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

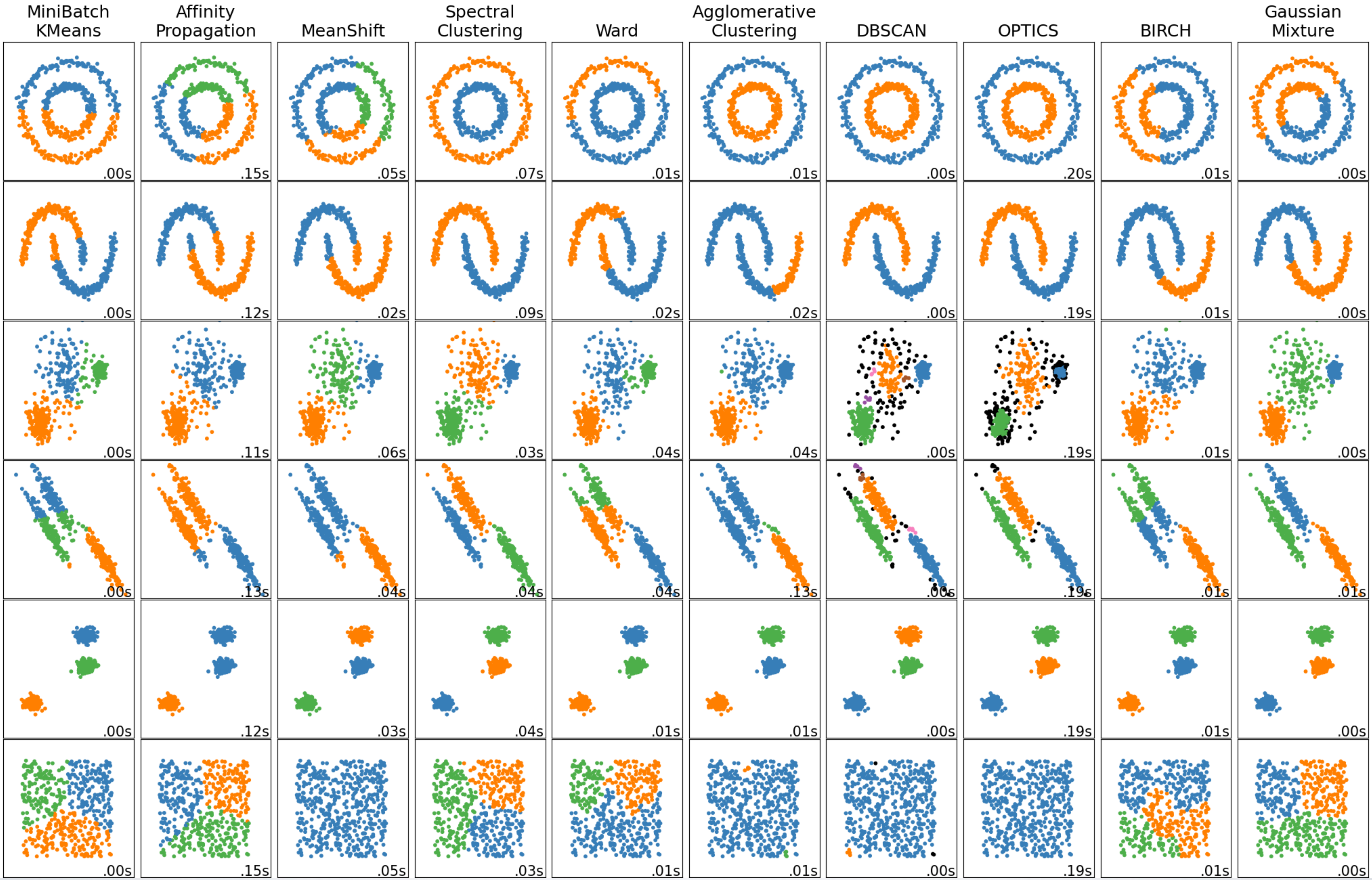
- The most famous unsupervised ML problem

- 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
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K-MEANS

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

K-MEANS

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

with

$\mathbf{S}$ a cluster assignment,

k a number of clusters

x a d dimensional item, and

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

K-MEANS

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

This is only one possible objective for clustering!

For instance, why using the **squared distance?**

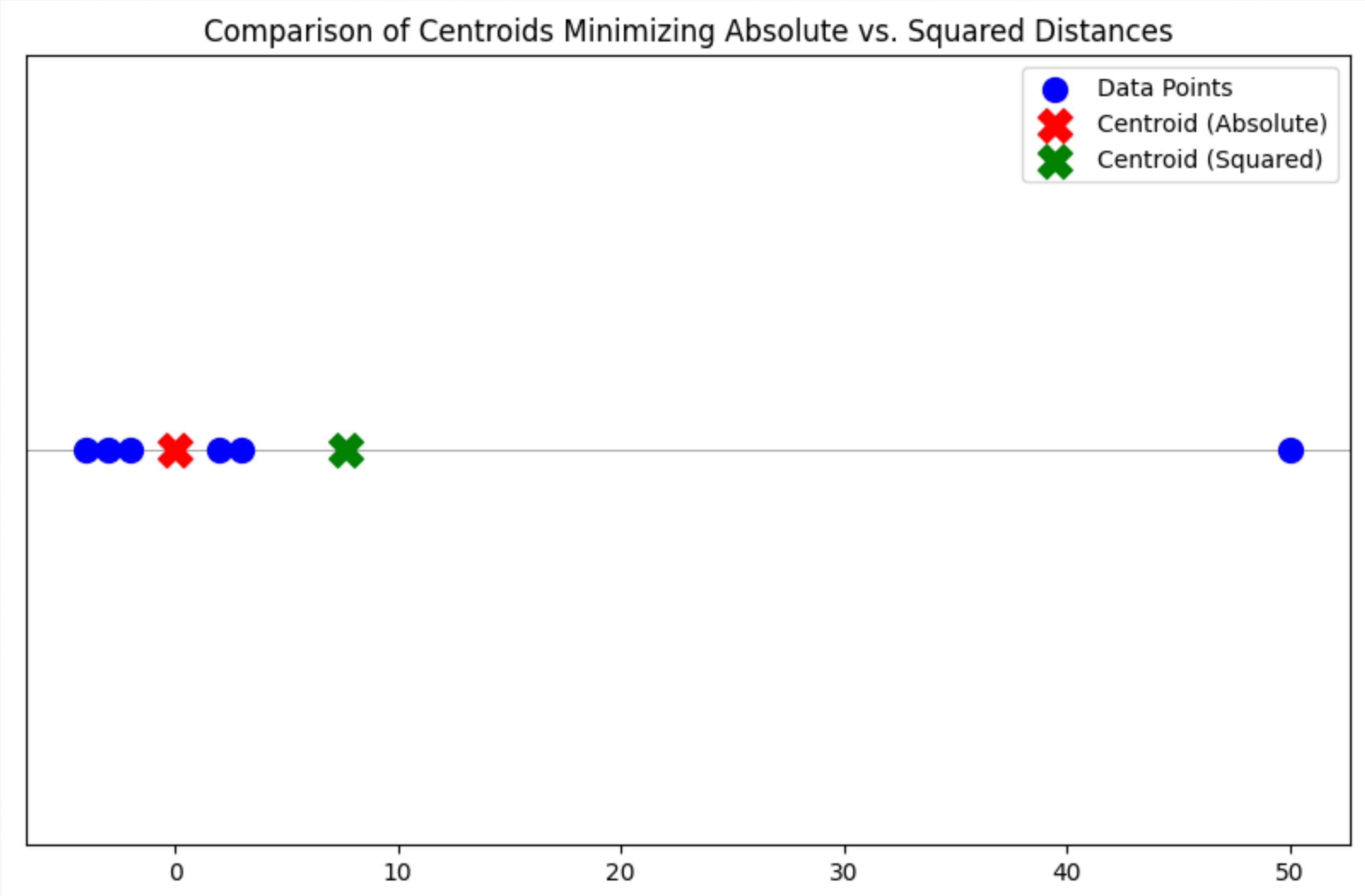
=>Good math properties (derivation), history

=>Consequence: outliers penalized more (pros and cons)

K-MEANS

=>Consequence: outliers penalized more (pros and cons)

Squared distance minimized by the **mean.**
Absolute distance minimized by the **median.**



K-MEDOIDS

Same method, replacing the squared distance by the absolute distance

K-MEANS

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

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…)

