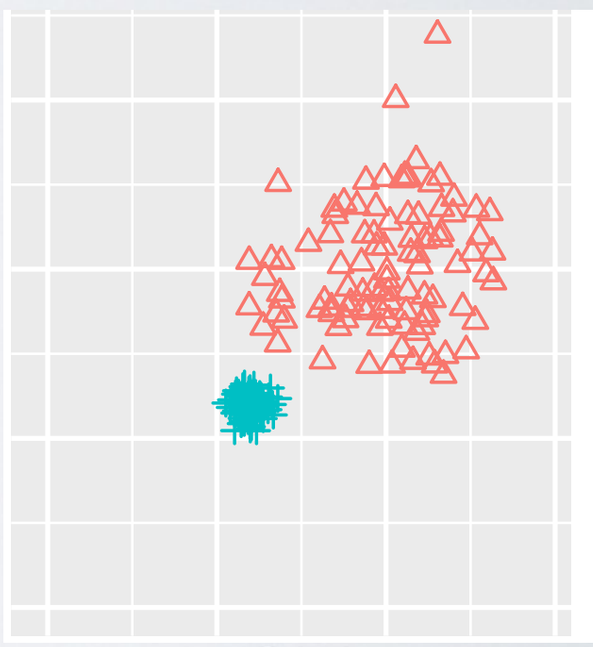
DENSITY HETEROGENEITY

- Allowing denser/sparser clusters
  - Consider the case in which gaussians are defined by a single value of variance (covariance=0)
  - If they differ for each clusters, some can be denser than others





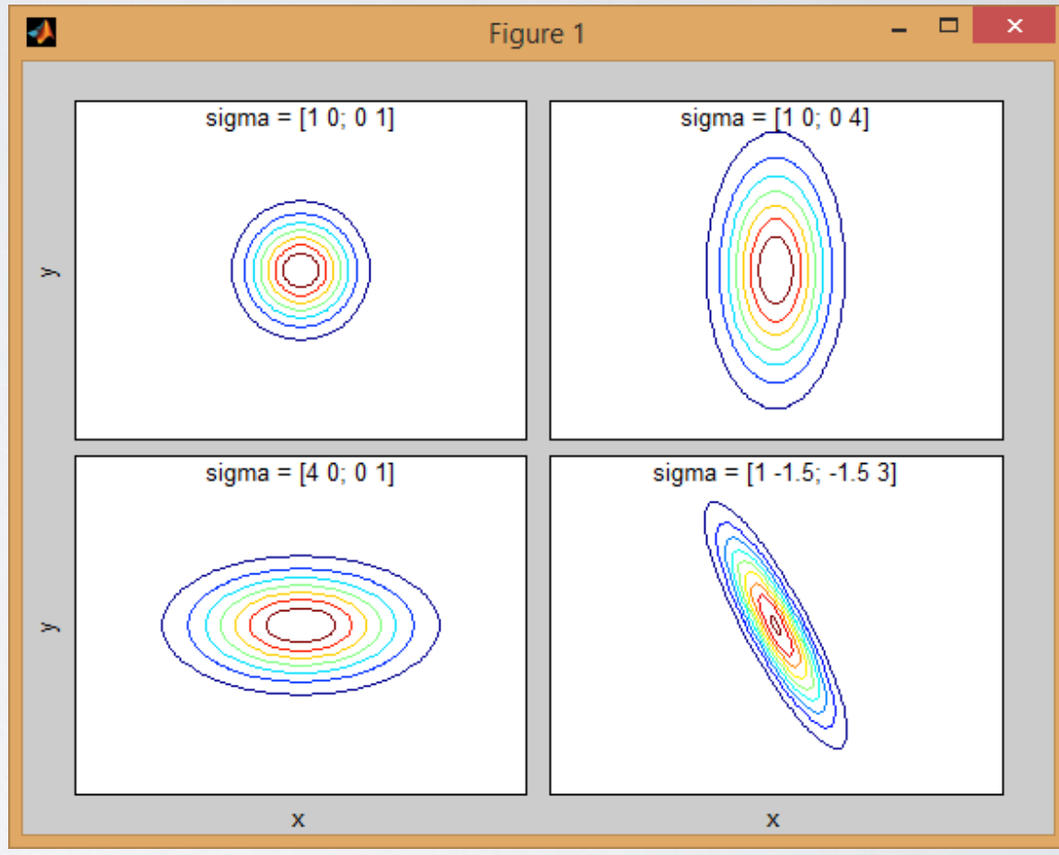
K-means



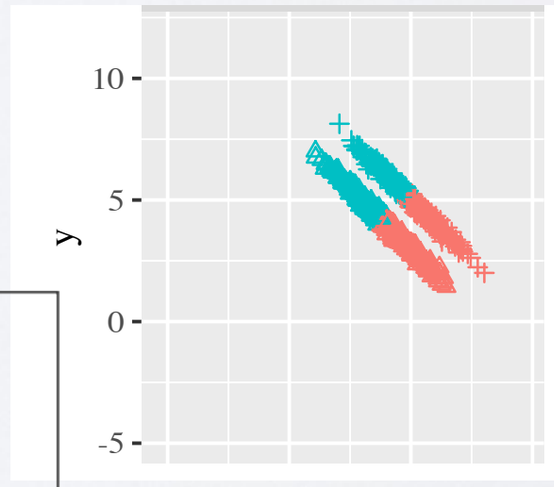
GM,
free variance

SHAPE VARIATIONS

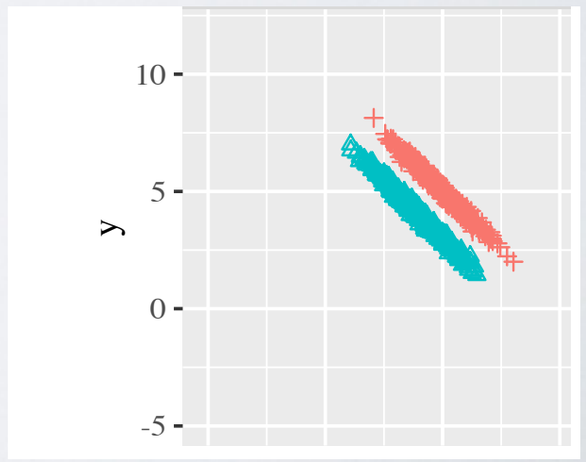
- Allowing non-circular shaped clusters
  - If values on the diagonal of the covariance matrix differs, the matrix can have ellipsoidal shape, in the direction of the axes
  - If the full covariance matrix is inferred, any ellipsoidal shape can be obtained



$$\begin{bmatrix} \mathrm{Var}(x_1) & \cdots & \mathrm{Cov}(x_n, x_1) \\ \vdots & \ddots & \vdots \\ \mathrm{Cov}(x_n, x_1) & \cdots & \mathrm{Var}(x_n) \end{bmatrix}$$

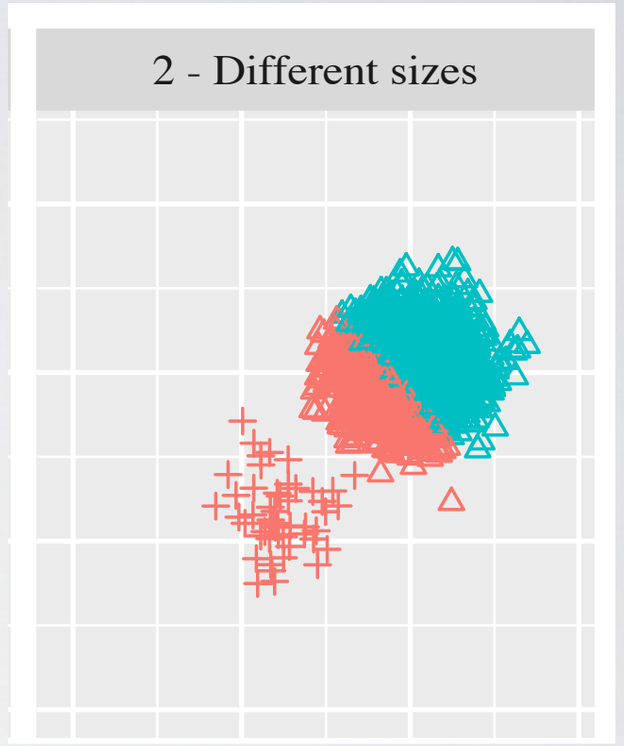


K-means

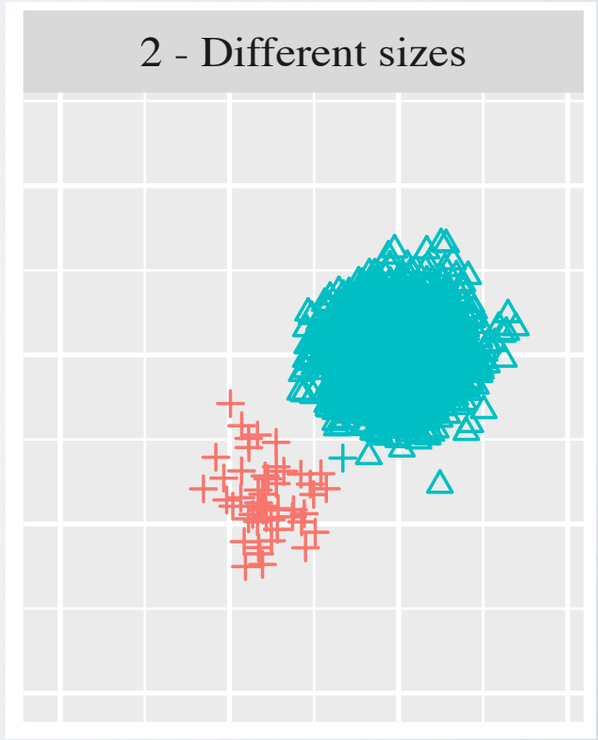


Full gaussian

SIZE HETEROGENEITY



- The fraction of all items generated by each generative gaussian (e.g., cluster) is the same.



- We usually add a *strength* parameter π to weight the fraction of items generated by each cluster