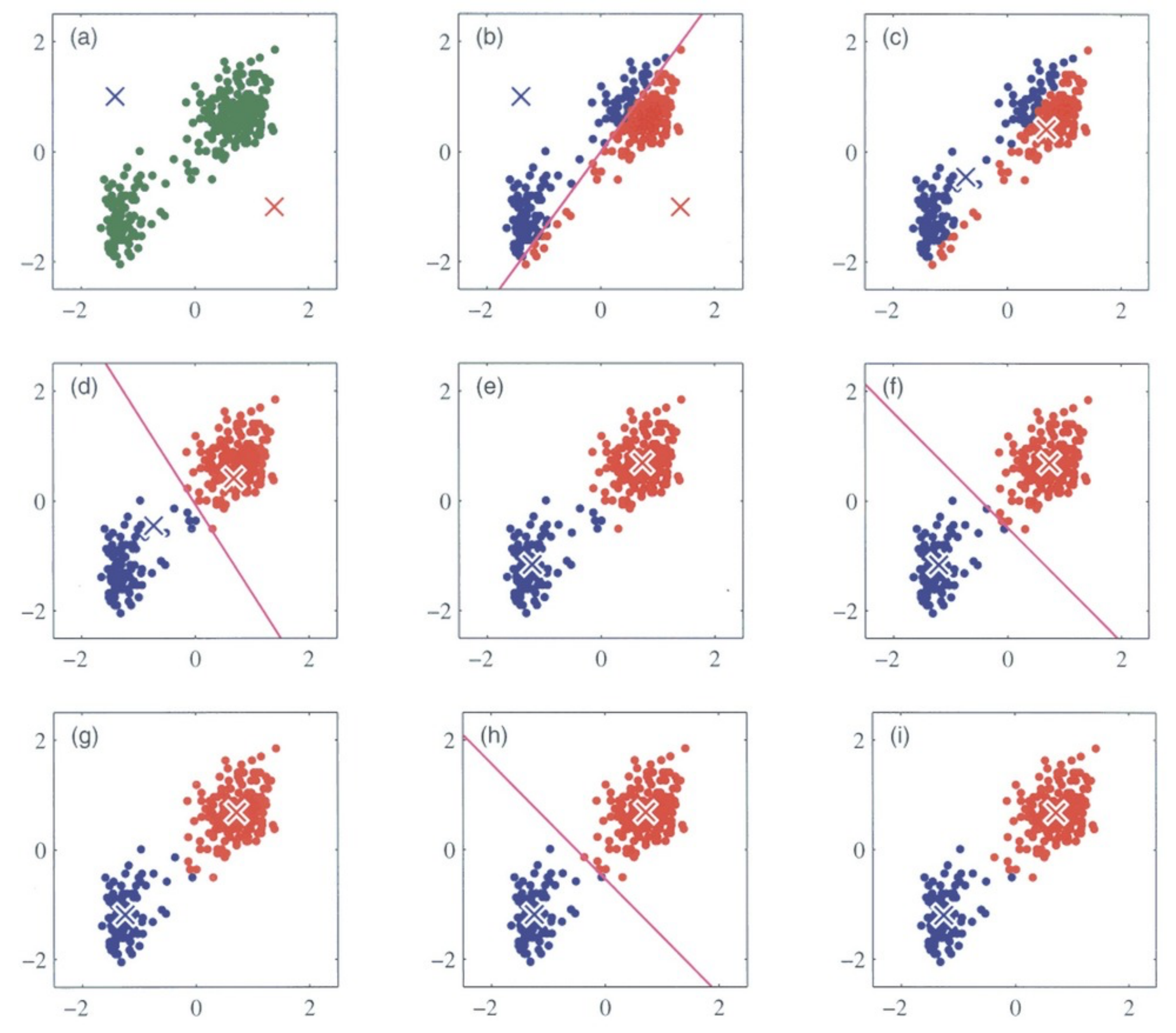
NAIVE K-MEANS

- 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

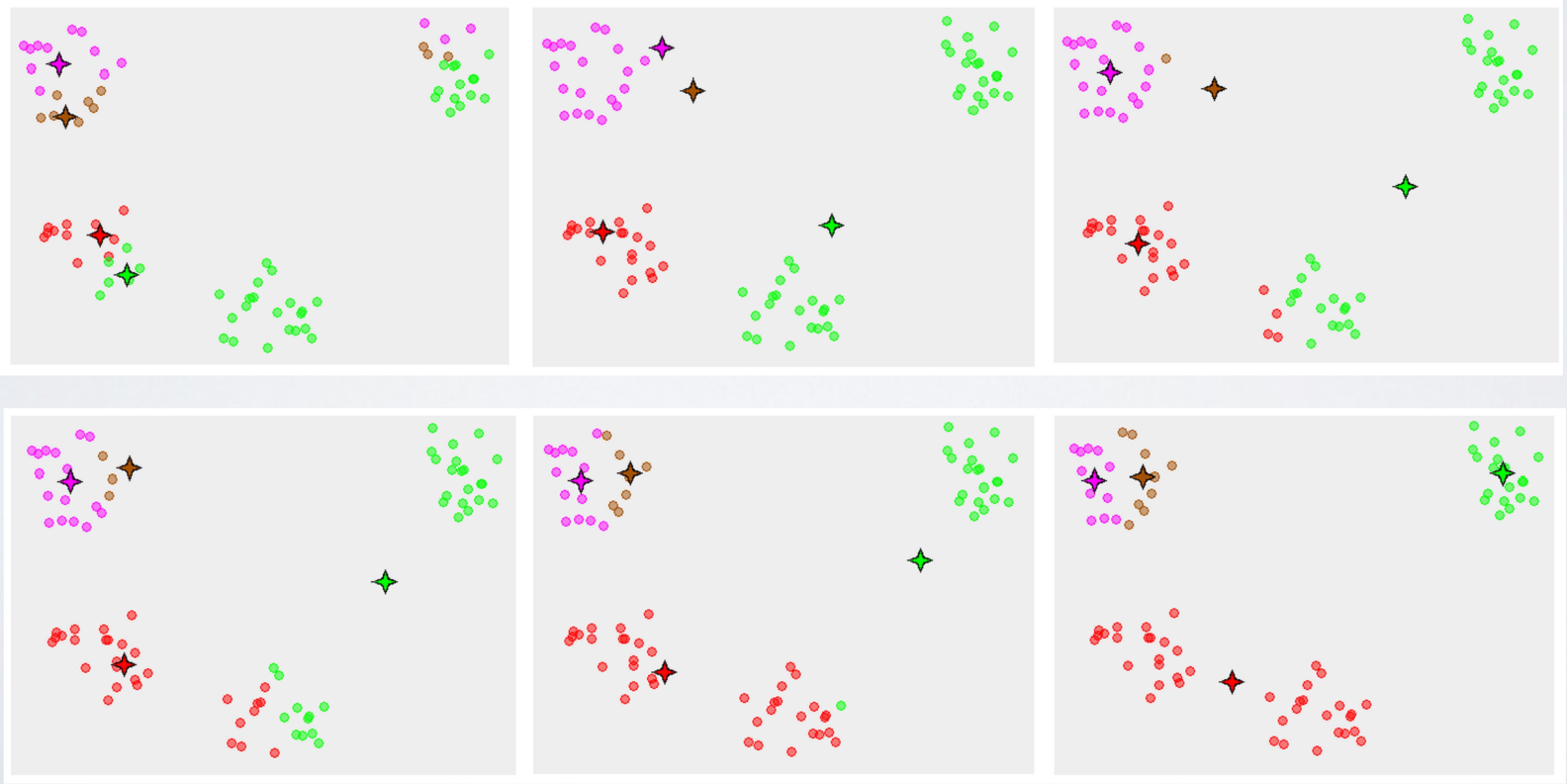
- Start with random centroids

NAIVE K-MEANS



NAIVE K-MEANS

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



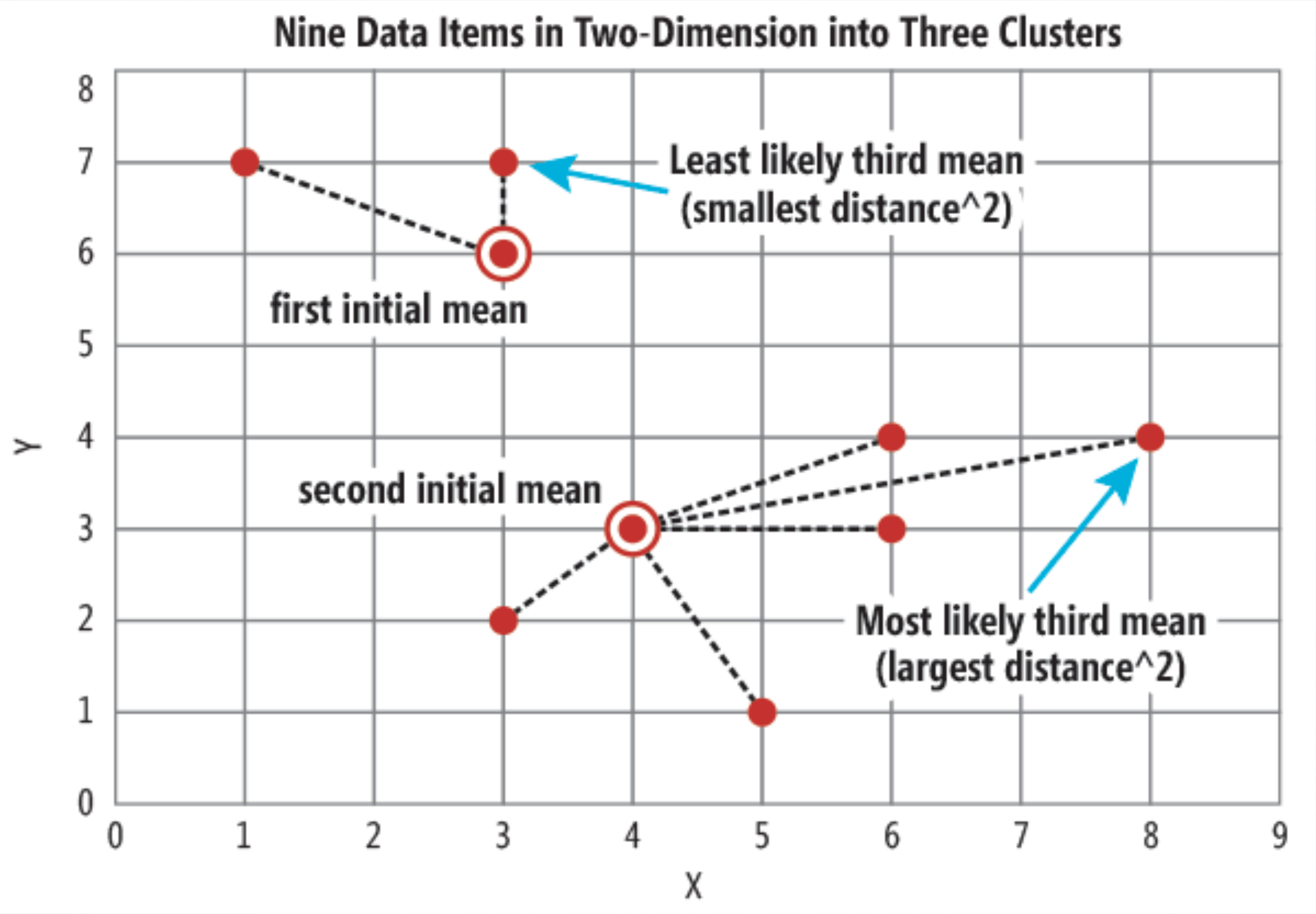
K-MEANS++

- 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++

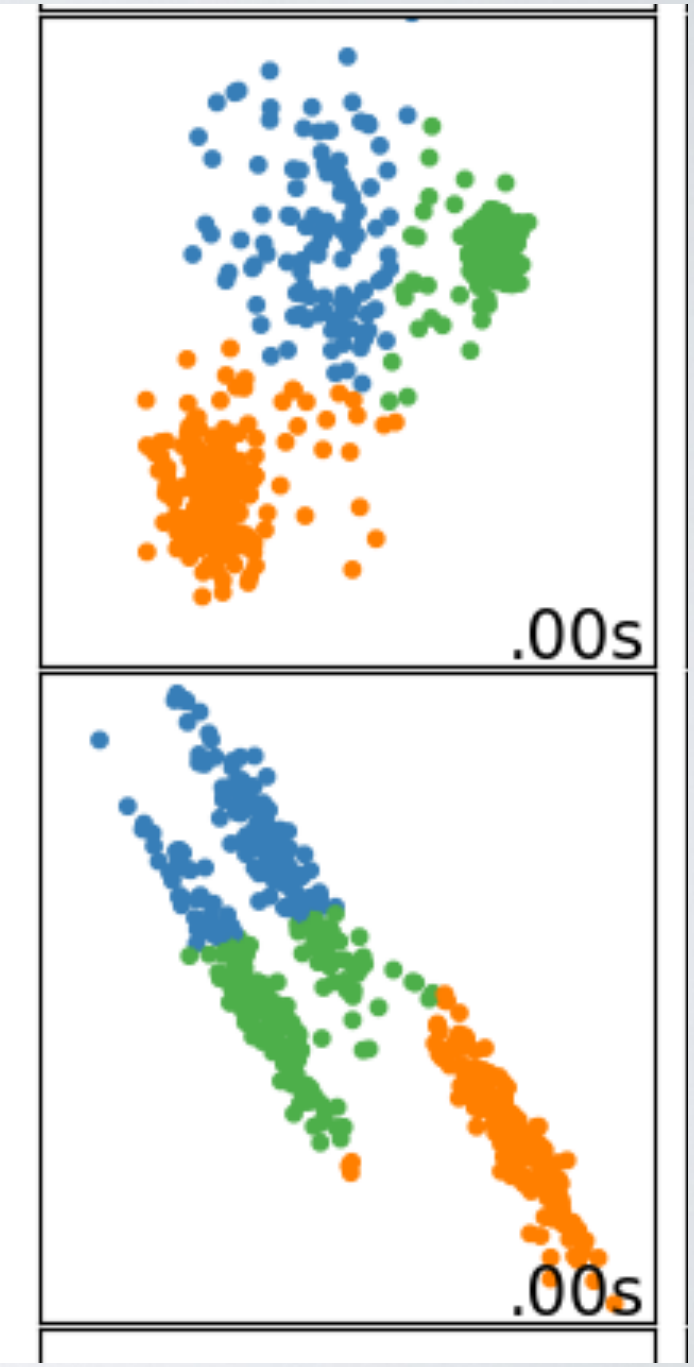
1. Choose one center uniformly at random among the data points.
2. For each data point x not chosen yet, compute $D(x)$, the distance between x and the nearest center that has already been chosen.
3. Choose one new data point at random as a new center, using a weighted probability distribution where 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

- 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

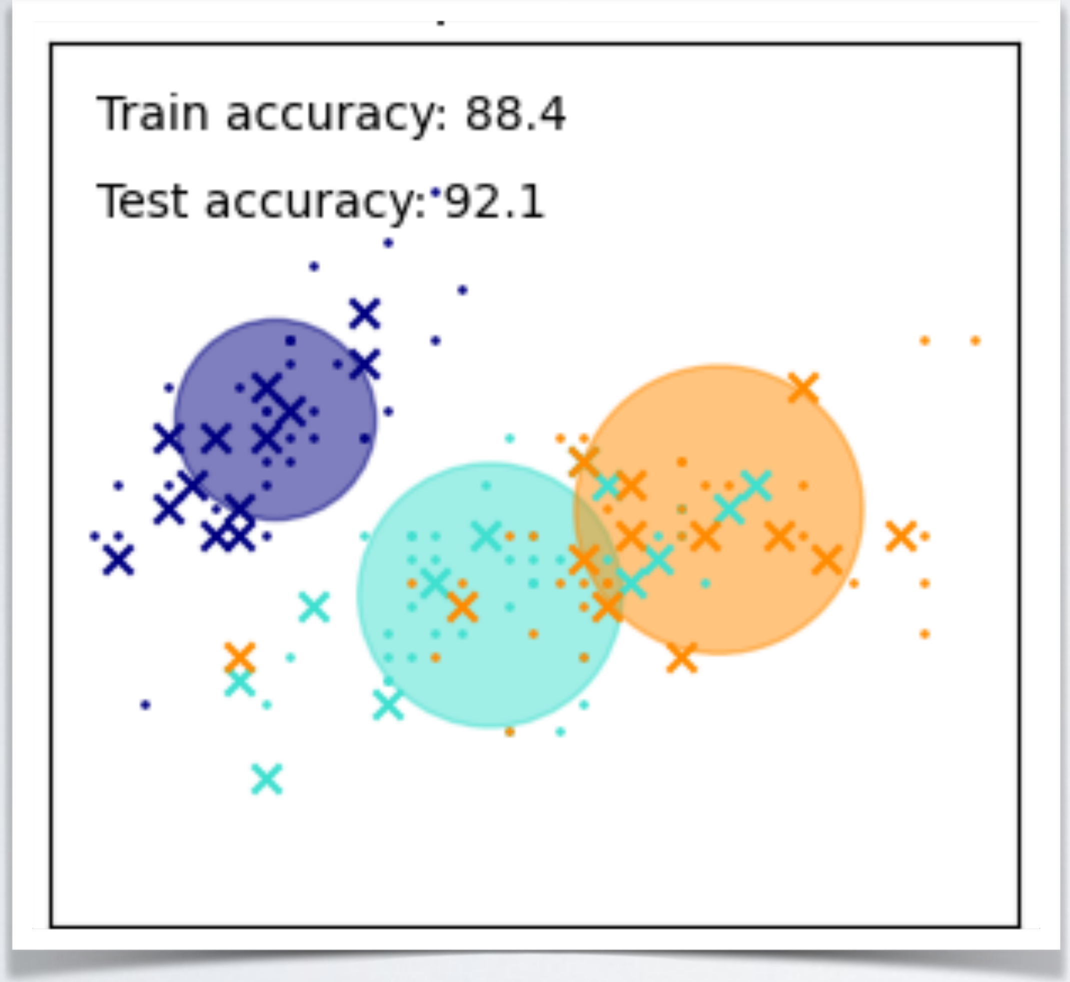
- Data needs to be **normalized/standardized**
  - Clustering based on age in years and revenue in $. The "distance" in $ will dominate
  - Remember: normalization/standardization are not fixing magically problems (outliers..)
    - You need to **think**: Is 1 unit in one dimension *worth* 1 unit in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