$$p(X) = \sum_{k=1}^{K} \pi_k G(X \mid \mu_k, \sigma_k)$$

ALL TOGETHER

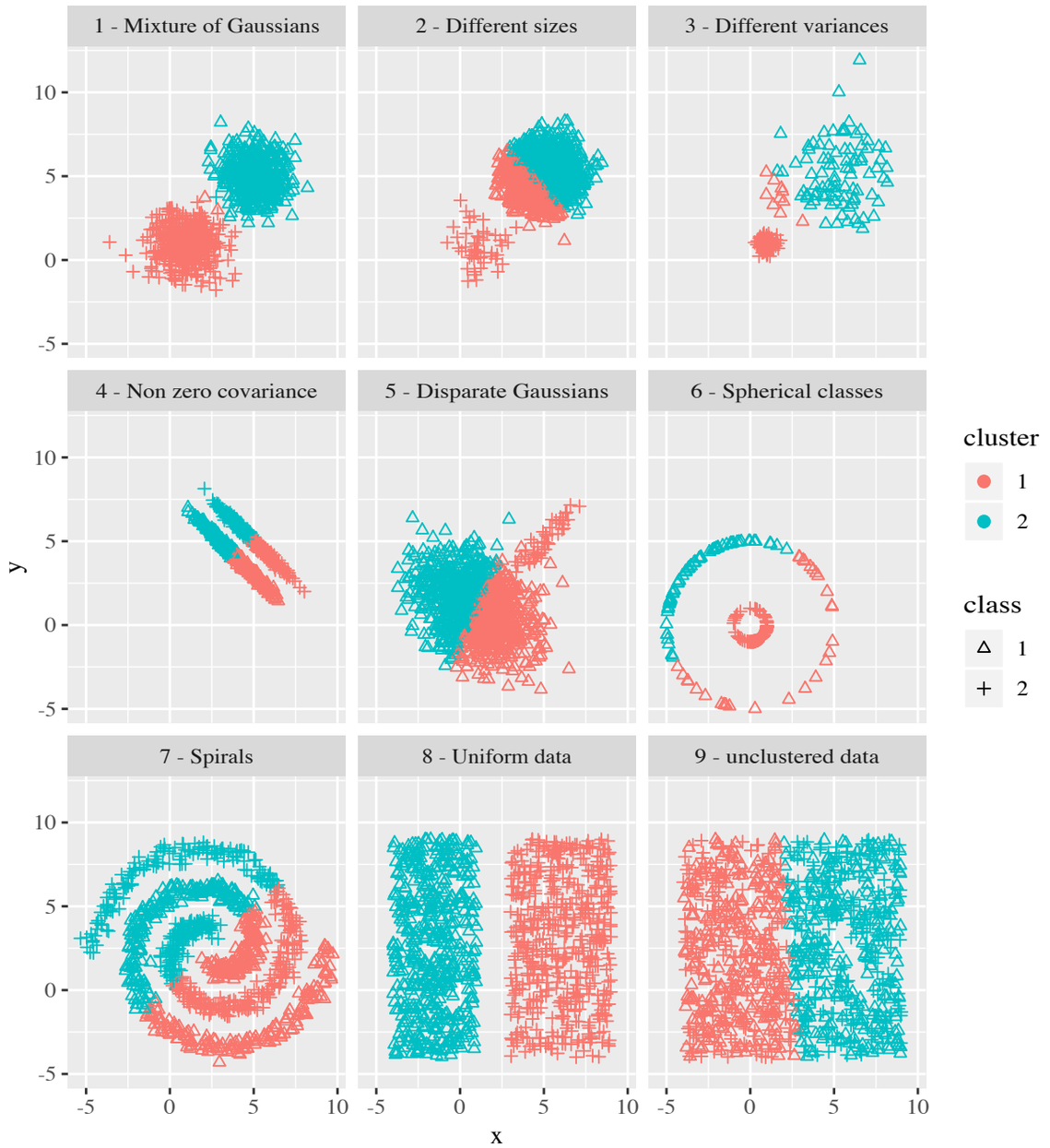
$$p(X) = \sum_{k=1}^{K} \pi_k G(X \mid \mu_k, \sigma_k)$$

$$\arg\max_{\Theta} p(X \mid \Theta)$$

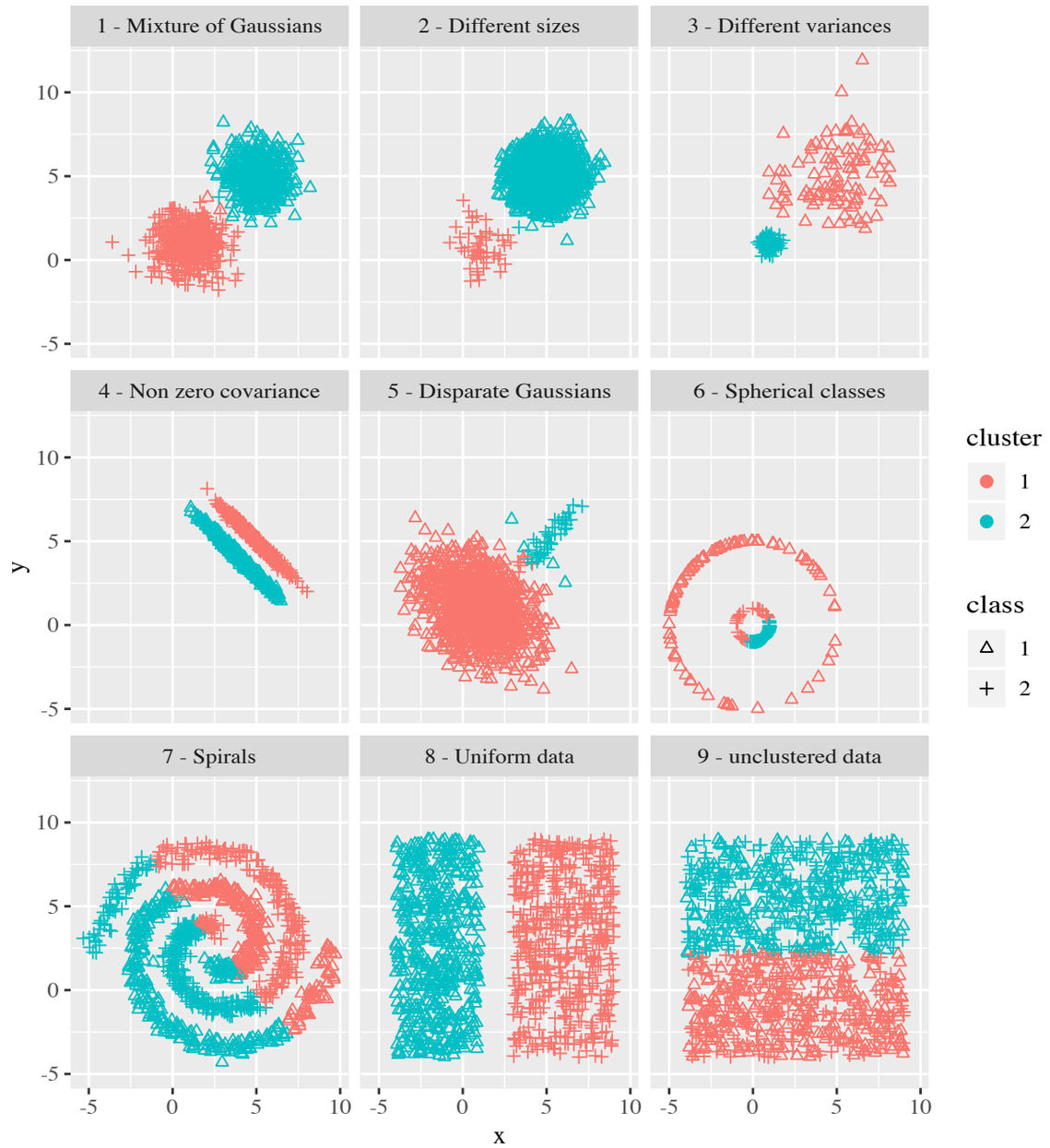
$$\Theta = \mu, \sigma, \pi$$

K-MEANS COMPARISON

K-means



Full Gaussian Mixture

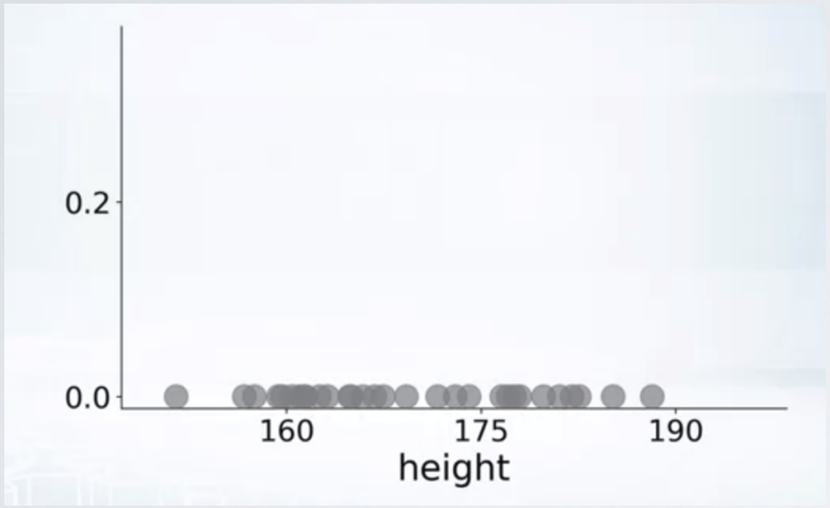


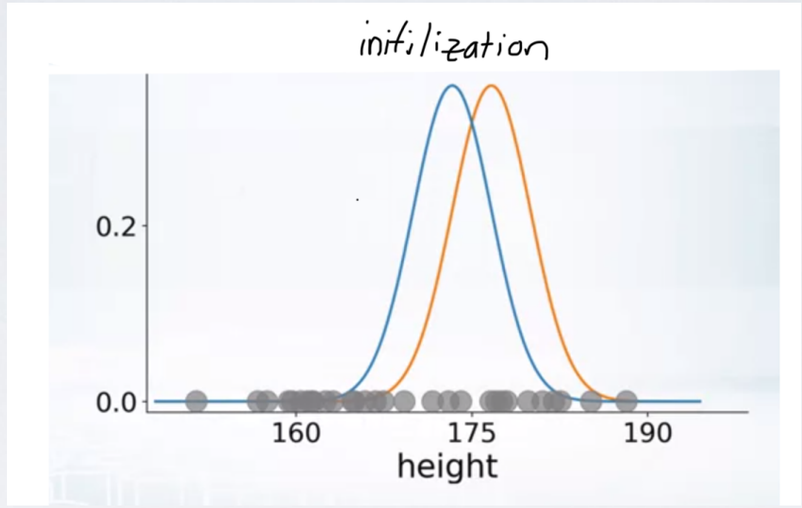
https://smorbieu.gitlab.io/gaussian-mixture-models-k-means-on-steroids/

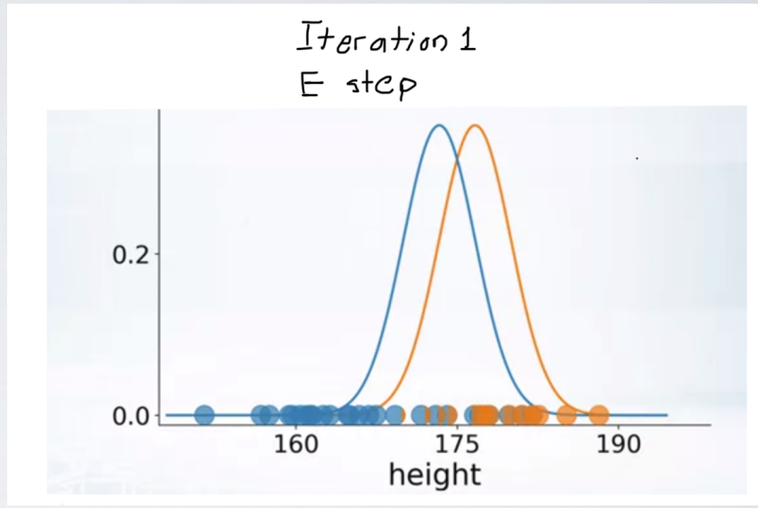
EM ALGORITHM

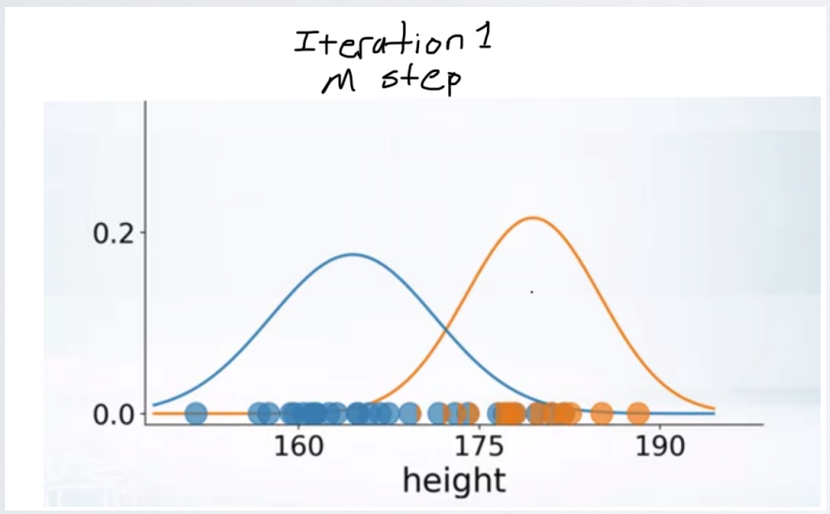
- To search for the parameters, we can use a method similar to naive k-means known as EM (Expectation Maximization)
  - Note Z the cluster assignation of items to their **most likely** clusters
  - 1)Initialize parameters Θ to random values
  - 2)(E) Compute Z, given Θ
  - 3)(M) Use assignations in Z to update values of Θ
  - 4)Iterate steps 2 and 3 until convergence

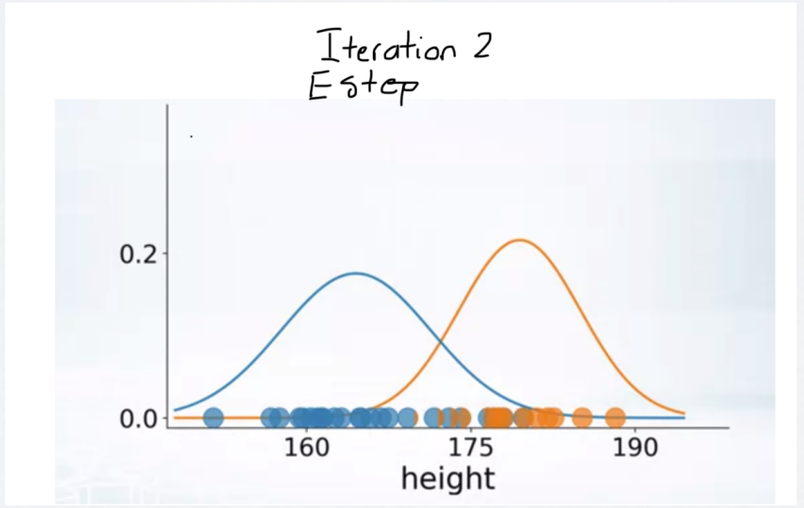
EM ALGORITHM

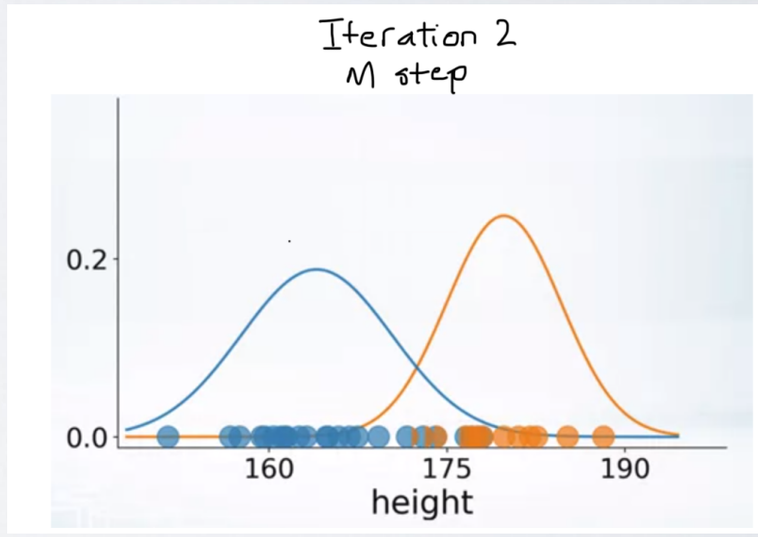








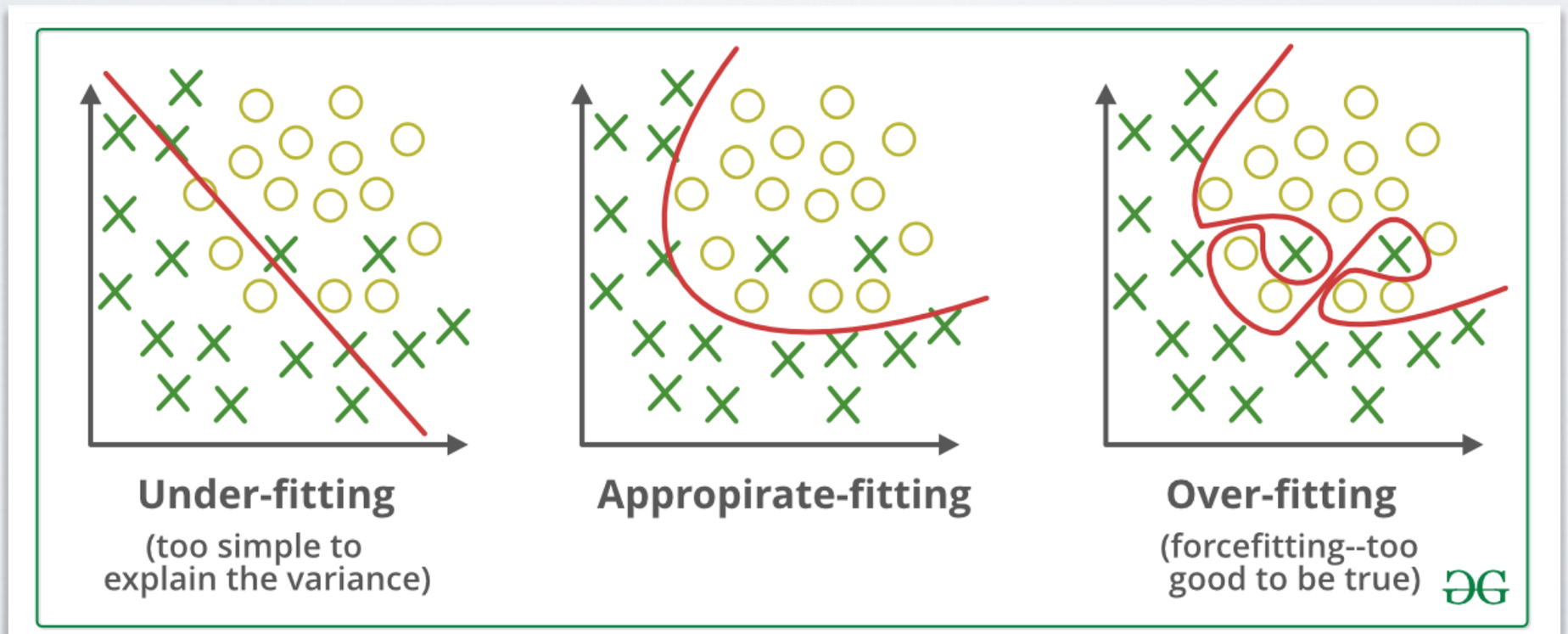




https://towardsdatascience.com/gaussian-mixture-models-d13a5e915c8e

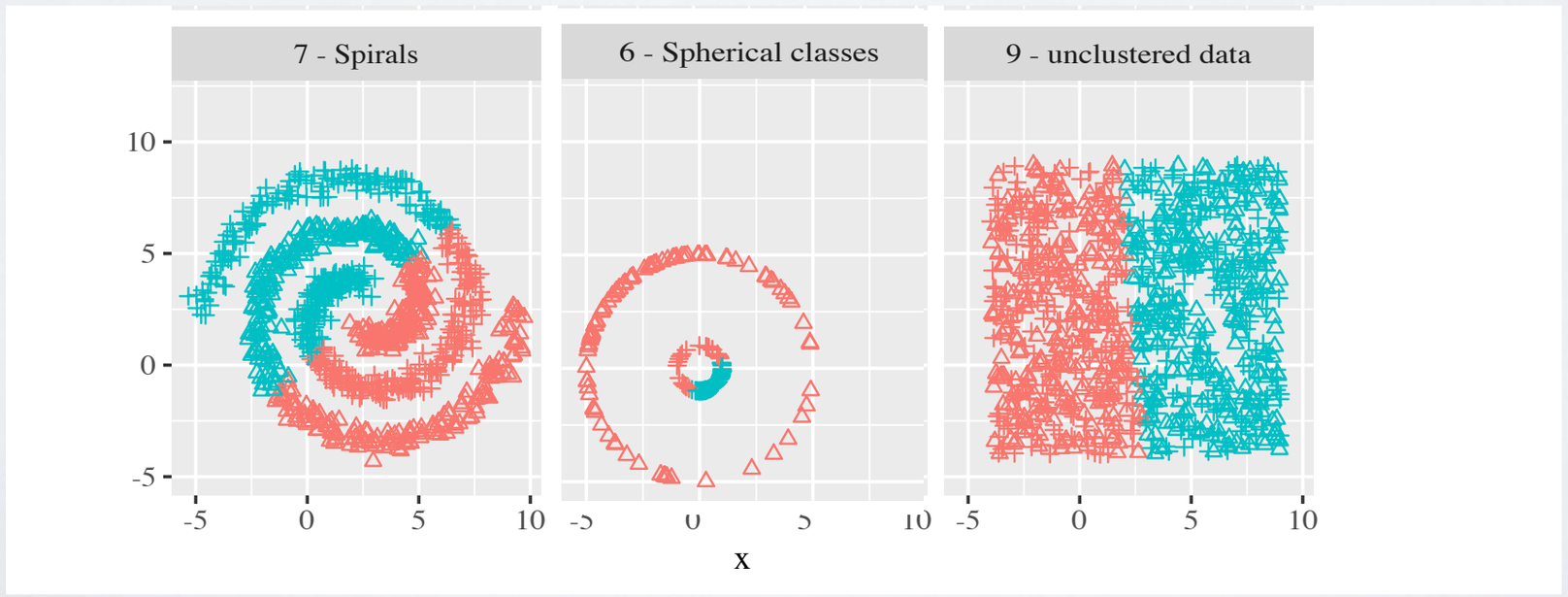
PROS AND CONS

- Gaussian mixture seems an improvement over k-means. Why not always using it?
  - Force of habits
  - Higher computational cost (More parameters => More complex problem)
  - Higher possibility of overfitting (More parameters =>More overfit risk)



REMAINING PROBLEMS

- We can mention 3 problems remaining (at least)
  - The number of clusters still need to be provided.
    - If allowed to change, it will always converge to the trivial solution with each item in its own cluster
  - If the data is completely random, the method still finds clusters
  - Impossible to discover non-convex structures, such as circles or spirals



MDL

- Discovering automatically the number of clusters —and thus finding no clusters in random data— is possible using an MDL approach

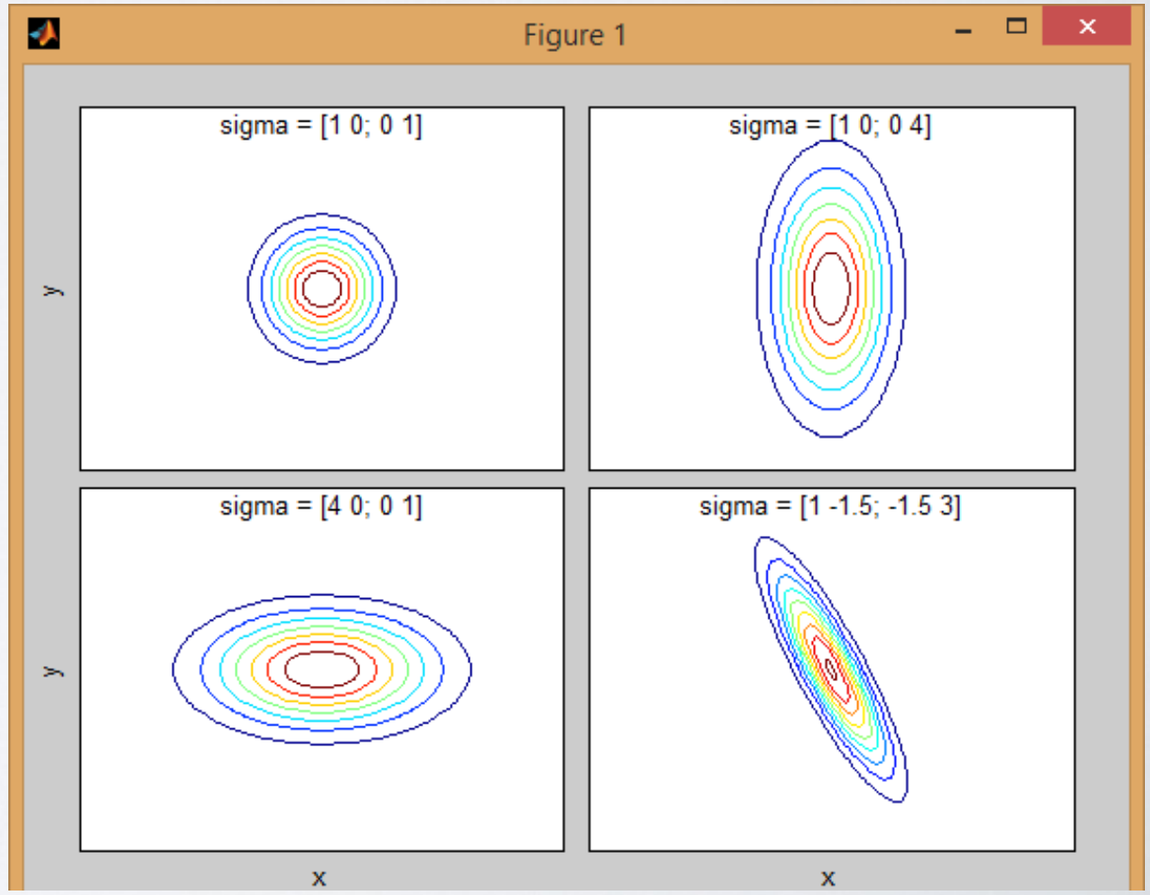
- MDL = Minimum Description Length

- The principle is to search a solution maximizing the compression rate, i.e., minimizing the *cost* of the description, e.g., in bits.