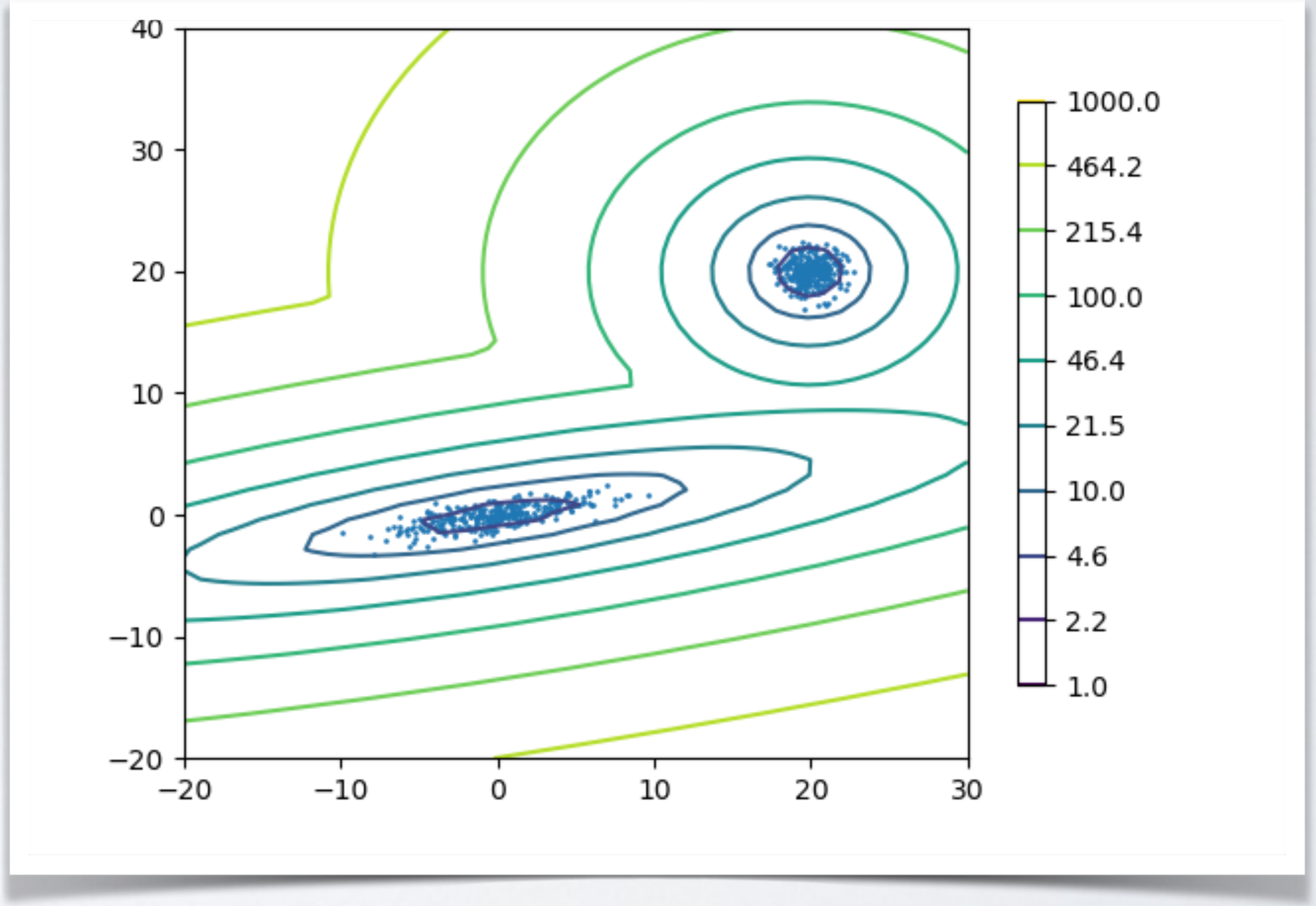
GAUSSIAN MIXTURES

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





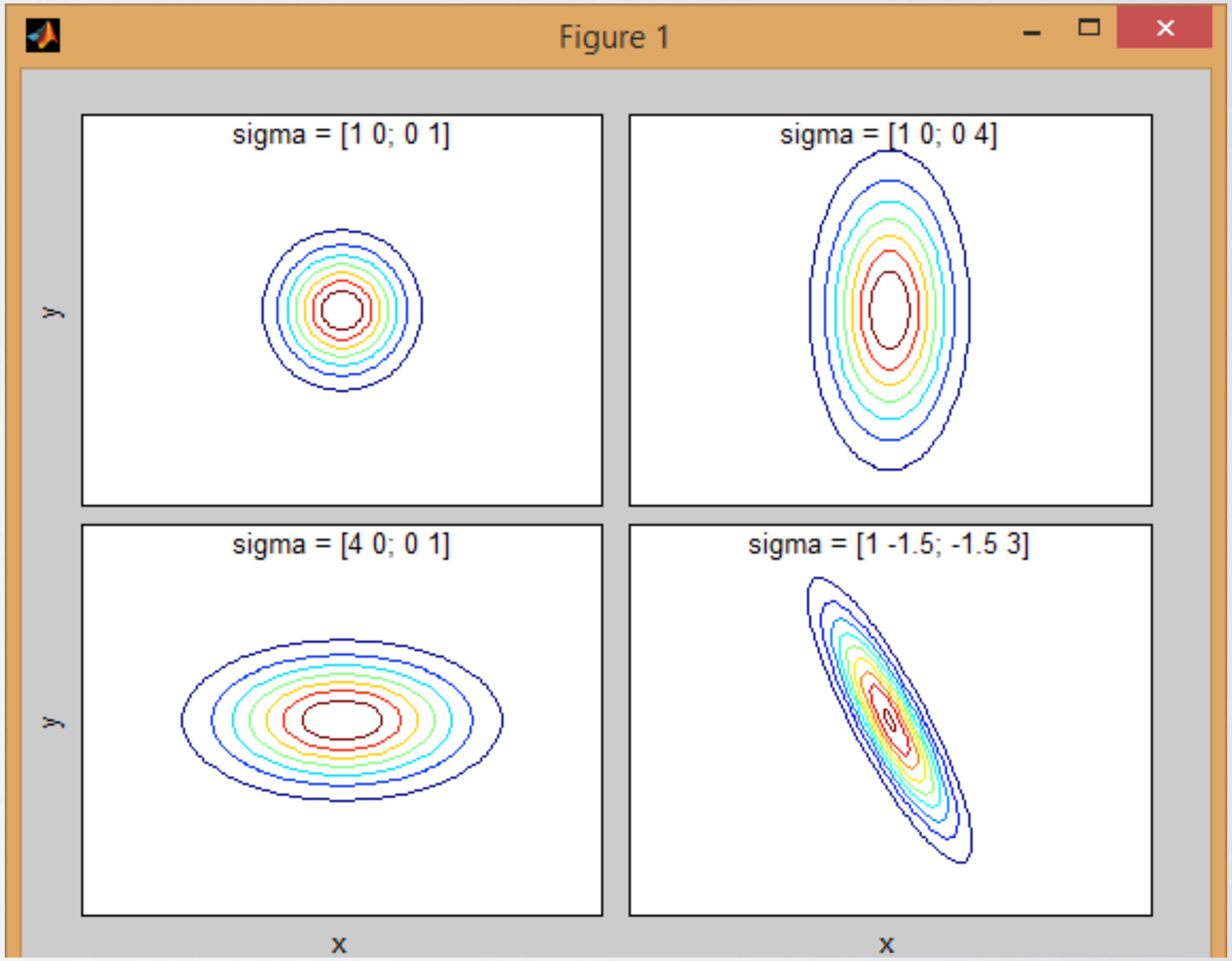
GAUSSIAN MIXTURES

- 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: $\arg\max_{\Theta} p(X|\Theta)$

MULTIVARIATE GAUSSIAN

- A gaussian is defined by
  - a mean
  - a variance

- A multivariate gaussian is defined by a
  - A center
  - a covariance matrix



K-MEANS EQUIVALENCE

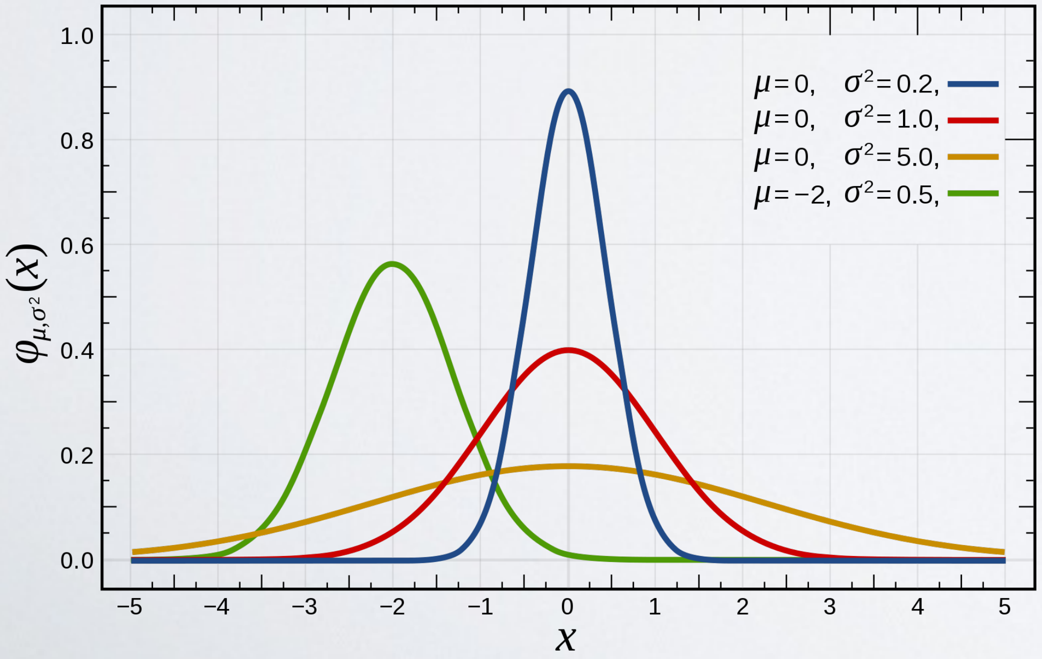
$$\begin{bmatrix} Var(x_1) & \cdots & Cov(x_n,x_1) \\ \vdots & \ddots & \vdots \\ Cov(x_n,x_1) & \cdots & Var(x_n) \end{bmatrix}$$

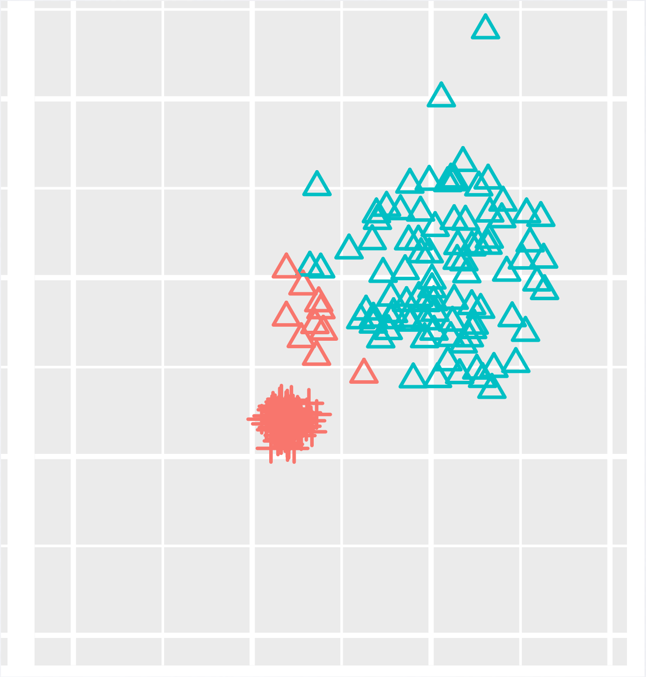
- If we assume that:
  - The gaussian distributions are defined only by their variance, not by complete covariance matrices
    - Similar in all directions, "spherical"
  - The variance value is the same for all gaussian distributions
    - Spheres of the same "size"
  - The probability for each item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

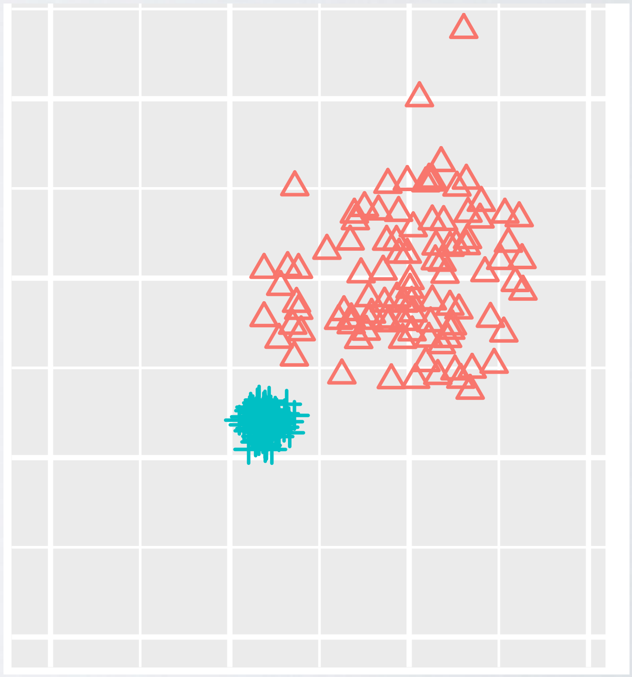
DENSITY HETEROGENEITY

- 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 cluster, some can be denser than others





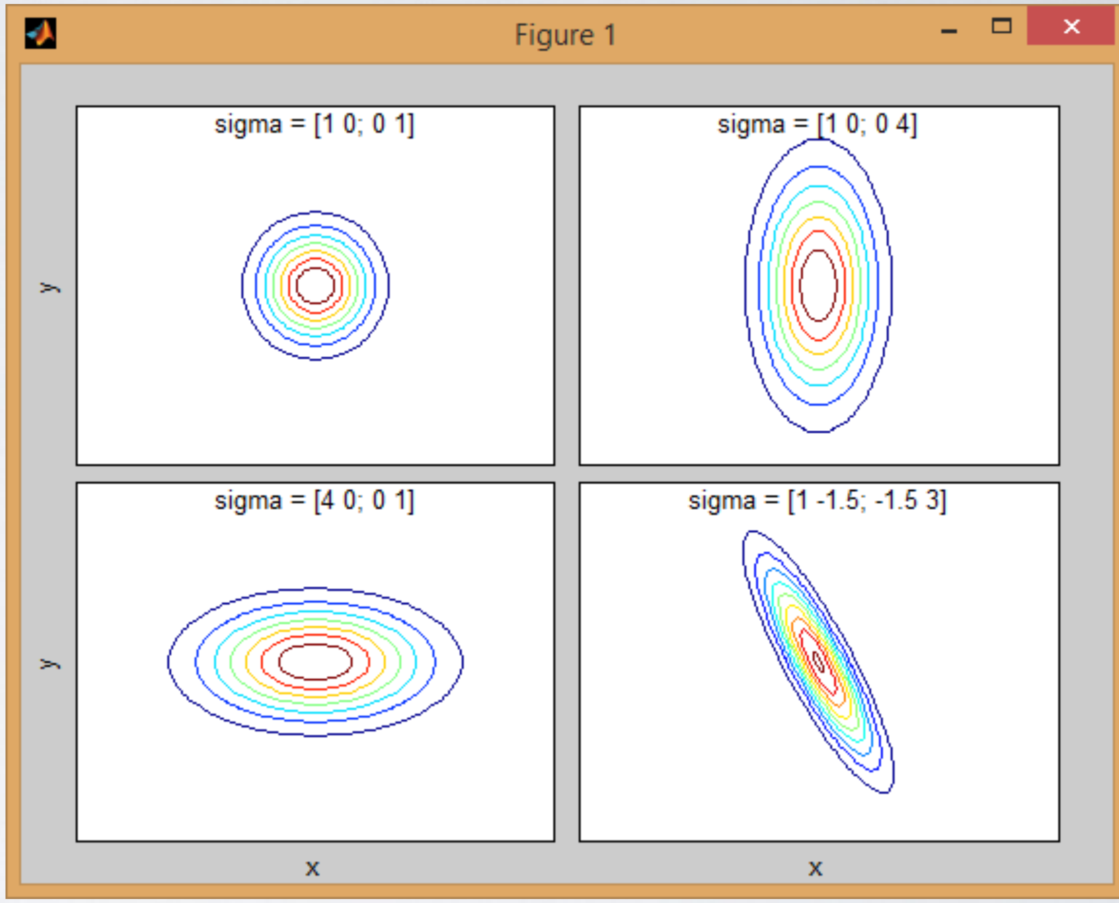
K-means



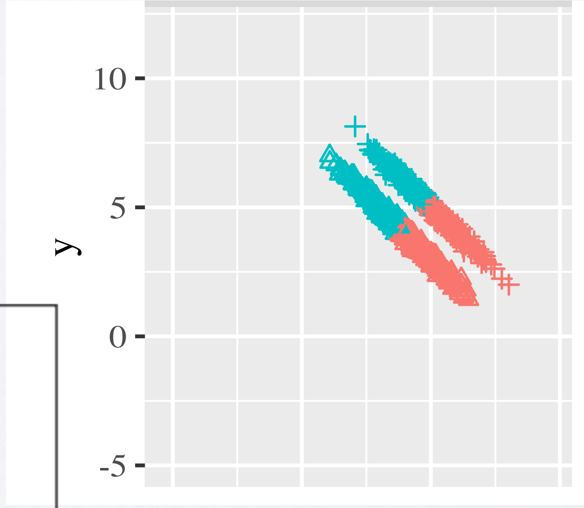
GM,
free variance

SHAPE VARIATIONS

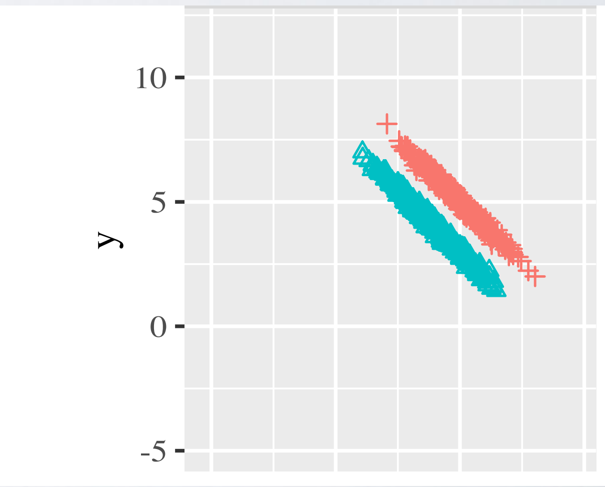
- Allowing non-circular shaped clusters
  - If values on the diagonal of the covariance matrix differs, the matrix can have ellipsoidal shape, in the direction of the axes
  - If the full covariance matrix is inferred, any ellipsoidal shape can be obtained