- Method introduced later

NORMALIZATION

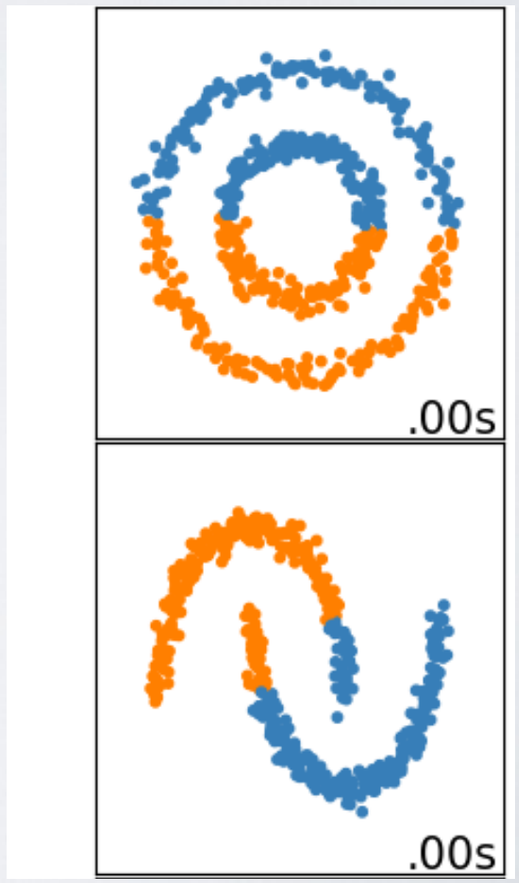
- Is normalization as important for full GM models as for k-means?



DBSCAN

K-MEANS/GM LIMITS

- The problem of spiral/Circulal/weird shaped clusters comes from the assumption that items of a cluster should be "normally distributed" around their mean



LOCAL DEFINITIONS

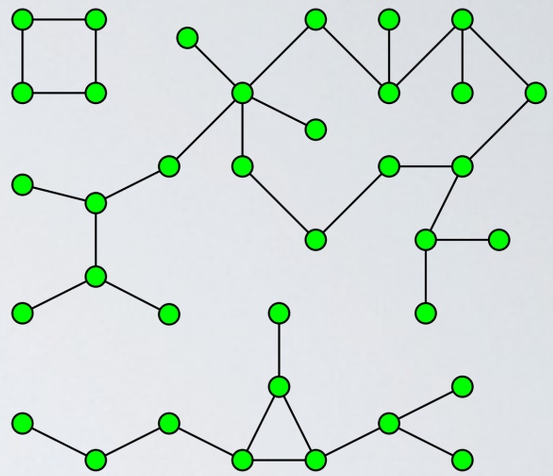
- To overcome this problem, several methods propose local definitions of clusters
  - Does not explicitly optimize a global function
  - Items belong to clusters because they are close enough, locally, to other items in that cluster
  - Clusters exist because there is continuum between all items in it, locally

DBSCAN

- Define some local parameters:
  - ϵ, the distance threshold above which items are considered "too different"
  - *minPts*, a minimal number of reachable points
  - No need to define a number of clusters !

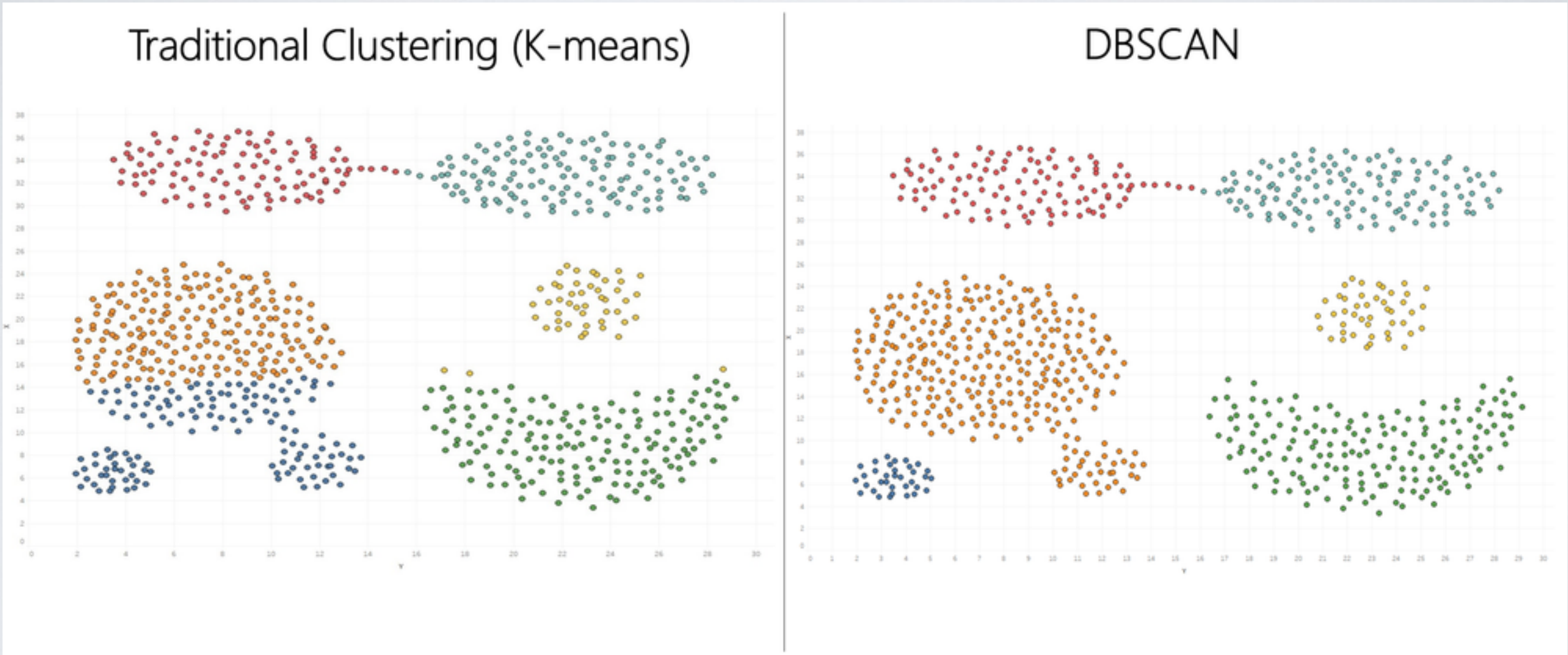
- Define:
  - An item p is a *core point* if it has at least *minPts* items at distance less than ϵ
    - Including p itself

DBSCAN: GRAPH DEFINITION

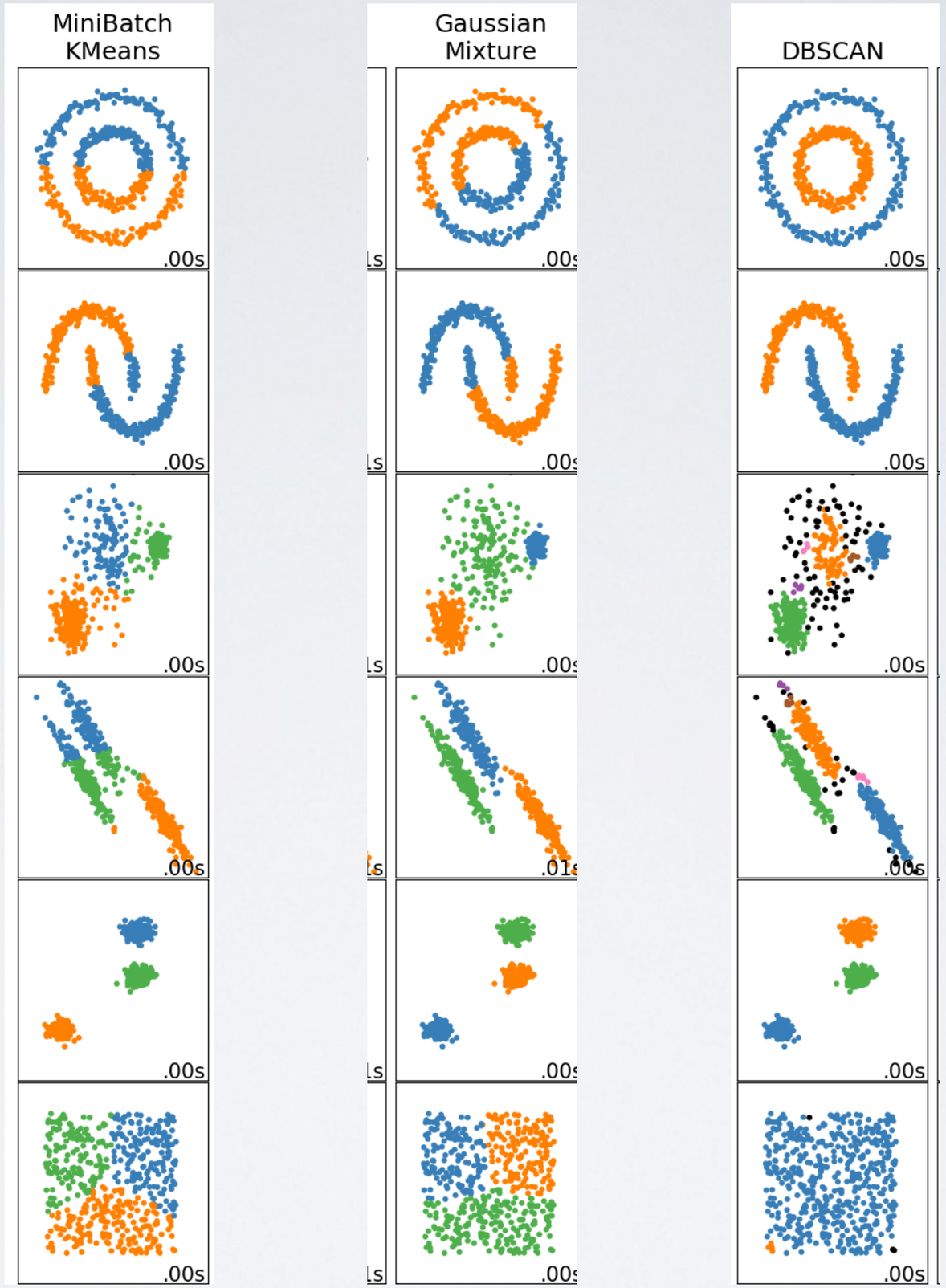


- 1)Build a graph such as
  - Each core node is a node
  - A link exist between core nodes if they are at d<ϵ
- 2)Detect the connected components of the graph
  - 2 nodes belong to the same connected components if there is a path between them
- 3) For all non-core nodes:
  - If they have no core points directly reachable, discard them as noise
  - Else, attribute them to (one of) the clusters for which one core point is directly reachable
    - Variant DBSCAN* =>ignore those points as noise

DBSCAN

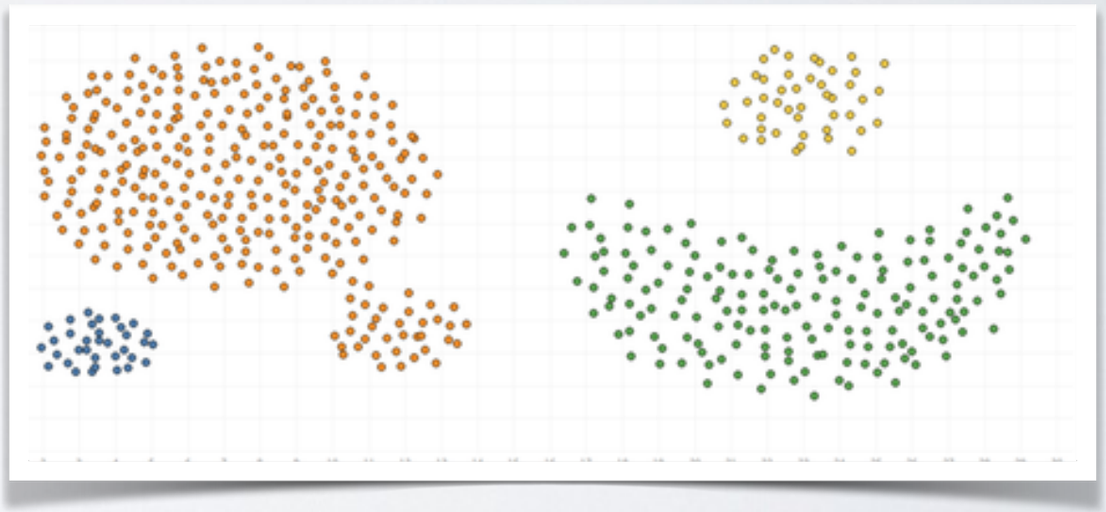


https://community.alteryx.com/t5/Data-Science/Partitioning-Spatial-Data-with-DBSCAN/ba-p/446273


MiniBatch
KMeans
Gaussian
Mixture
DBSCAN
.00s
.01s

DBSCAN

- Strength:
  - No need to define the number of clusters
  - Can discover arbitrarily-shaped clusters
  - A notion of noise



- Weaknesses
  - Defining ϵ is extremely difficult
    - Similar to the number of clusters.
    - In fact it determines the number of clusters…
  - Despite safeguards, risk of the stretched clusters effect

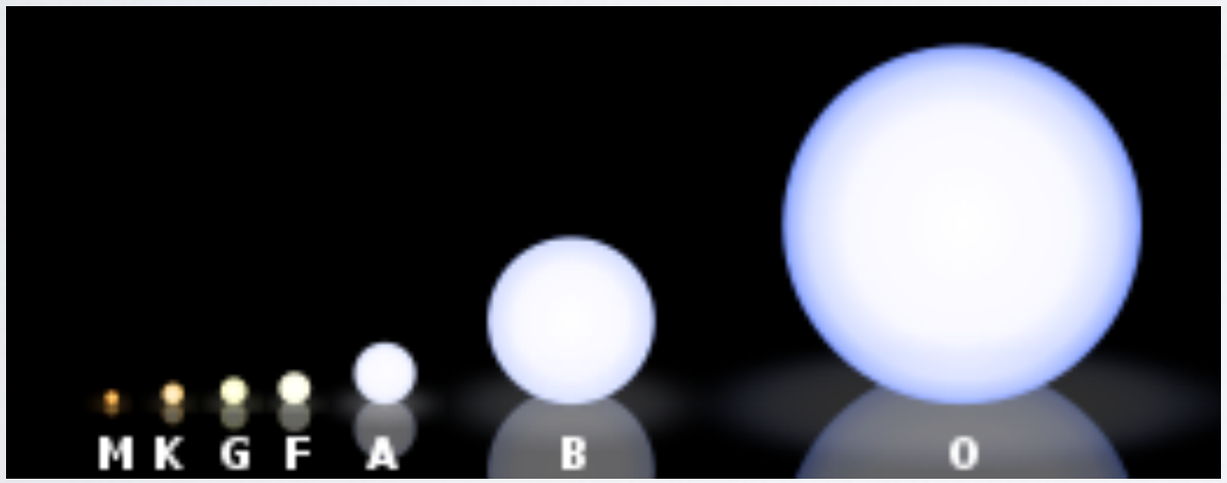
CLUSTERING EVALUATION

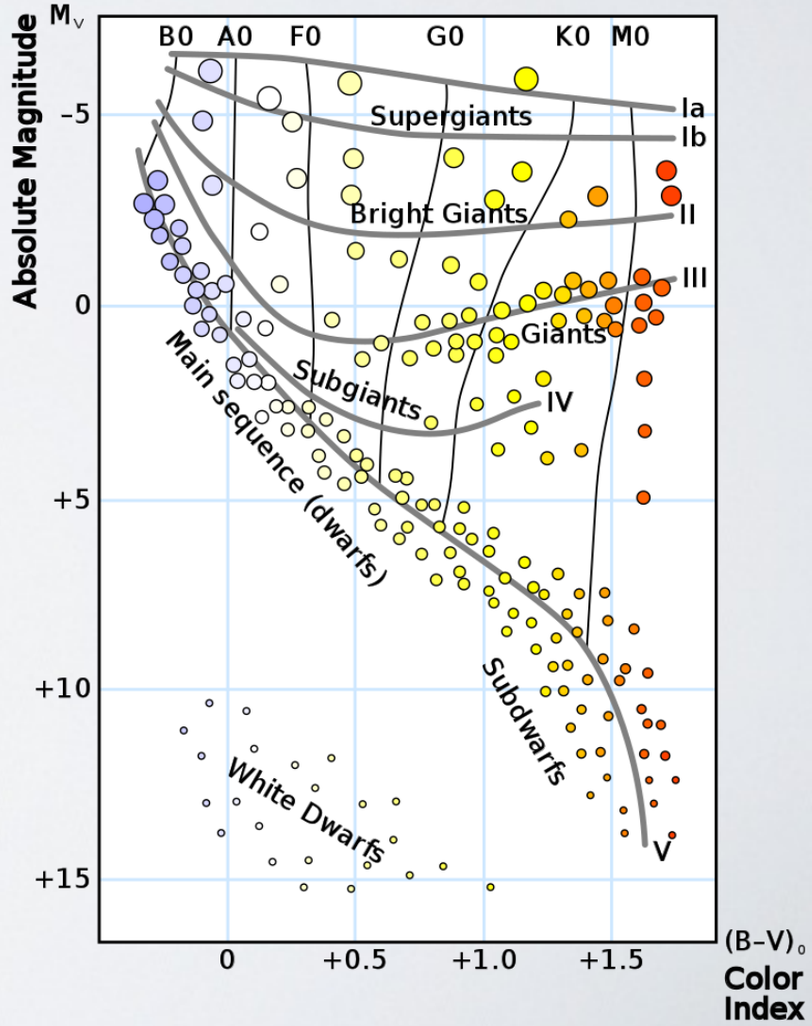
INTERNAL/EXTERNAL

- Two types of evaluation: internal or external
- External Evaluation (extrinsic):
  - Similarly to supervised learning, compares the clusters found with a "ground truth"
  - The ground truth can be exactly the right clustering desired
    - So we are just validating the method, since we already know the answer…
  - The ground truth can be a proxy to what we want
    - e.g., we want to cluster stars based on their characteristics (size, temperature, color…). We already have a manual historic categorization (red dwarf, Brown dwarfs, Red giants…). We assume that the new categories found should be somewhat similar

INTERNAL/EXTERNAL

Class	Effective temperature[2][3]	Vega-relative chromaticity[4][5][a]	Chromaticity (D65)[6][7][4][b]	Main-sequence mass[2][8] (solar masses)	Main-sequence radius[2][8] (solar radii)	Main-sequence luminosity[2][8] (bolometric)	Hydrogen lines	Fraction of all main-sequence stars[9]
O	≥ 30,000 K	blue	blue	≥ 16 $M_\odot$	≥ 6.6 $R_\odot$	≥ 30,000 $L_\odot$	Weak	~0.00003%
B	10,000–30,000 K	blue white	deep blue white	2.1–16 $M_\odot$	1.8–6.6 $R_\odot$	25–30,000 $L_\odot$	Medium	0.13%
A	7,500–10,000 K	white	blue white	1.4–2.1 $M_\odot$	1.4–1.8 $R_\odot$	5–25 $L_\odot$	Strong	0.6%
F	6,000–7,500 K	yellow white	white	1.04–1.4 $M_\odot$	1.15–1.4 $R_\odot$	1.5–5 $L_\odot$	Medium	3%
G	5,200–6,000 K	yellow	yellowish white	0.8–1.04 $M_\odot$	0.96–1.15 $R_\odot$	0.6–1.5 $L_\odot$	Weak	7.6%
K	3,700–5,200 K	light orange	pale yellow orange	0.45–0.8 $M_\odot$	0.7–0.96 $R_\odot$	0.08–0.6 $L_\odot$	Very weak	12.1%
M	2,400–3,700 K	orange red	light orange red	0.08–0.45 $M_\odot$	≤ 0.7 $R_\odot$	≤ 0.08 $L_\odot$	Very weak	76.45%





INTERNAL/EXTERNAL

- Two types of evaluation: internal or external

- Internal Evaluation (Intrinsic):
  - We have no ground truth to compare to
  - We evaluate the intrinsic properties of our clusters, typically
    - If their elements are similar
    - If clusters are far appart /if elements in different clusters are different.

INTERNAL EVALUATION

AD-HOC SCORES

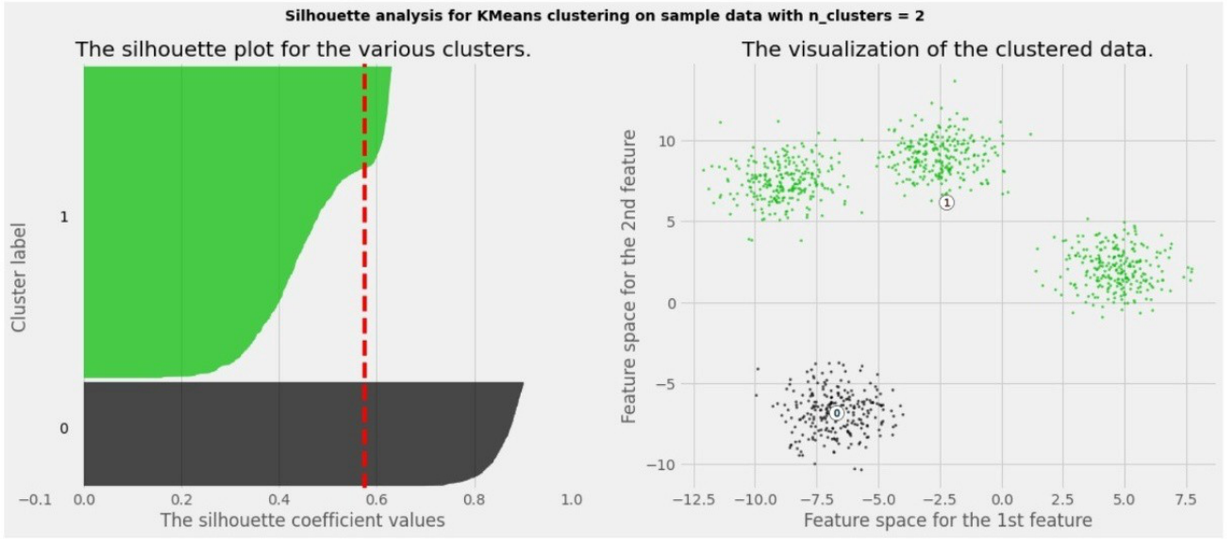
- Several clustering method define their own objective to minimize. This objective can be used as a score for clusters obtained by this method or others
  - k-means minimizes inter-cluster variance
  - Gaussian mixture maximize likelihood