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

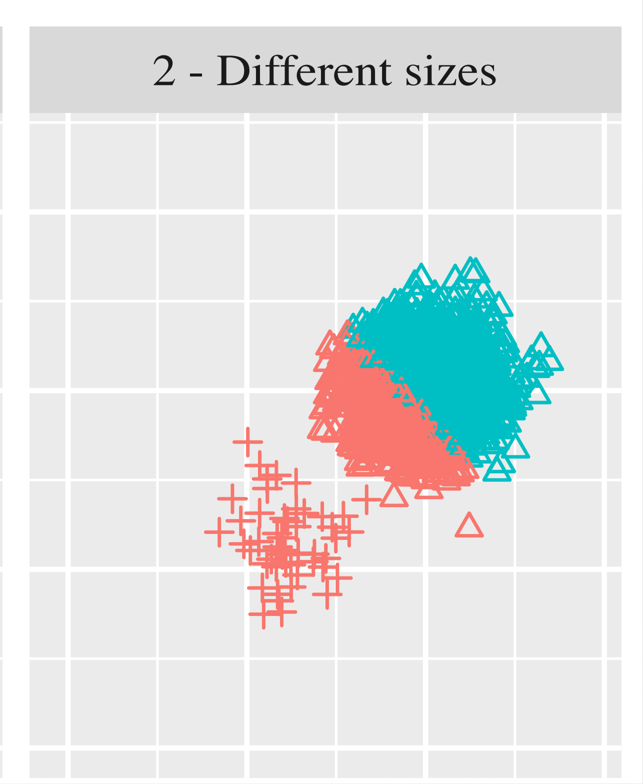


K-means



Full gaussian

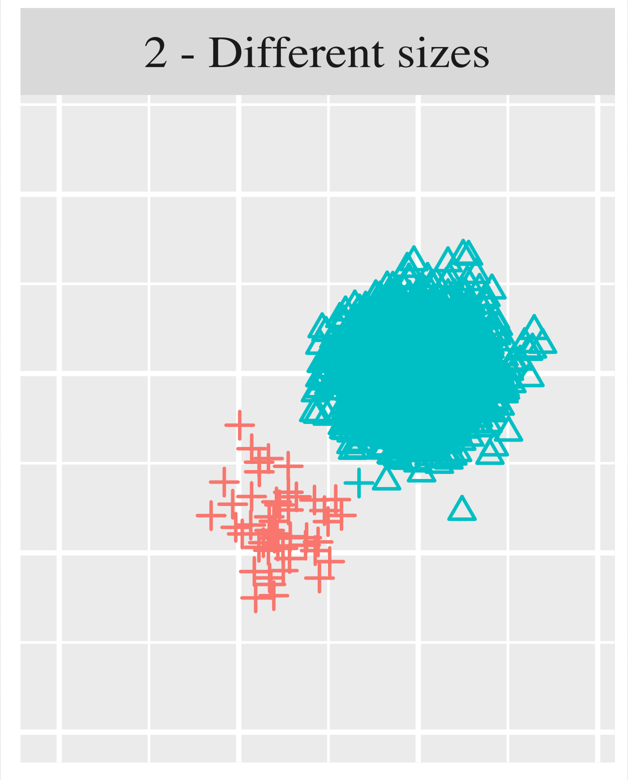
SIZE HETEROGENEITY



- 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

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



ALL TOGETHER

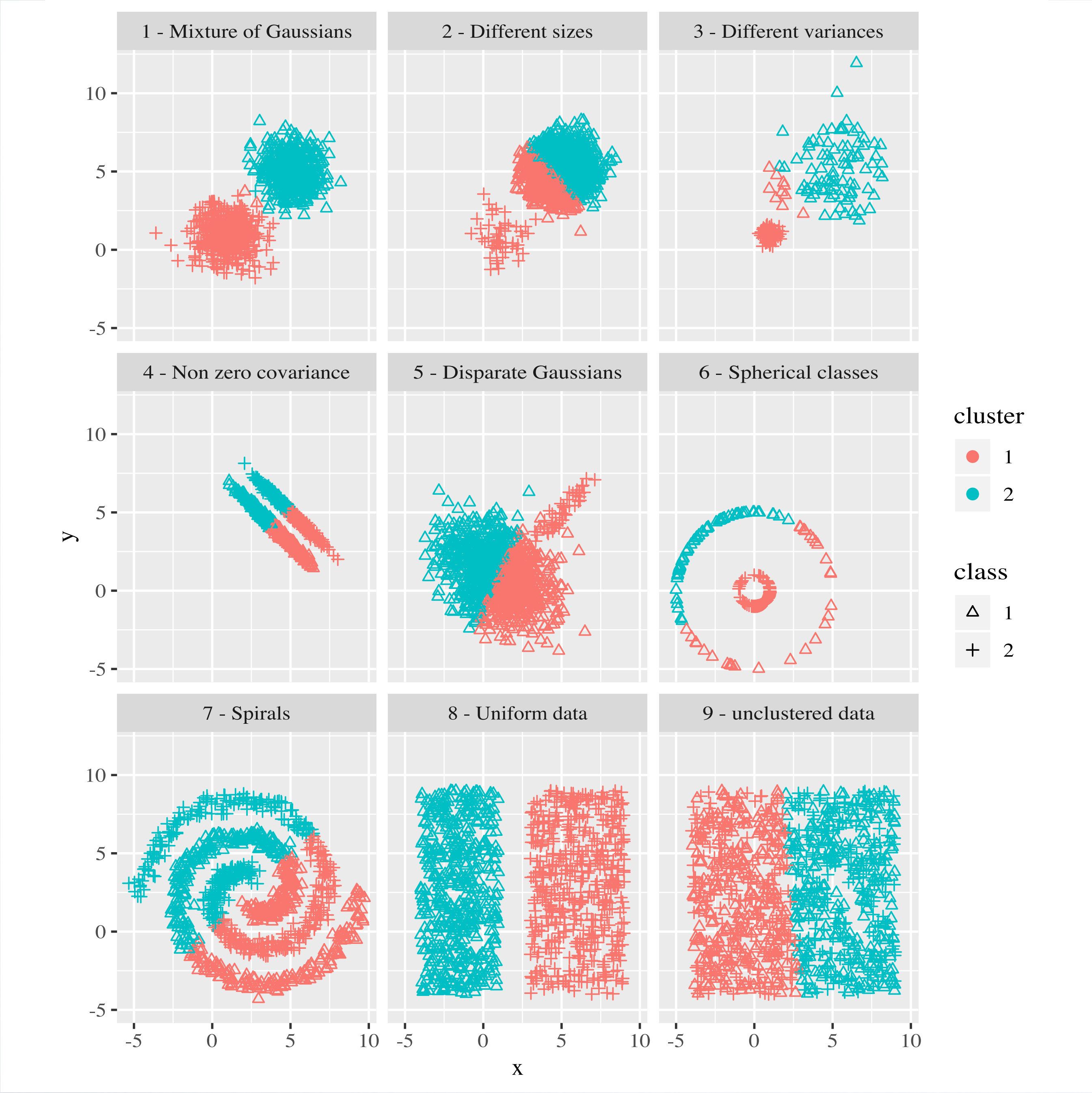
$$p(X) = \sum_{k=1}^{K} \pi_k G(X \mid \mu_k, \sigma_k)$$

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

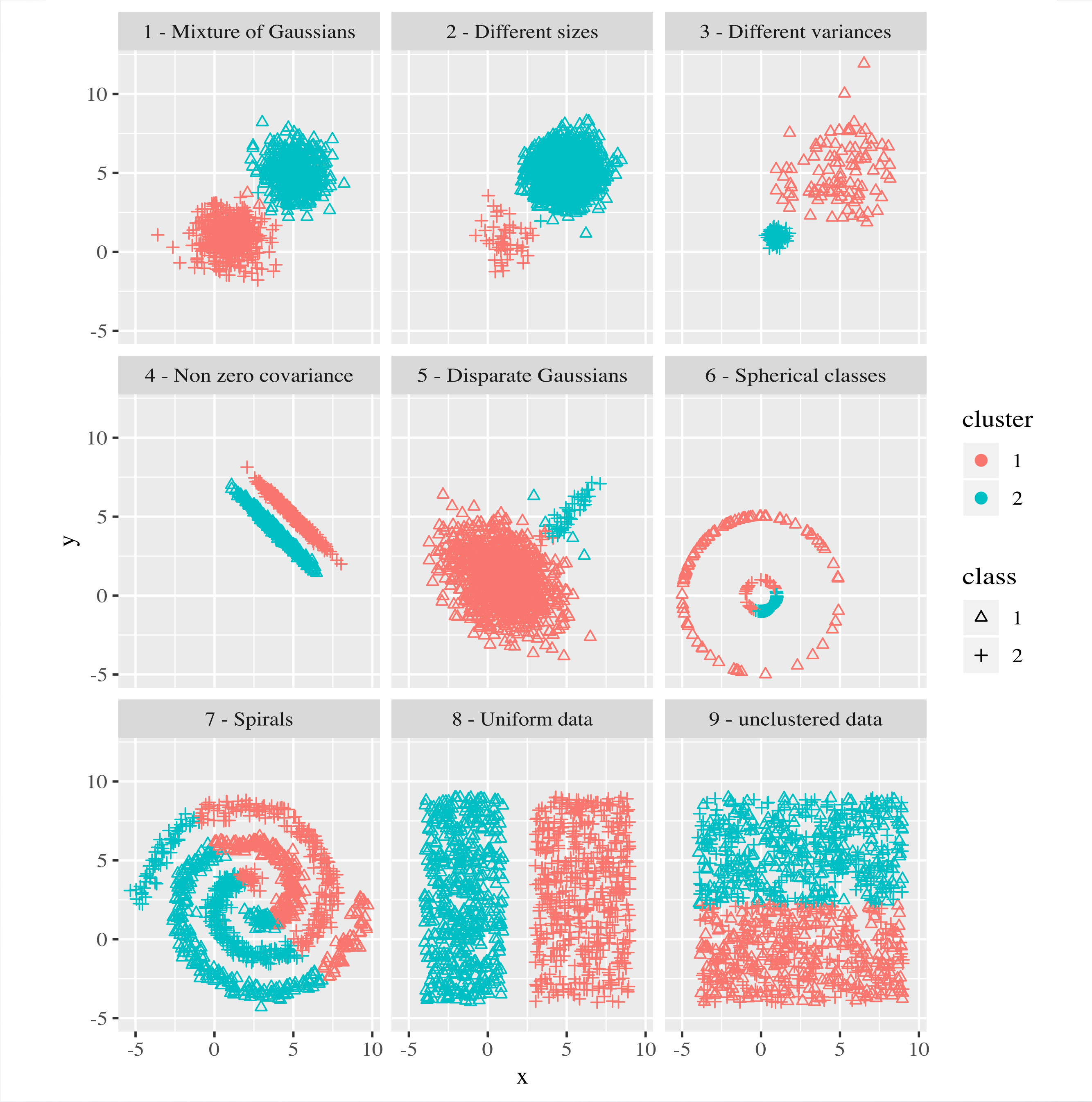
$$\Theta = \mu, \sigma, \pi$$

K-MEANS COMPARISON

K-means



Full Gaussian Mixture

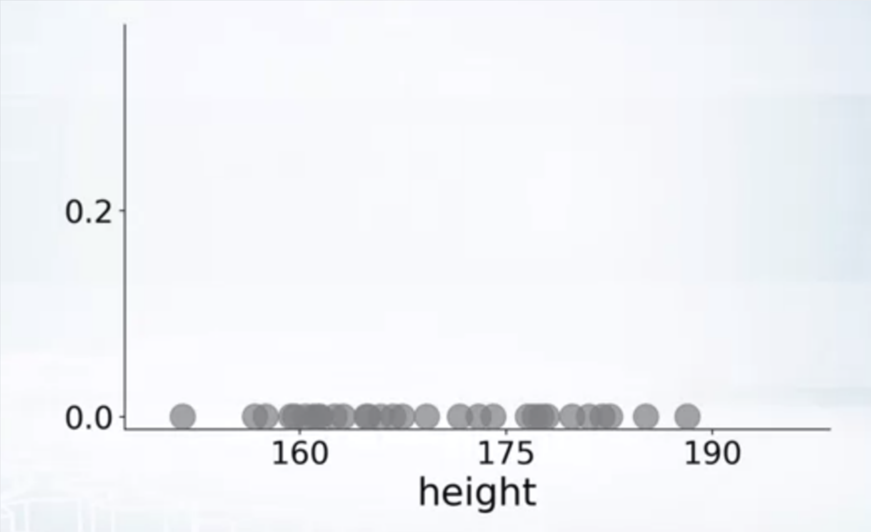


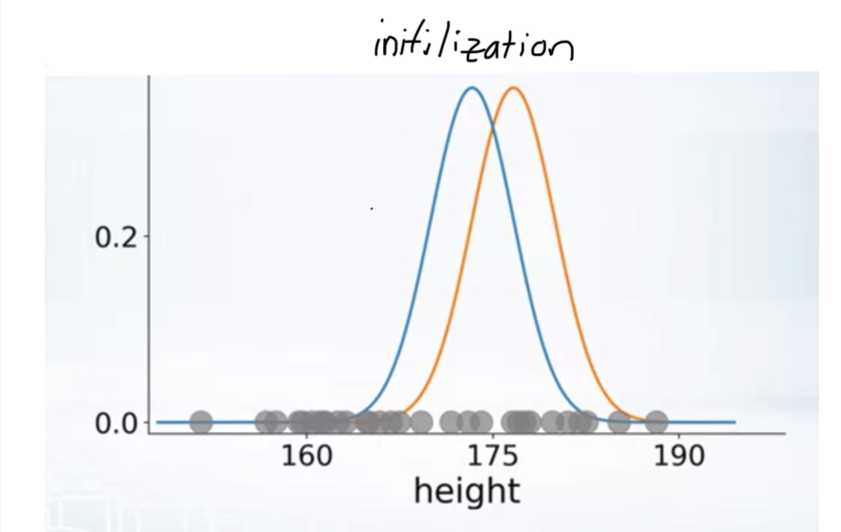
https://smorbieu.gitlab.io/gaussian-mixture-models-k-means-on-steroids/