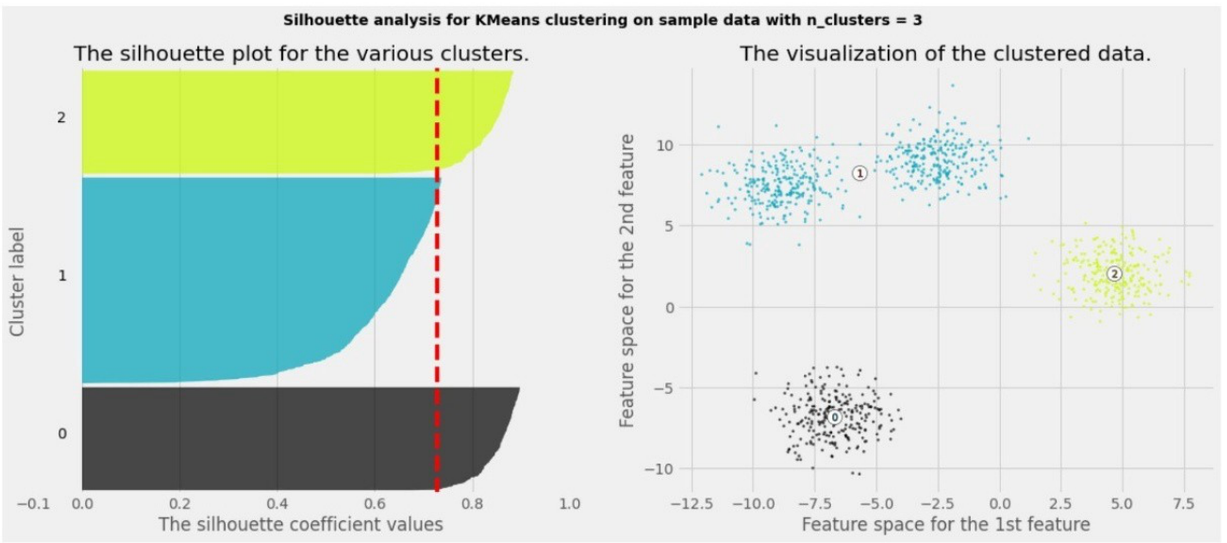
- But can lead to unfair comparison:
  - Using inter-cluster variance to compare k-means and another method such as DBscan is unfair.
    - One explicitly minimizes this objective, the other no…

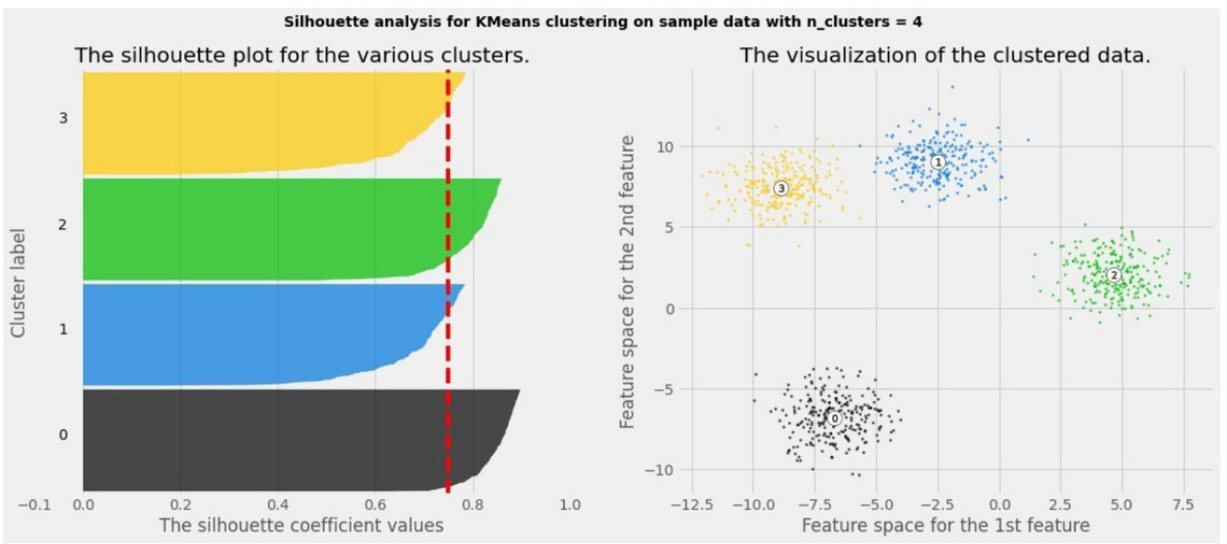
- As always, the choice of a score is equivalent to choosing a definition of cluster…

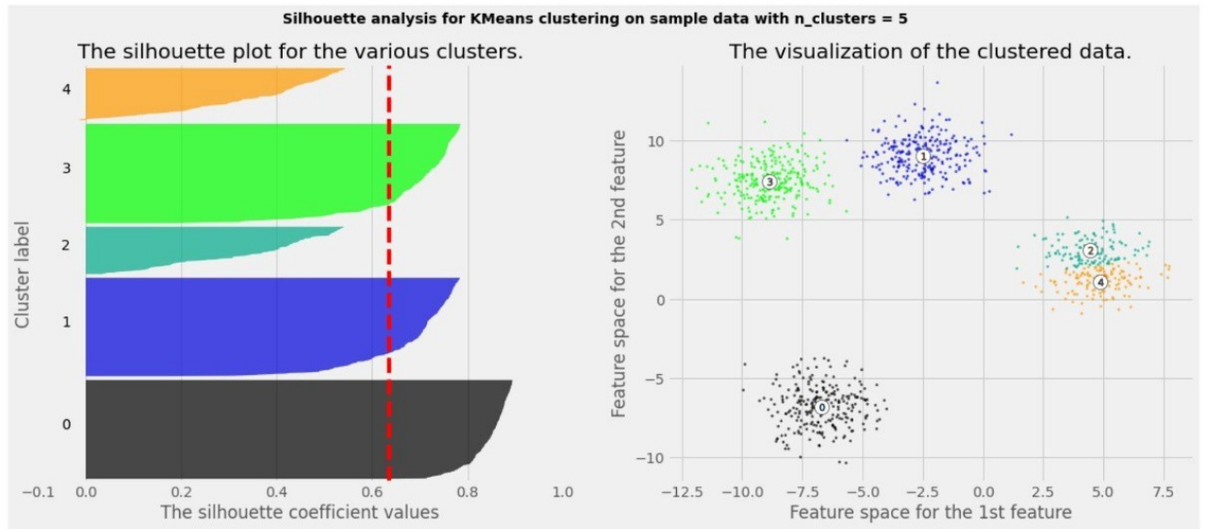
SILHOUETTE SCORE

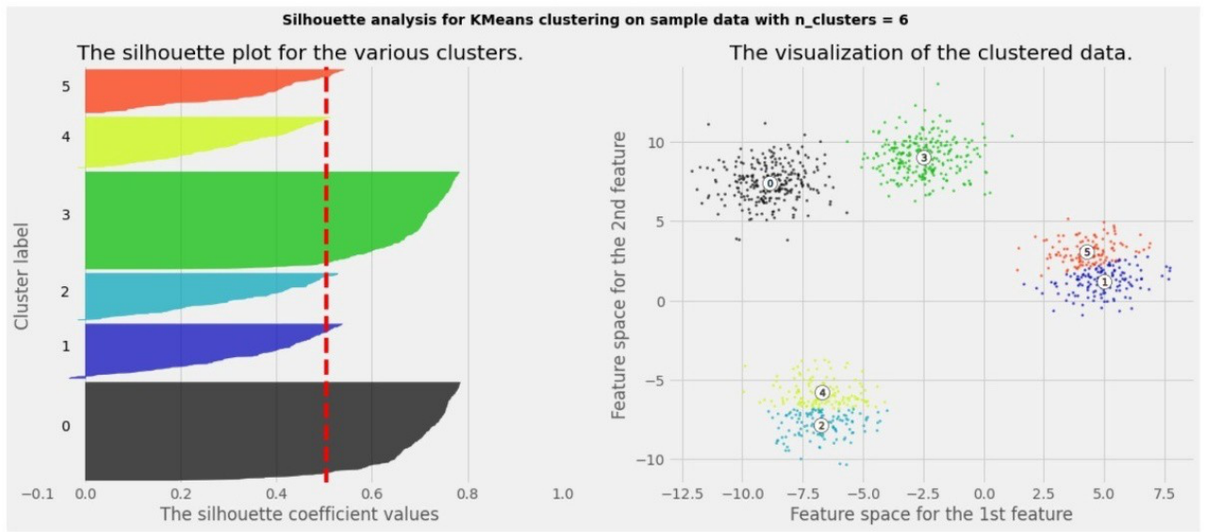
- Intrinsic score
- Silhouette score of 1 item:
  - 1)Compute $a(i)$, average distance to all other points of the same cluster
  - 2)Compute $b(i)$, min average distance to all points of another cluster
  - 3) Silhouette: $s(i) = \begin{cases} 1 - a(i)/b(i), & \text{if } a(i) < b(i) \\ 0, & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1, & \text{if } a(i) > b(i) \end{cases}$
- Silhouette coefficient:
  - Average of all individual Silhouette scores.


Silhouette analysis for KMeans clustering on sample data with n_clusters = 2
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature


Silhouette analysis for KMeans clustering on sample data with n_clusters = 3
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature

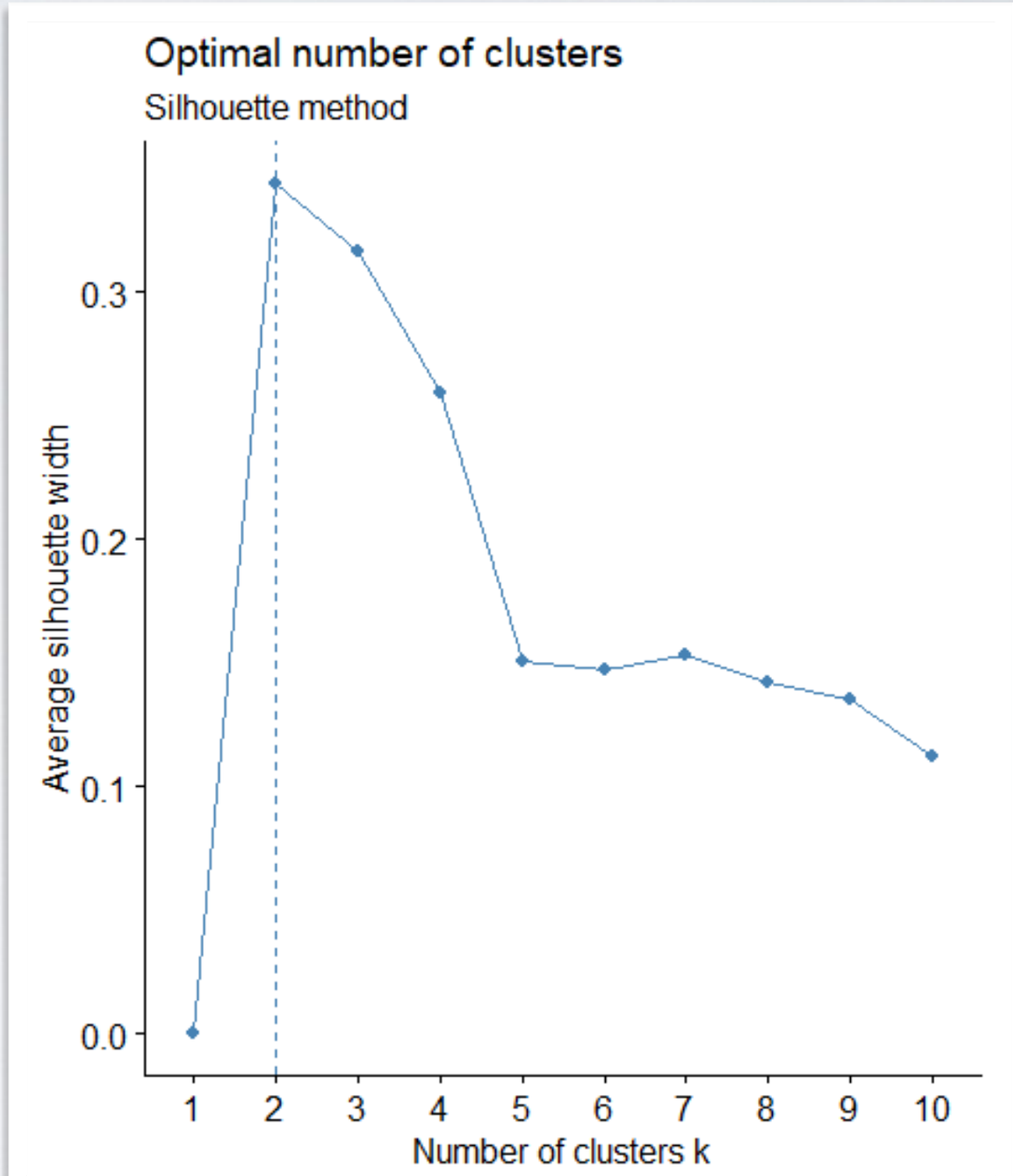

Silhouette analysis for KMeans clustering on sample data with n_clusters = 4
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature