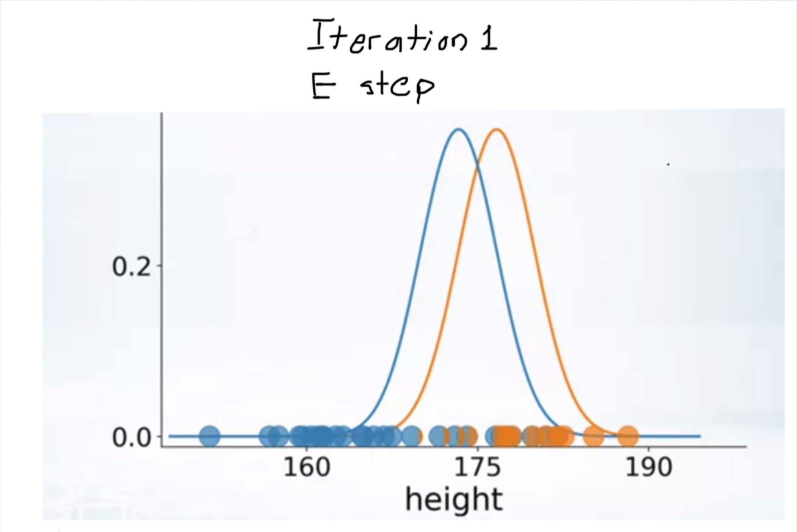
EM ALGORITHM

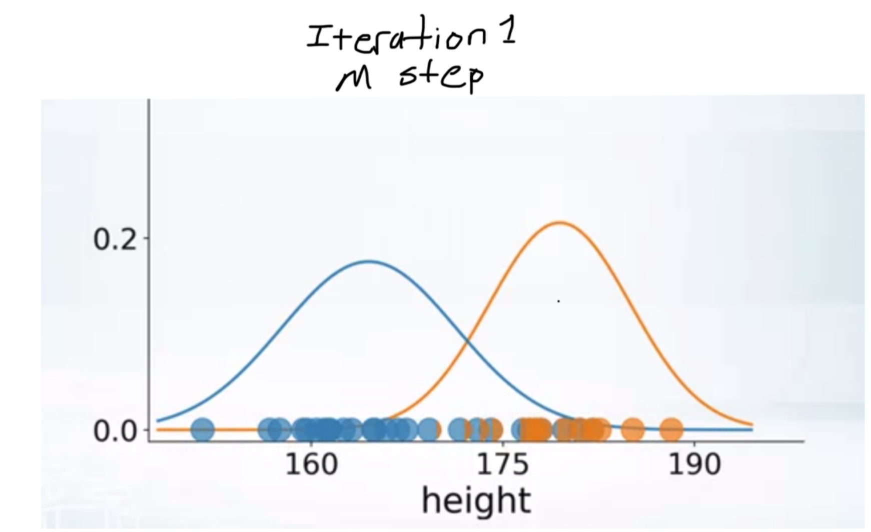
- To search for the parameters, we can use a method similar to naive k-means known as EM (Expectation Maximization)
  - Note Z the cluster assignation of items to their **most likely** clusters
  - 1)Initialize parameters Θ to random values
  - 2)(E) Compute Z, given Θ
  - 3)(M) Use assignations in Z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

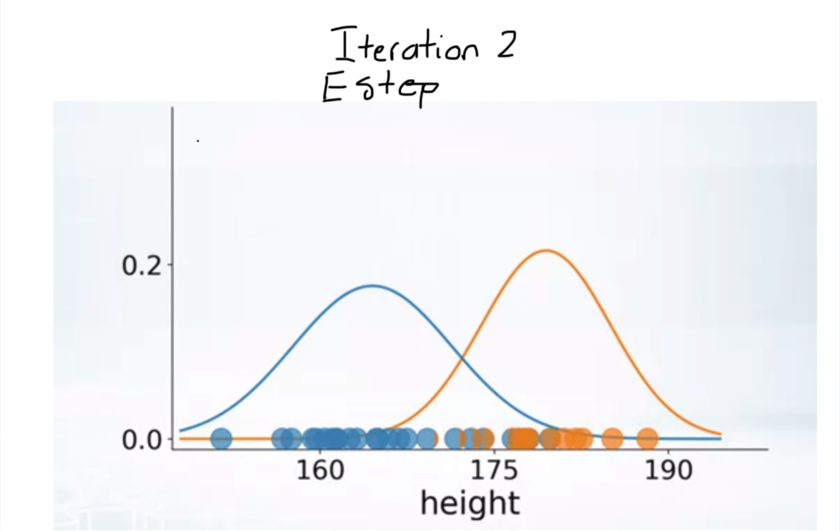
EM ALGORITHM

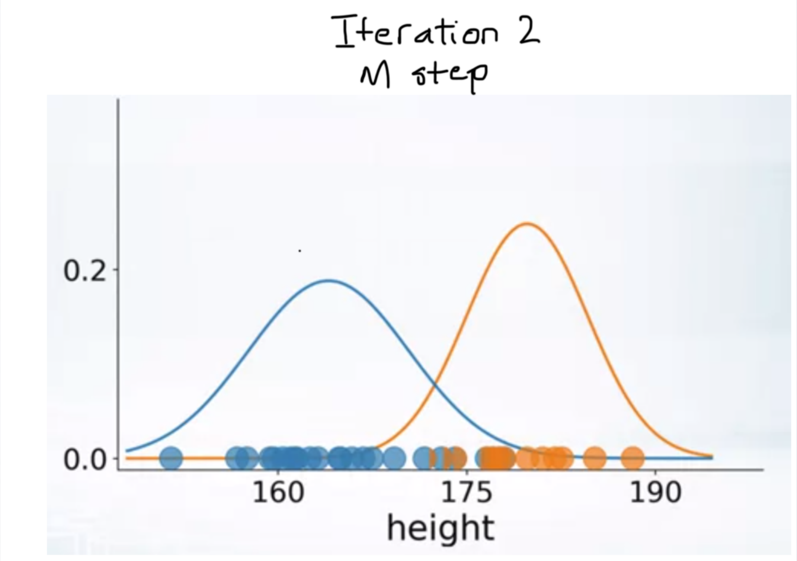



initilization


Iteration 1
E step


Iteration 1
M step

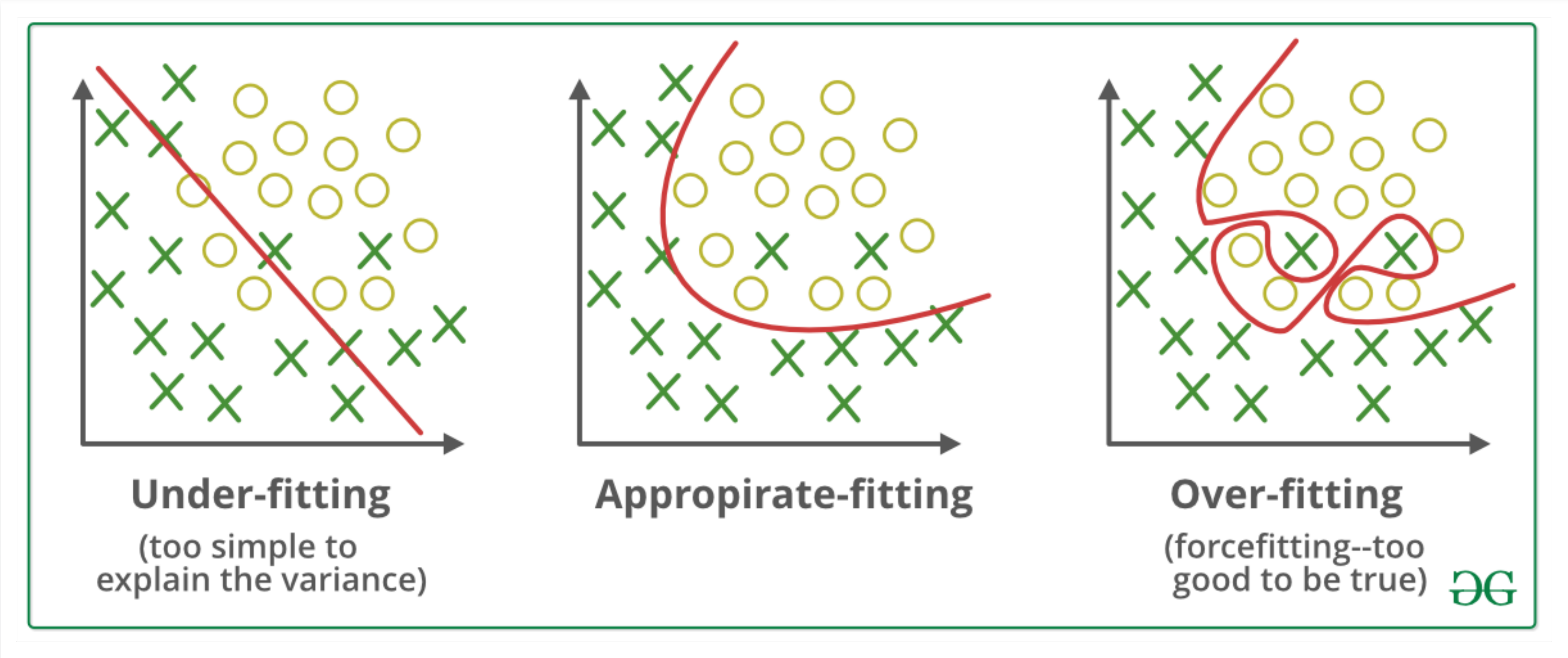

Iteration 2
E step


Iteration 2
M step

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

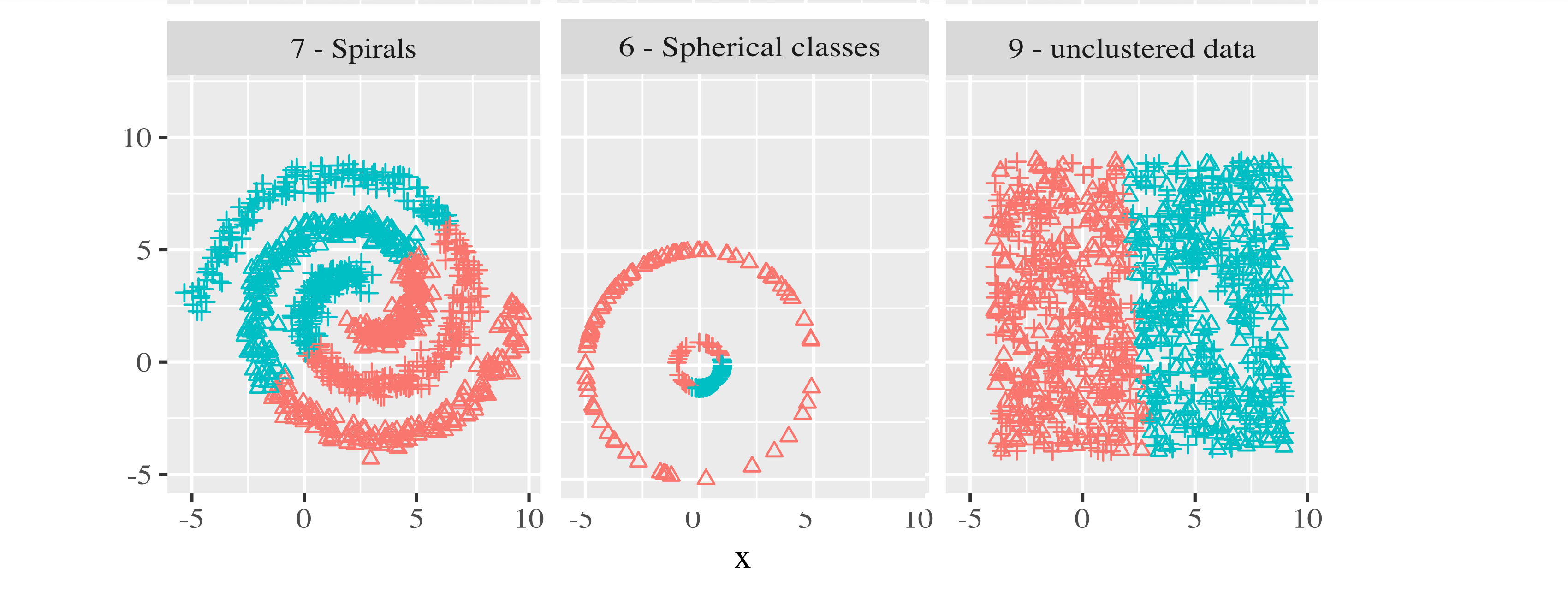
PROS AND CONS

- 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)


Under-fitting
(too simple to explain the variance)
Appropirate-fitting
Over-fitting
(forcefitting--too good to be true)
GG

REMAINING PROBLEMS

- We can mention 3 problems remaining (at least)
  - The number of clusters still needs 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

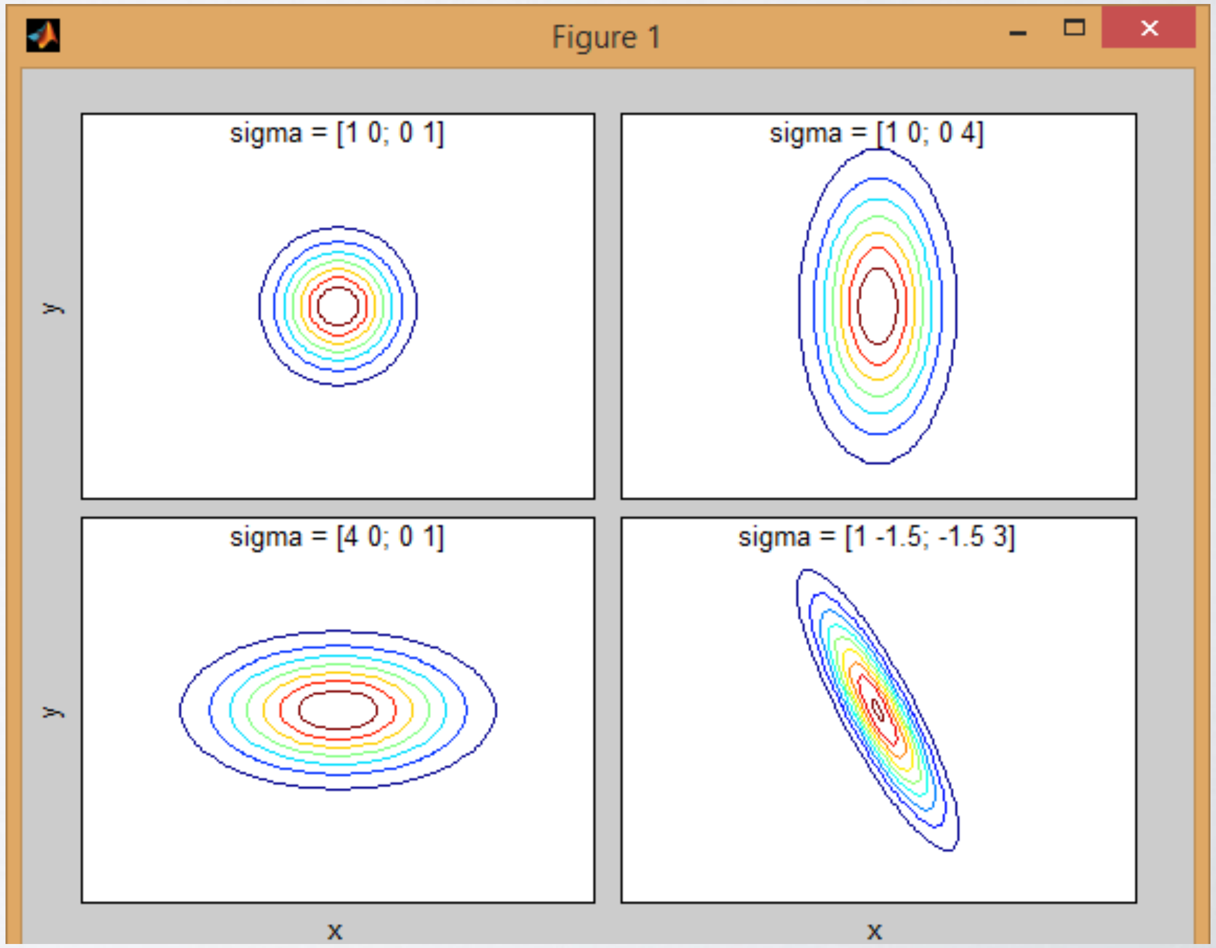


MDL

- 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.
- https://en.wikipedia.org/wiki/Minimum_description_length

NORMALIZATION

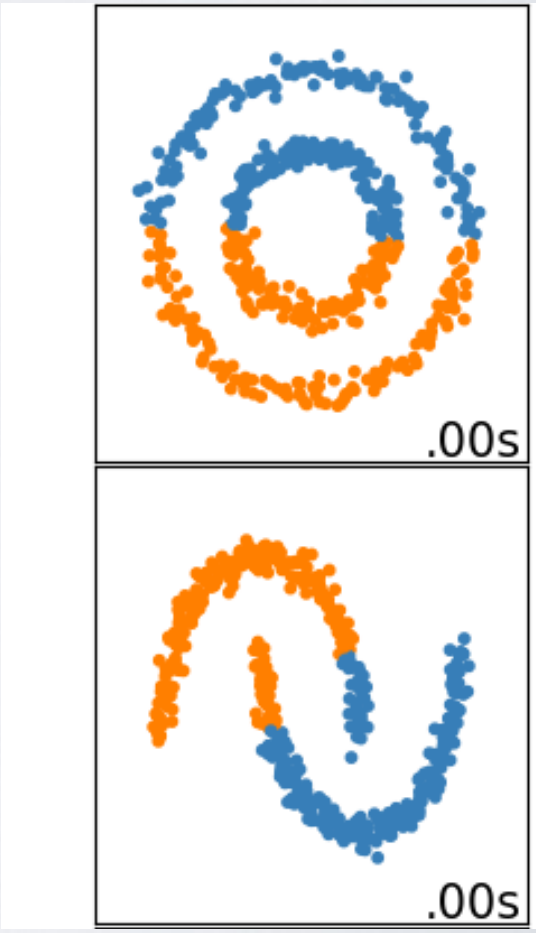
- Is normalization as important for full GM models as for k-means?



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

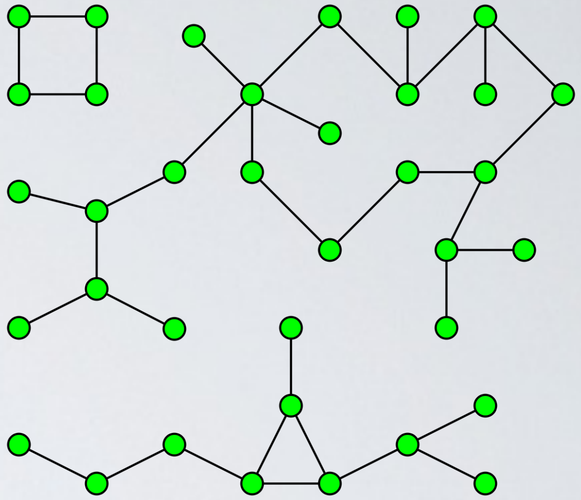
- To overcome this problem, several methods propose local definitions of clusters
  - Does not explicitly optimize a global function
  - Items belong to clusters because they are close enough, locally, to other items in that cluster
  - Clusters exist because there is continuum between all items in it,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

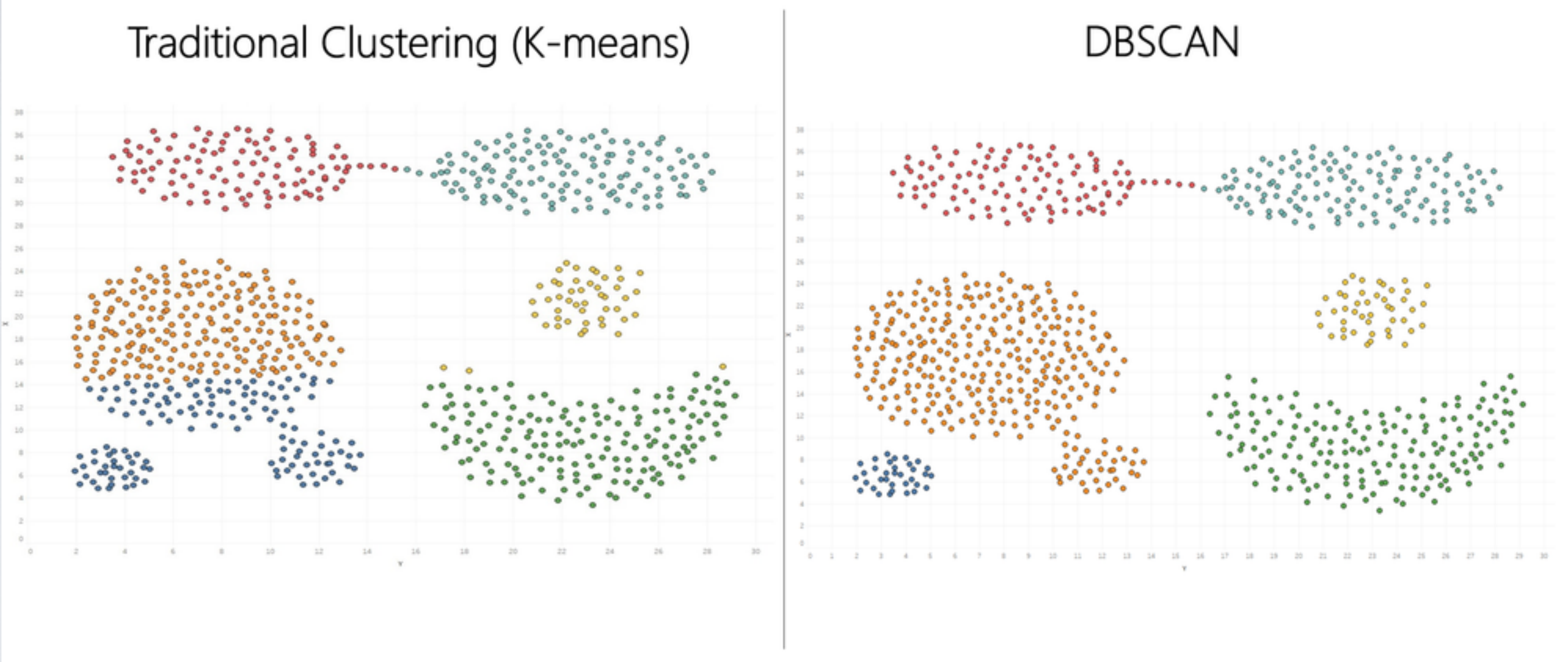
- Define:
  - An item p is a *core point* if it has at least *minPts* items at distance less than ϵ
    - Including p itself

DBSCAN: GRAPH DEFINITION

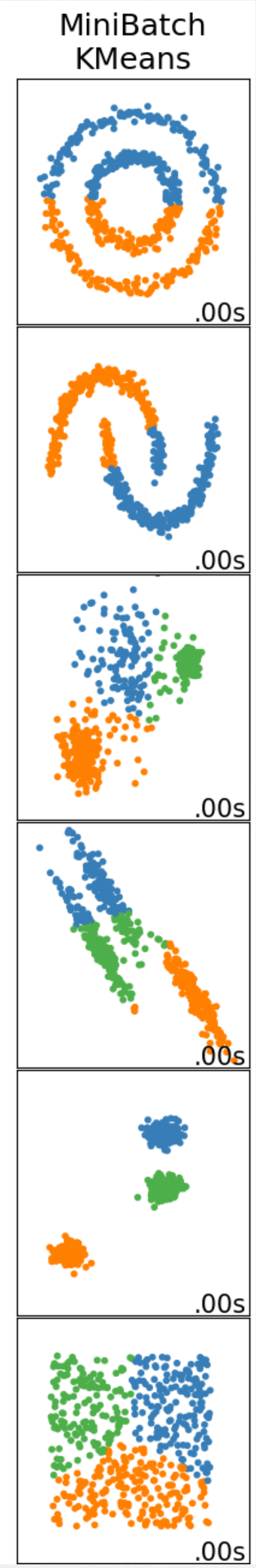


- 1)Build a graph such as
  - Each core node is a node
  - A link exist between core nodes if they are at d<ϵ
- 2)Detect the connected components of the graph
  - 2 nodes belong to the same connected components if there is a path between them
- 3) For all non-core nodes:
  - If they have no core points 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
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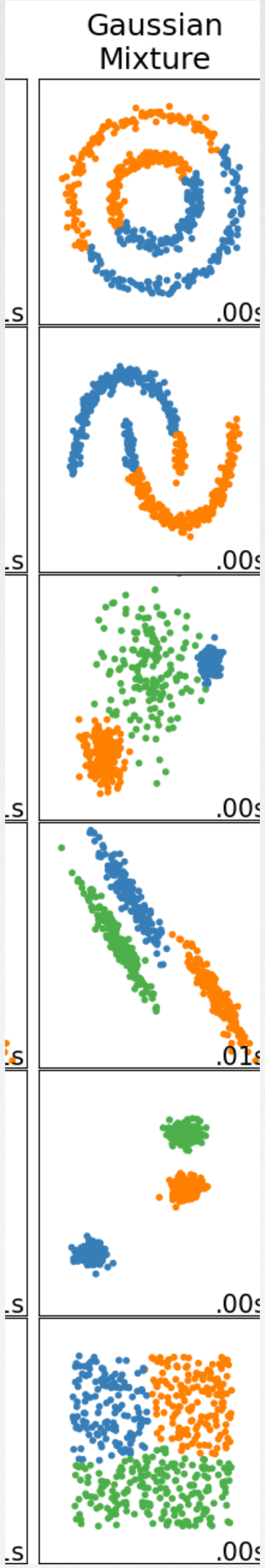
Gaussian Mixture
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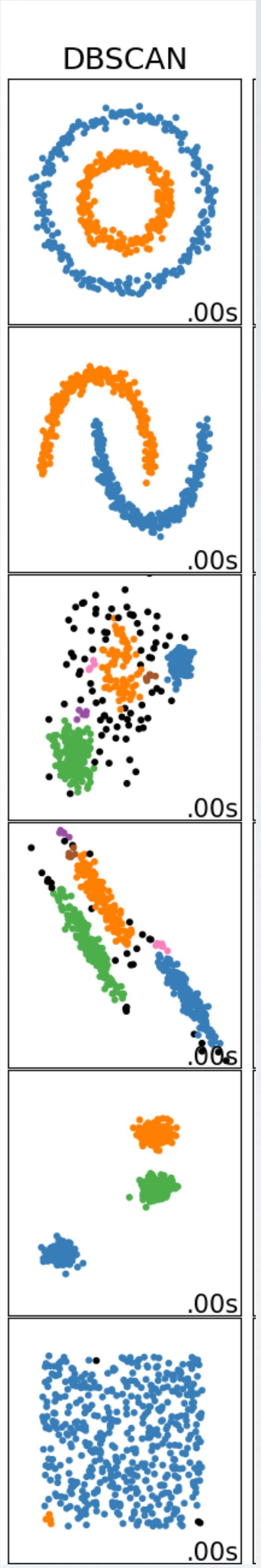
DBSCAN
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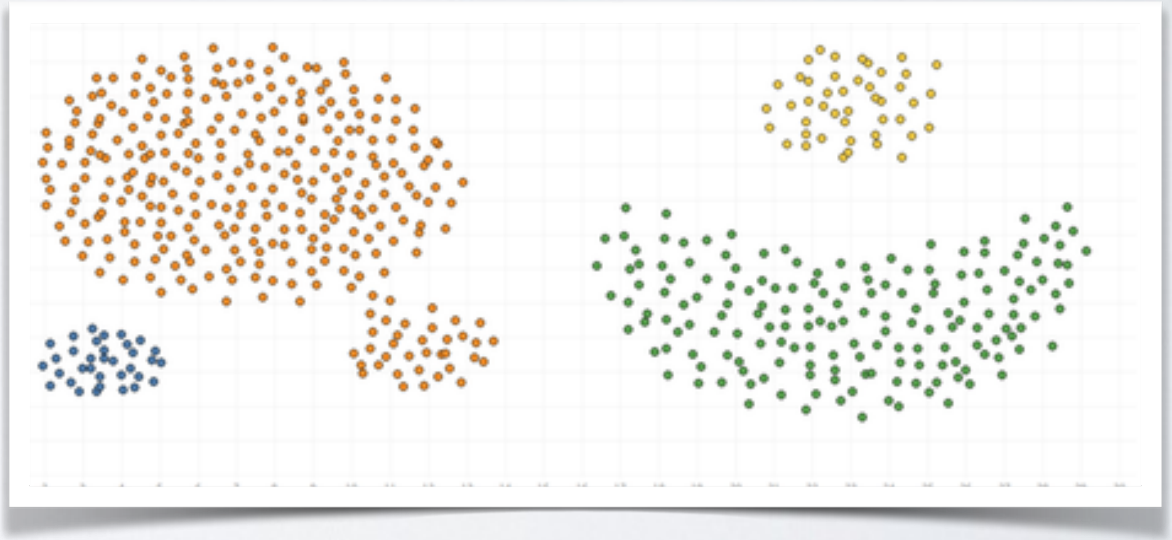
DBSCAN