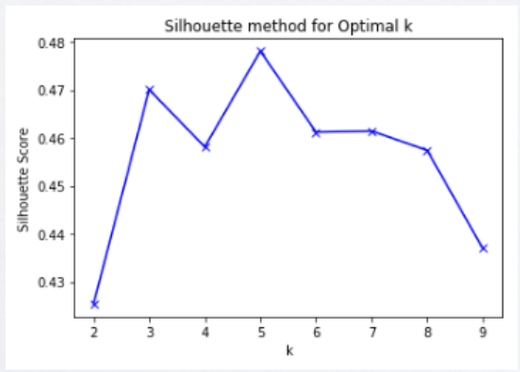

Silhouette analysis for KMeans clustering on sample data with n_clusters = 5
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature


Silhouette analysis for KMeans clustering on sample data with n_clusters = 6
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature

AUTOMATIC K SELECTION

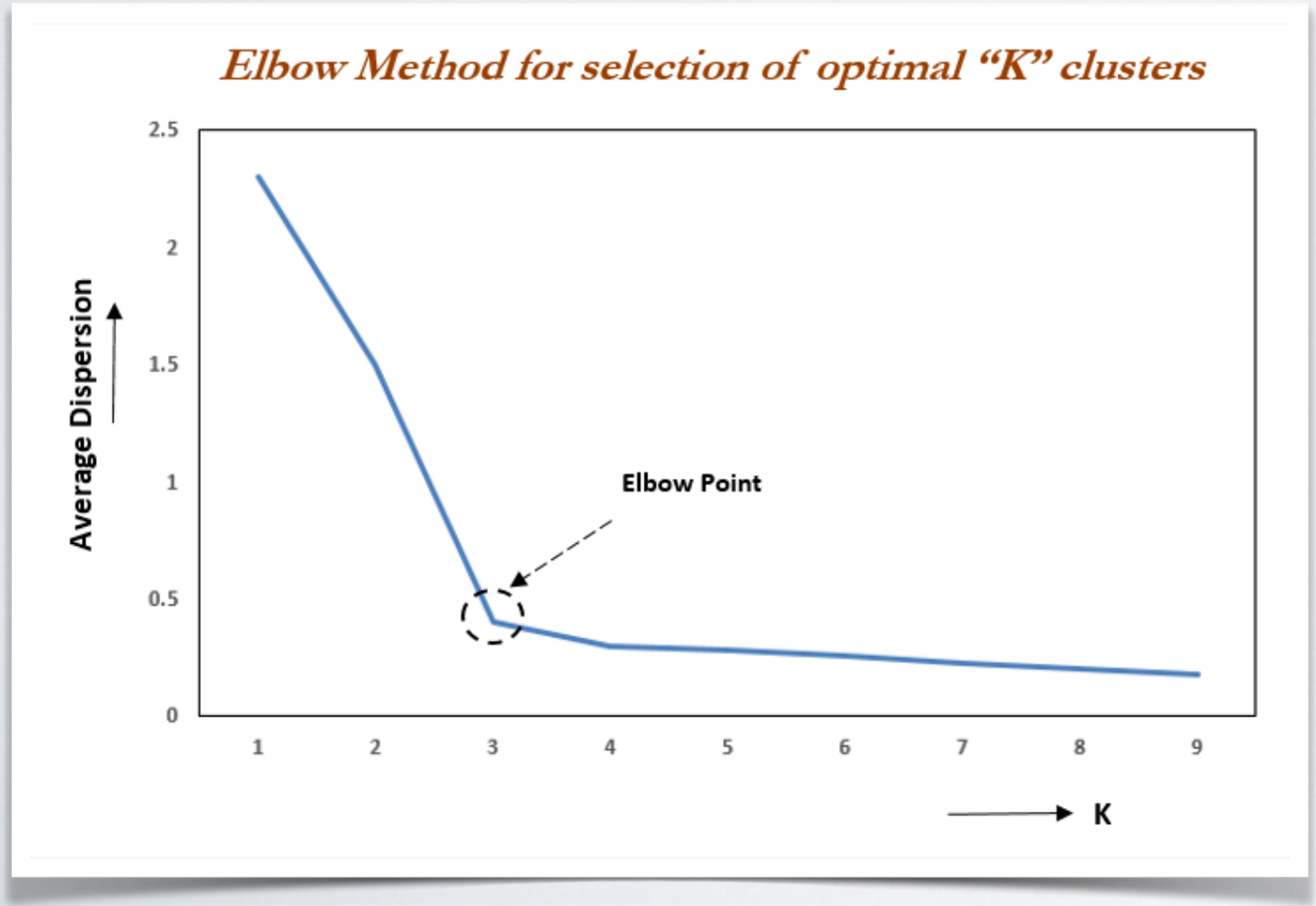
- The Silhouette score can be used to choose automatically the number of clusters:
  - We vary the number of clusters k, and search for the maximum

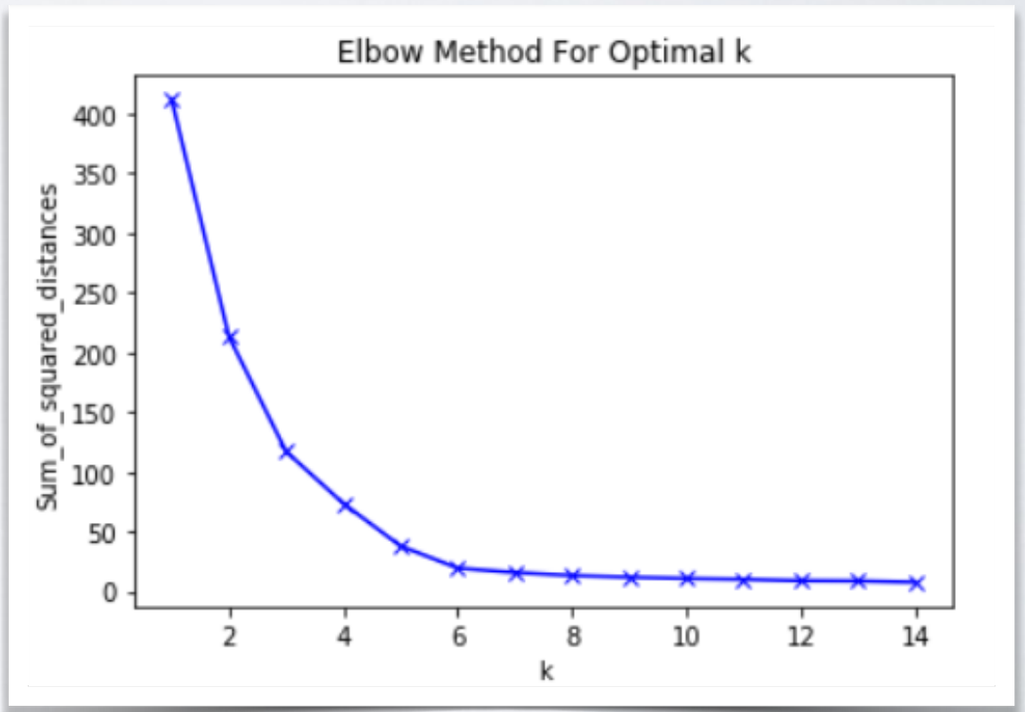




VARIANT: ELBOW METHOD

- Another well known method to find automatically the number of clusters consists in plotting a measure of quality such as the inter-cluster variance, and cut at an "elbow"
  - Diminishing returns=> less "worthy" to continue





EXTERNAL EVALUATION

EXTERNAL EVALUATION

- Rand Index = Accuracy over node pairs

$$RI = \frac{TP + TN}{TP + FP + FN + TN}$$

  - TP:two nodes in same cluster in both GT and solution
  - TN:two nodes in different clusters in both GT and solution
  - TP+FP+FN+TN=all possible node pairs

- Problem: complexity. #of pairs= $\mathcal{O}(n^2)$
  - 100k items: 10 Billion pairs…

RAND INDEX

- Fast computation: Contingency table
  - Same as a confusion matrix, but not necessarily square

	S1	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**NA**
K1	95									
K2		**18**								
K3			**17**							
K4				*31*	*1*	*1*	*6*		*11*	*6*
K5					***45***	*1*				*1*
K6					***3***	*21*	***12***	**8**	***6***	*4*
K7					***44***	*1*			***3***	*1*

$$\binom{x}{2} = \frac{(x(x-1))}{2}$$

RAND INDEX

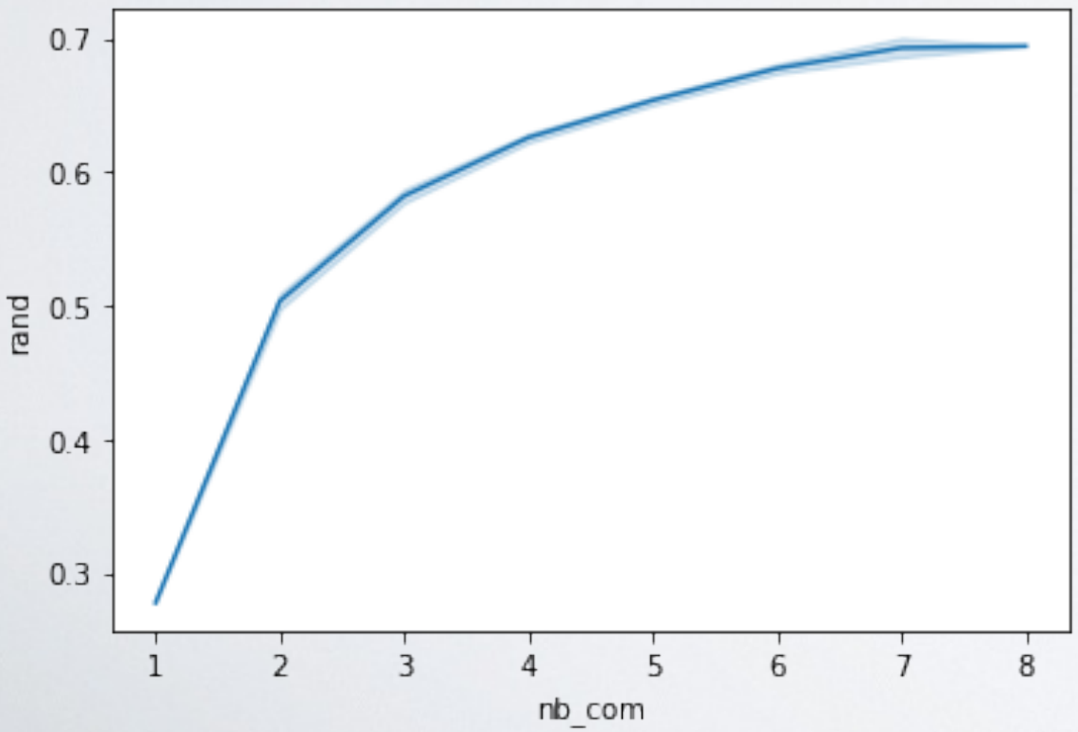
	x1	x2	x3		Sums
y1	1	1	0		2
y2	1	2	0		3
y3	0	0	4		4
Sums	2	3	4		