- 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

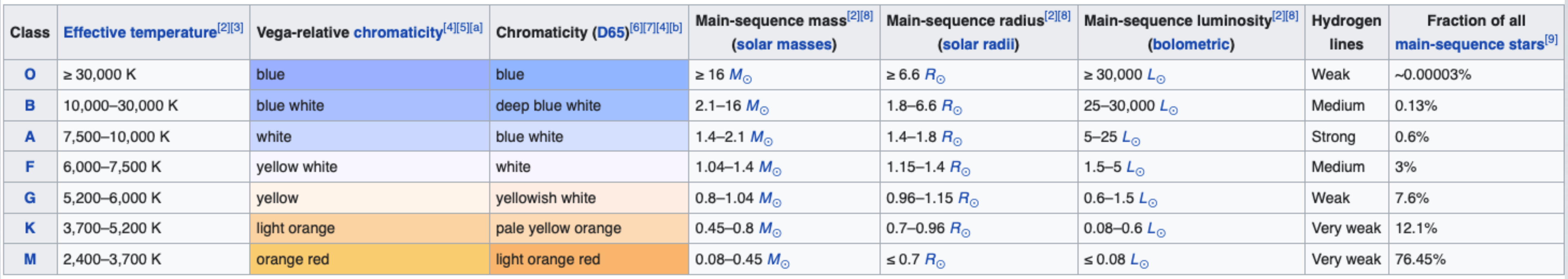
CLUSTERING EVALUATION

INTERNAL/EXTERNAL

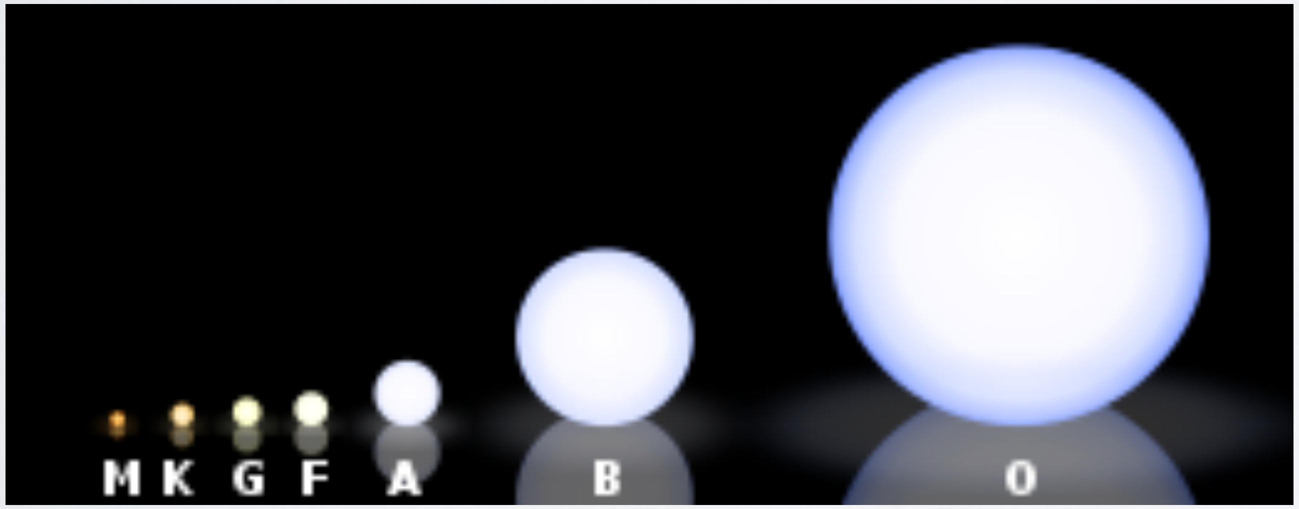
- Two types of evaluation: internal or external

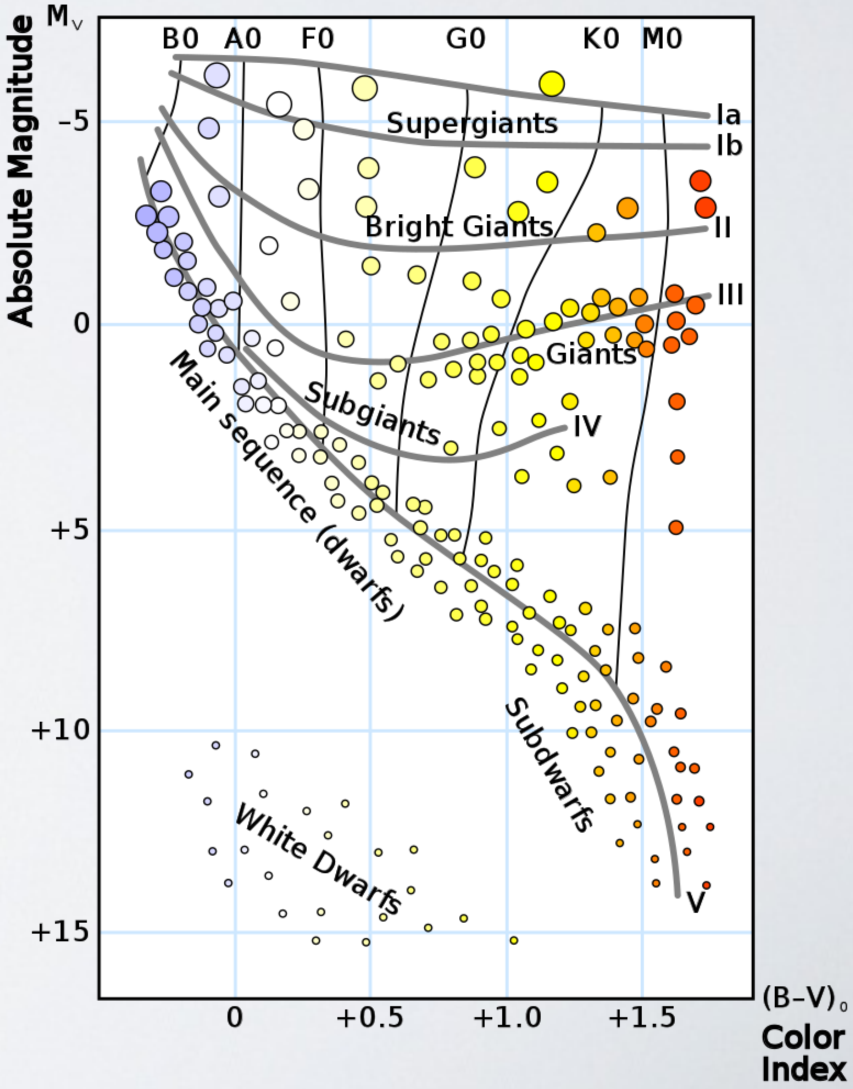
- **External** Evaluation (extrinsic):
  - Similarly to supervised learning, compares the clusters found with a "ground truth"
  - The ground truth can be exactly the right clustering desired
    - So we are just validating the method, since we already know the answer…
  - The ground truth can be a proxy to what we want
    - e.g., we have a manual ground truth, done by an expert. Not perfect, costly, and not generalizable to newer data, so supervised cannot work. We can check that clustering find something close.

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 maximizes the likelihood

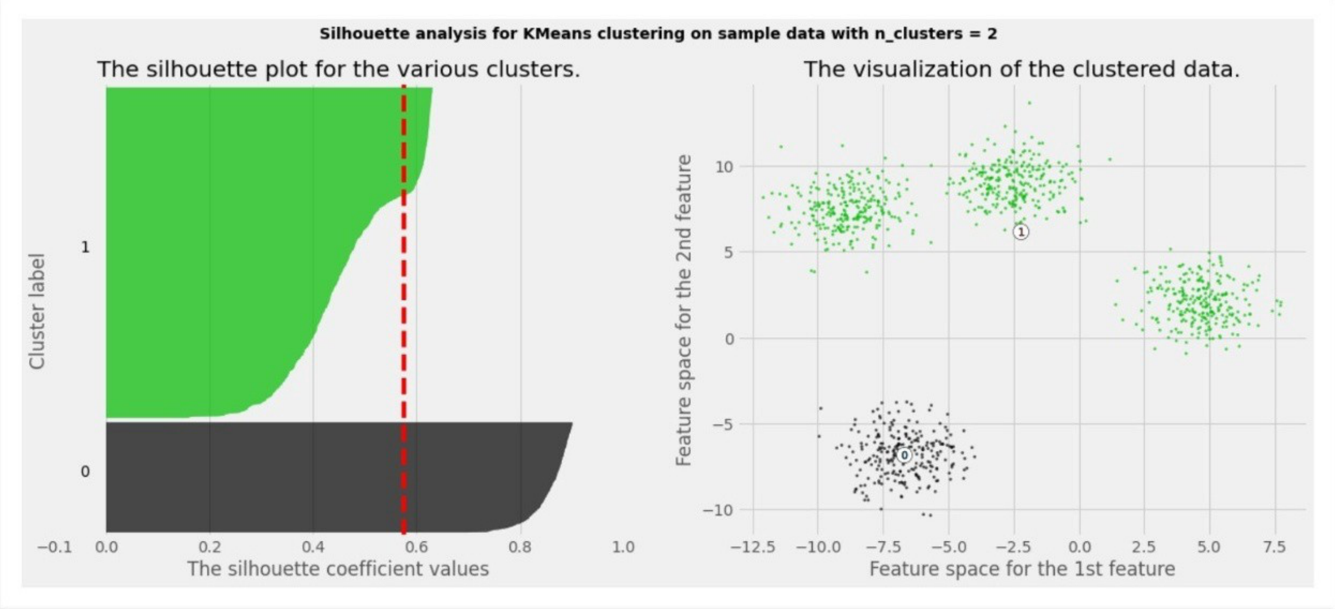
- But can lead to unfair comparisons:
  - Using inter-cluster variance to compare k-means and another method such as DBscan is unfair.
    - One explicitly minimizes this objective, the other no…

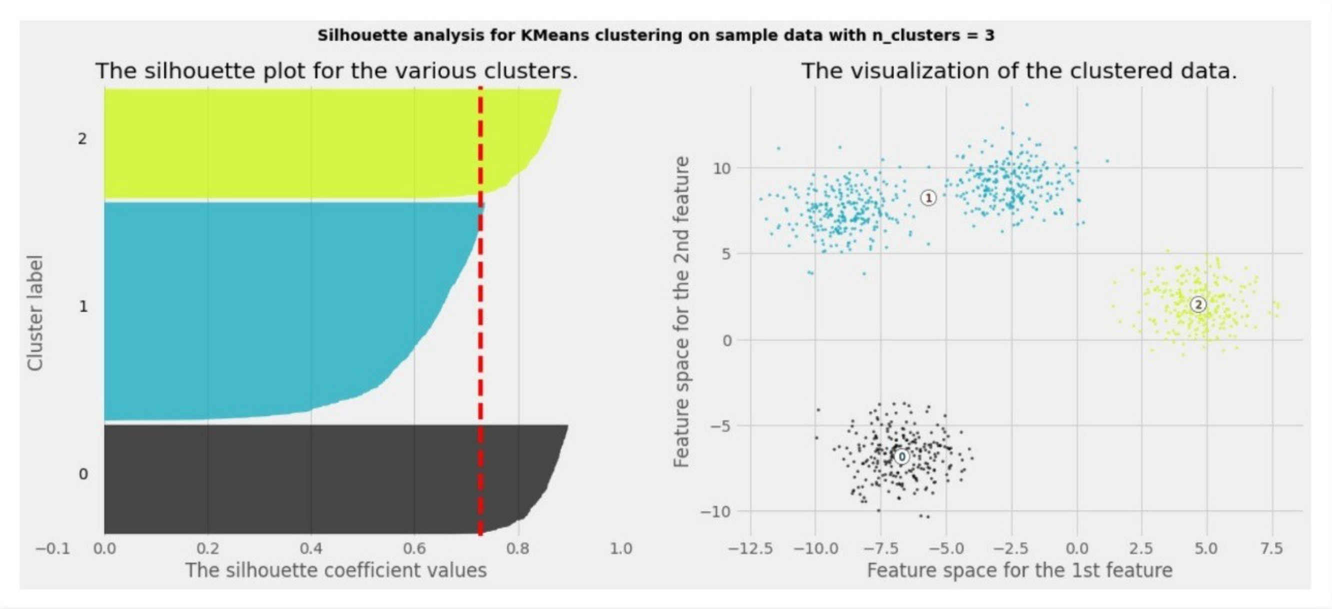
- The choice of a score is equivalent to choosing a definition of cluster…

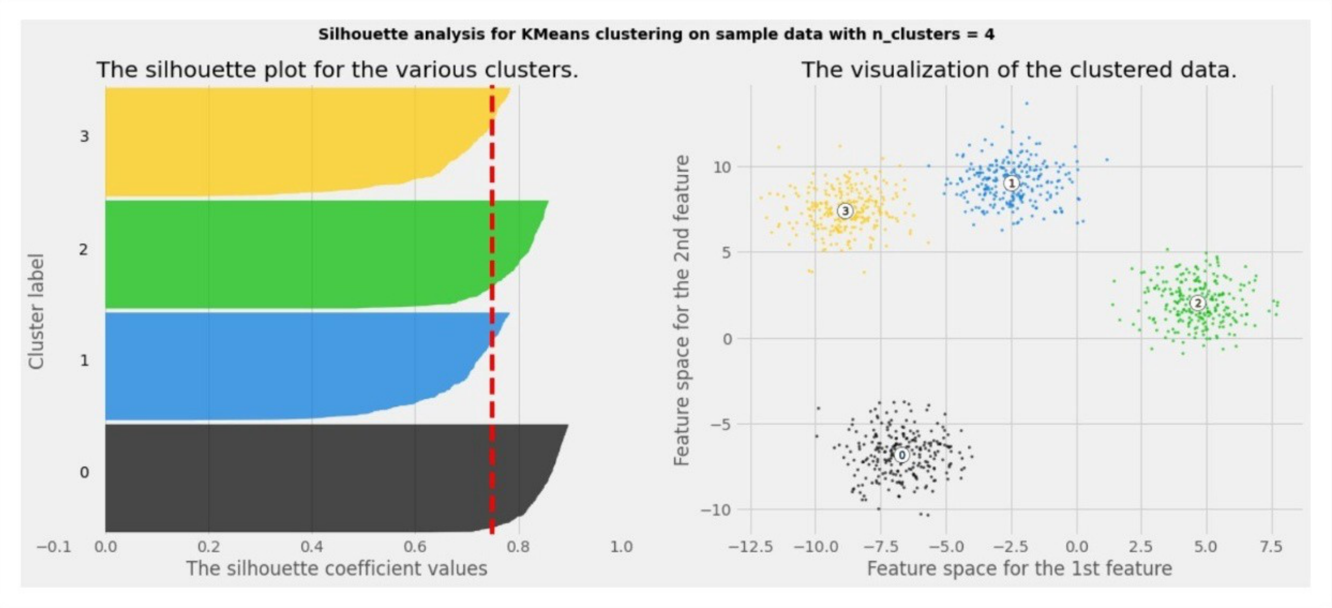
SILHOUETTE SCORE

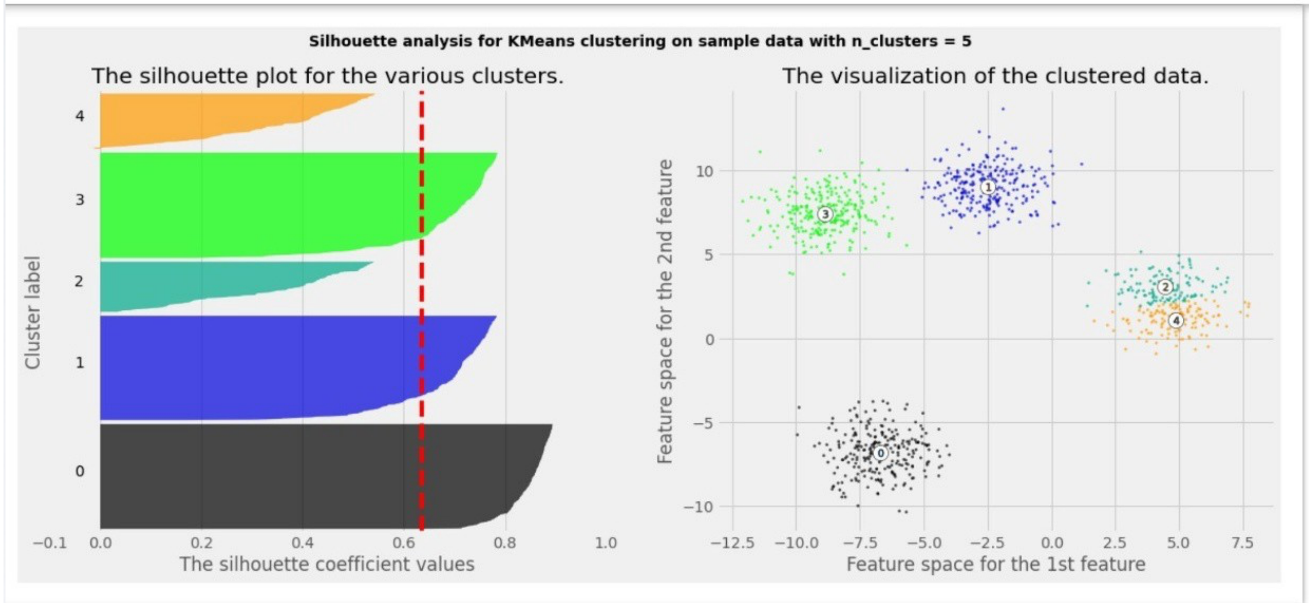
- Silhouette score of 1 observation:
  - 1)Compute $a(i)$, average distance to all other observations of the same cluster
  - 2)Compute $b(i)$, <u>min</u> of "average distance to all observations of another cluster"
  - 3) Silhouette: $s(i) = \begin{cases} 1 - a(i)/b(i), & \text{if } a(i) < b(i) \\ 0, & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1, & \text{if } a(i) > b(i) \end{cases}$

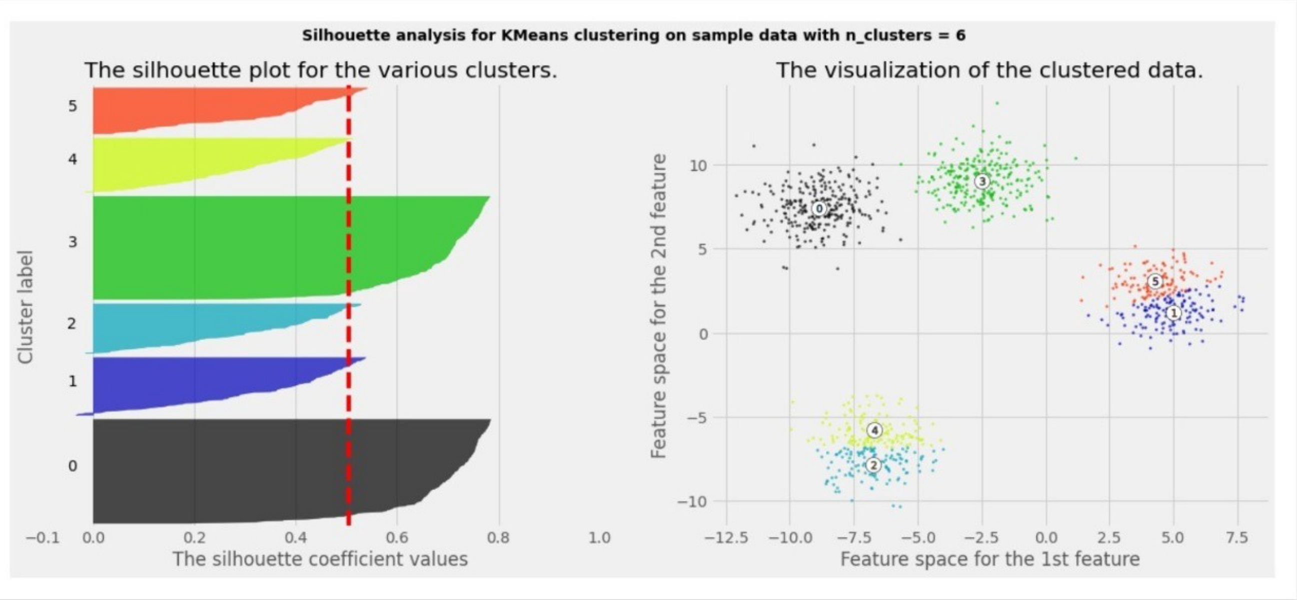
- Silhouette coefficient:
  - Average of all individual Silhouette scores.


Silhouette analysis for KMeans clustering on sample data with n_clusters = 2
The silhouette plot for the various clusters.
Cluster label
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Feature space for the 1st feature
1
0


Silhouette analysis for KMeans clustering on sample data with n_clusters = 3
The silhouette plot for the various clusters.
Cluster label
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Feature space for the 1st feature
1
2
0

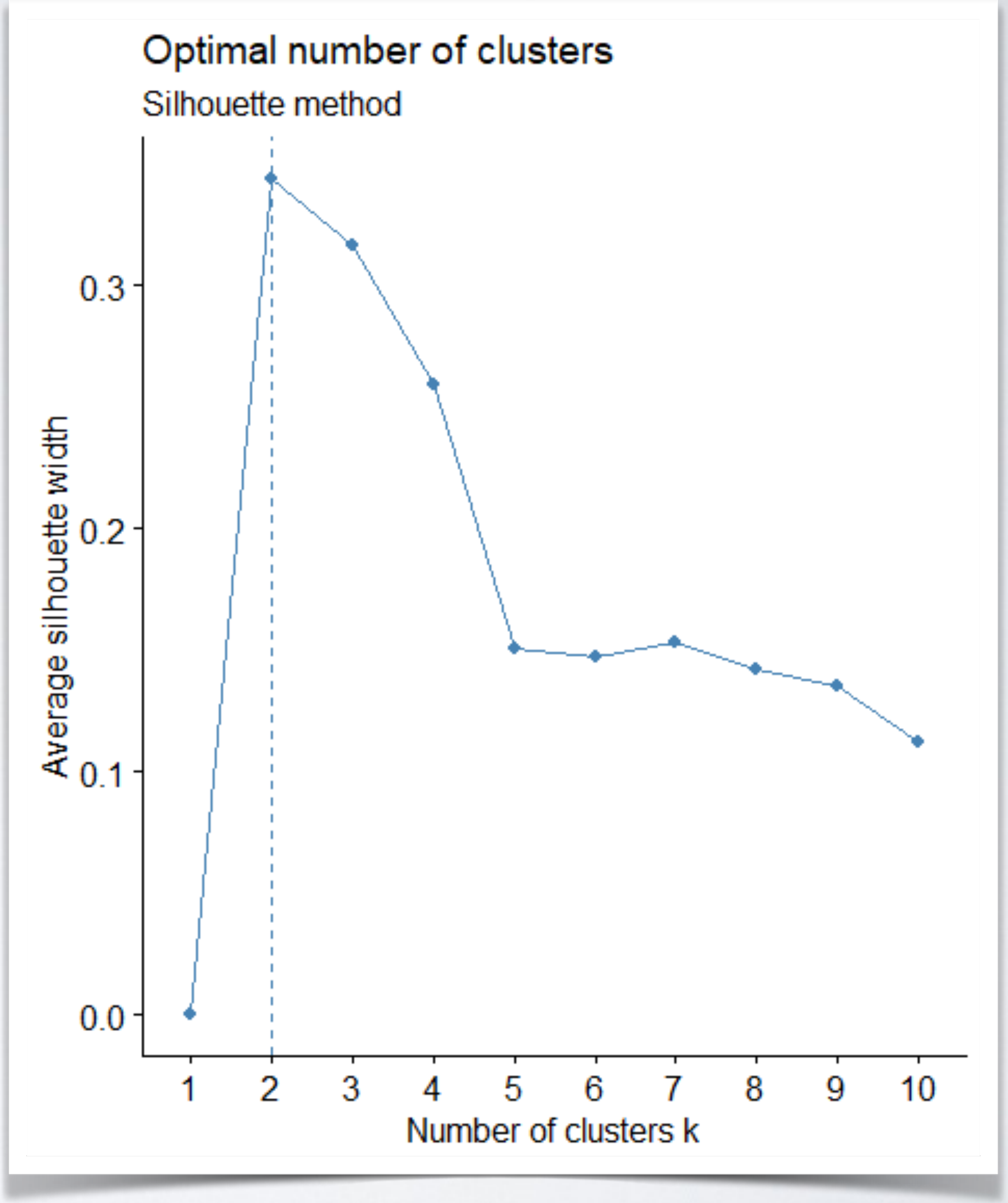

Silhouette analysis for KMeans clustering on sample data with n_clusters = 4
The silhouette plot for the various clusters.
Cluster label
3
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Feature space for the 1st feature
3
1
2
0

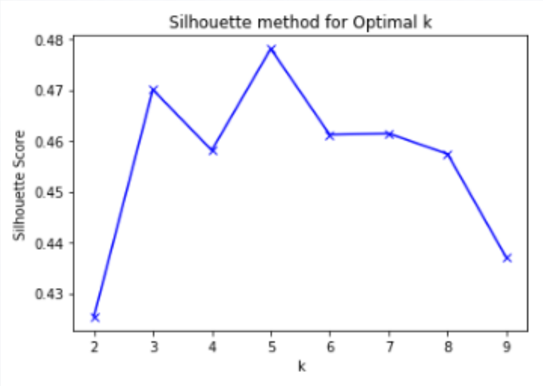

Silhouette analysis for KMeans clustering on sample data with n_clusters = 5
The silhouette plot for the various clusters.
Cluster label
4
3
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Feature space for the 1st feature
3
1
2
4
0


Silhouette analysis for KMeans clustering on sample data with n_clusters = 6
The silhouette plot for the various clusters.
Cluster label
5
4
3
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Feature space for the 1st feature
0
3
5
1
4
2

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





AUTOMATIC K SELECTION

- Better than the elbow method on real data

OTHER SCORE FUNCTIONS

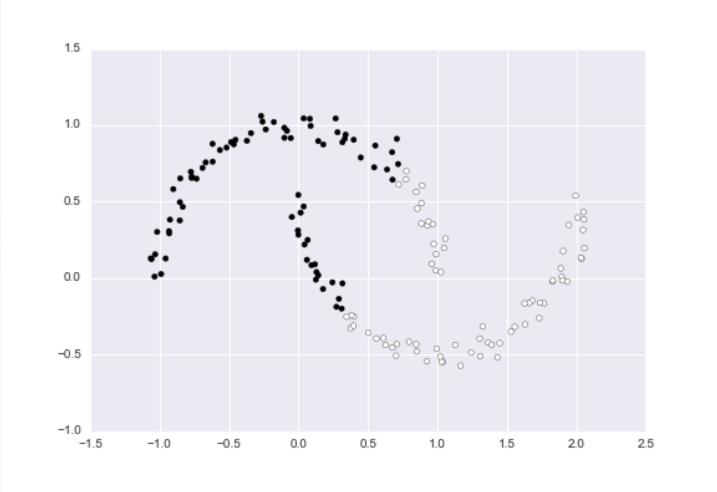
- **Davies-Bouldin Index (DBI)**: The average similarity ratio of each cluster with its most similar cluster,
  - where similarity is the ratio of within-cluster distances to between-cluster distances;
  - lower DBI values suggest better clustering.

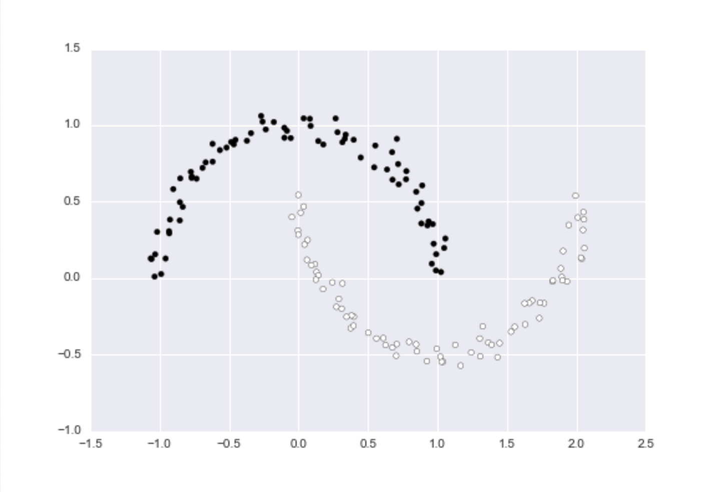
DUNN INDEX

$$DI_m = \frac{\min\limits_{1 \leqslant i < j \leqslant m} \delta(C_i, C_j)}{\max\limits_{1 \leqslant k \leqslant m} \Delta_k}$$

- With
  - $\delta(C_i, C_j)$ a measure of distance between clusters
    - e.g., distance between closest points, average distance…
  - Δ_k a measure of the dispersion of the cluster
    - e.g., max distance between two cluster points

NON-SPHERICAL CLUSTERS





- Remember the difference between k-means clusters and DB-scan clusters
- Previous scores are reliable only in k-means-like clusters.
- Specific (less known) scores for arbitrary clusters
    - Density-based silhouette
    - DBCV(Density-Based Clustering Validation)

STABILITY

- If clusters are not clear, multiple runs of the same method might discover different clusters

- Evaluating the stability of those clusters might be a way to assess their quality

- To better assess the quality, one can introduce noise:
  - Comparing clustering on sub-sets (random samples, independent samples…)
  - Adding noise (fake data points, outliers, removing low-quality data…)

CONSENSUS CLUSTERING

- Let’s consider that we have multiple candidate clusterings
  - From the same method ran multiple times
  - From the same method with different parameters
  - From different methods

- One can compute a “consensus”
  - Create the consensus matrix C_{ij} counts the number of times data points i, j were grouped together
  - Apply your favorite clustering method on that matrix, considering that $\frac{1}{C_{ij}}$ gives the *distance* between data points.

MANY OTHER CLUSTERINGS

- Hierarchical clustering
- Spectral clustering
- Mean-Shift clustering
- Affinity Propagation
- OPTICS (Ordering Points To Identify the Clustering Structure)

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.