- TP: $\sum_{ij} \binom{n_{ij}}{2} = 3\binom{1}{2} + \binom{2}{2} + \binom{4}{2} = 6 + 1 = 7$
- TN: $\binom{n}{2} - \sum_i \binom{n_i}{2} - \sum_j \binom{n_j}{2} + TP$ = 36-(1+3+6)-(1+3+6)+7=23
  - All pairs - pairs inside clusters in our solution($\sum_i \binom{n_i}{2}$)= N(all negatives) in our solution.
  - Remove those that are positive in GT ($\sum_j \binom{n_j}{2}$) But retain among them those in common in our solution too (TP)
- Rand=(23+7)/36=0.833

RAND INDEX

- Rand Index has the same weakness as Accuracy:
  - If the classes are imbalanced, i.e., the size and number of communities vary between GT and clustering, results can be counterintuitive

- In practice:
  - Random communities have different scores depending on their size
  - =>Prefer certain types of communities



Previous example,
With random communities

ARI

- Solution: Use an **adjusted for chance** score.
  - Principle: adjust (normalize) such as 0 is the score obtained with a "random" solution, 1 is the highest possible score.
  - Negative solutions are worst than random

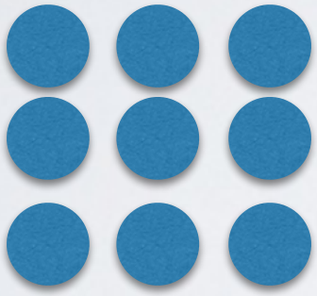
$$\frac{\text{Index} - \text{Expected index}}{\text{Max index - Expected index}}$$

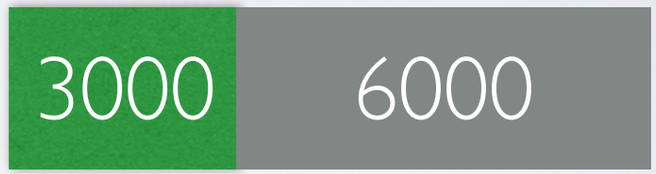
Expected nb of TP

$$E(n_{ij}) = \binom{n_i}{2} \frac{\binom{n_j}{2}}{\binom{n}{2}}$$

ARI

- Simple interpretation,
  - Forget about clusters: we had X blue chocolates, we distribute at random in a box having a total of Y free spaces. The green part of the box has Z free spaces. How many blue chocolates do you expect in the green part?





Chocolate/ pairs

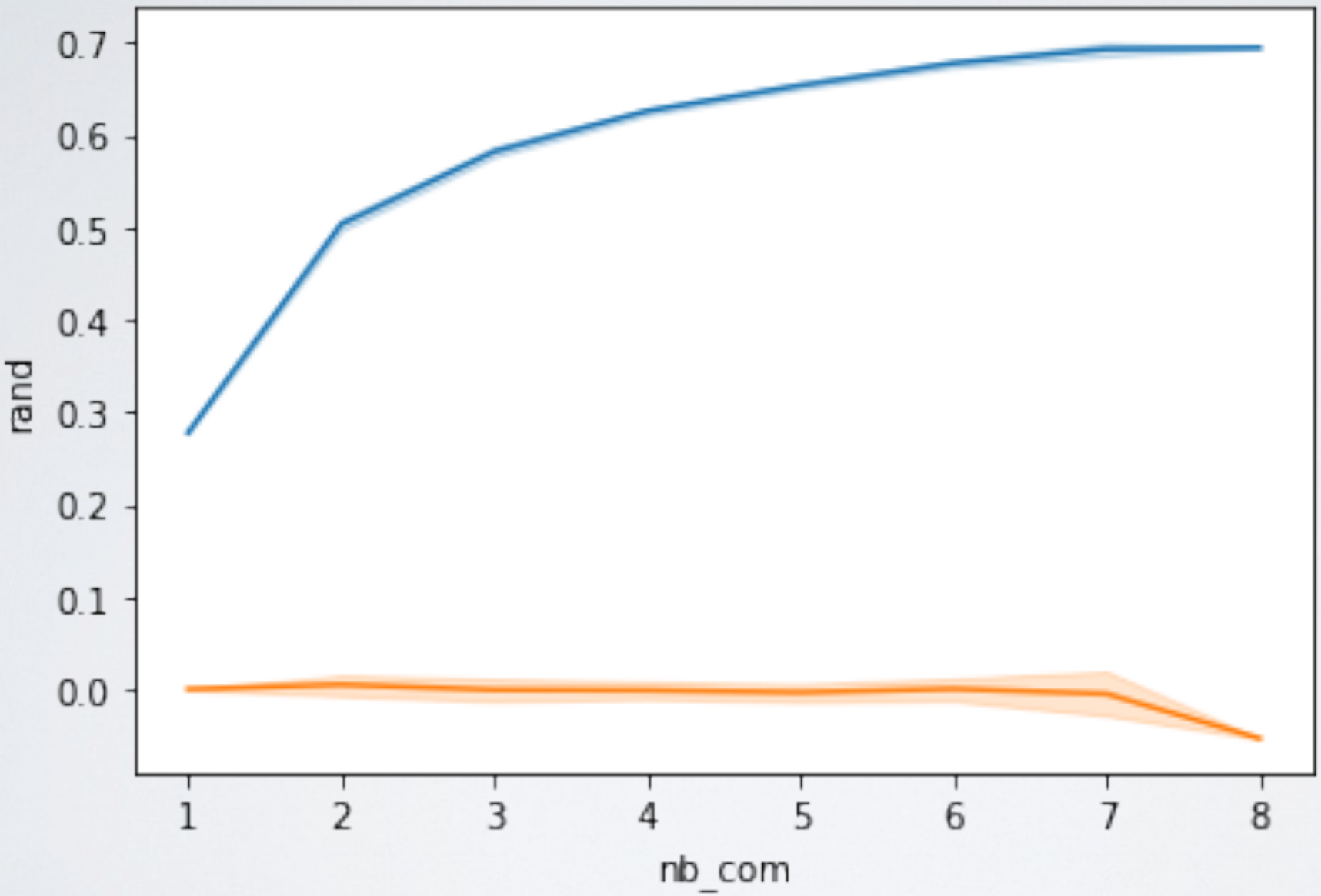
	x1	x2	x3		Sums
y1	1	1	0		2
y2	1	2	0		3
y3	0	0	4		4
Sums	2	3	4		

Space

	x1	x2	x3		Sums
y1	1/36	3/36	6/36		2
y2	3/36	9/36	18/36		3
y3	6/36	18/36	36/36		4
Sums	2	3	4		

=100/36=2.77 expected TP

ARI



Lawrence Hubert and Phipps Arabie (1985). "Comparing partitions". *Journal of Classification*. **2** (1)

HOMOGENEITY/ COMPLETENESS

- Similar idea than Precision and Recall
  - Scores based on Information Theory

- Homogeneity
  - Items inside a same cluster belong to the same class (GT cluster)
  - $\in [0,1]$, 1: each cluster contains only items of the same class
    - But several clusters can be composed of the same class…

- Completeness
  - Items belonging to the same class (GT cluster) are found in the same cluster
  - $\in [0,1]$, 1: All items of a same class are found in the same clusters
    - But a same cluster might contain different classes…

- Trivial solutions: Each in its own cluster, a single cluster…

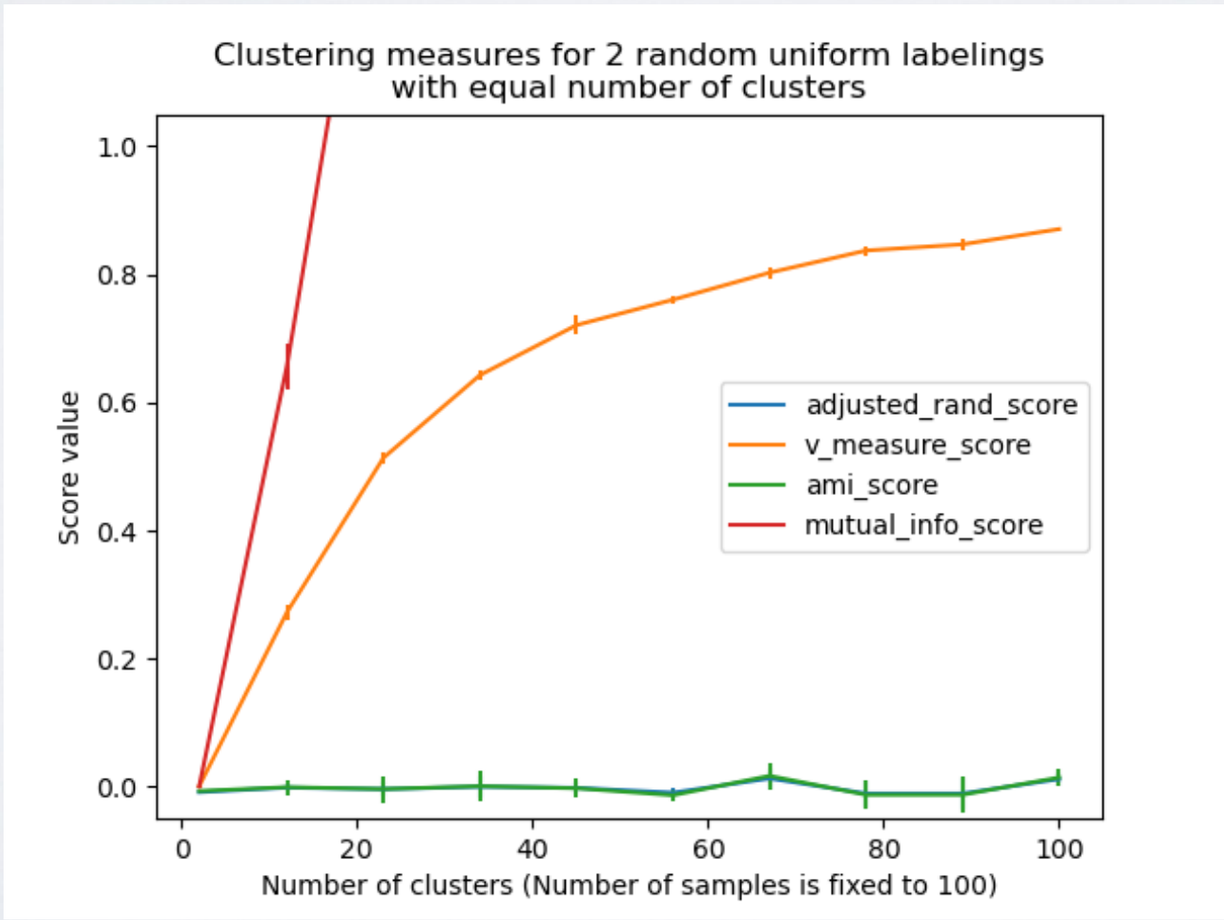
V-SCORE / NMI

- As with f1-score, Homogeneity and Completeness can be combined in a single score, using harmonic mean
  - Called the v-score.
  - $$v = \frac{2 \times \text{homogeneity} \times \text{completeness}}{\text{homogeneity} + \text{completeness}}$$

- The exact same score (defined differently, still from Information Theory) is also called NMI
  - NMI: Normalized Mutual Information

AMI

- NMI/v-score is known to suffer from the exact same problem as Rand Index
  - An adjusted for chance version exist, called AMI (adjusted Mutual Information)



NO FREE LUNCH THEOREM

- "Any two optimization algorithms are equivalent when their performance is averaged across all possible problems"
  - Two clustering algorithms with different objective functions are fully comparable, one is not intrinsically better than another.
  - Each is the best for the objective function it defines
  - What is "the best" cluster? Depends on your definition.

- Does not mean that some methods are not more appropriate than other for what most people consider as clusters…

Wolpert, D.H., Macready, W.G. (1997), "No Free Lunch Theorems for Optimization", *IEEE Transactions on Evolutionary Computation* **1**, 67.