Clustering algorithms

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Clustering is a key process in data exploration

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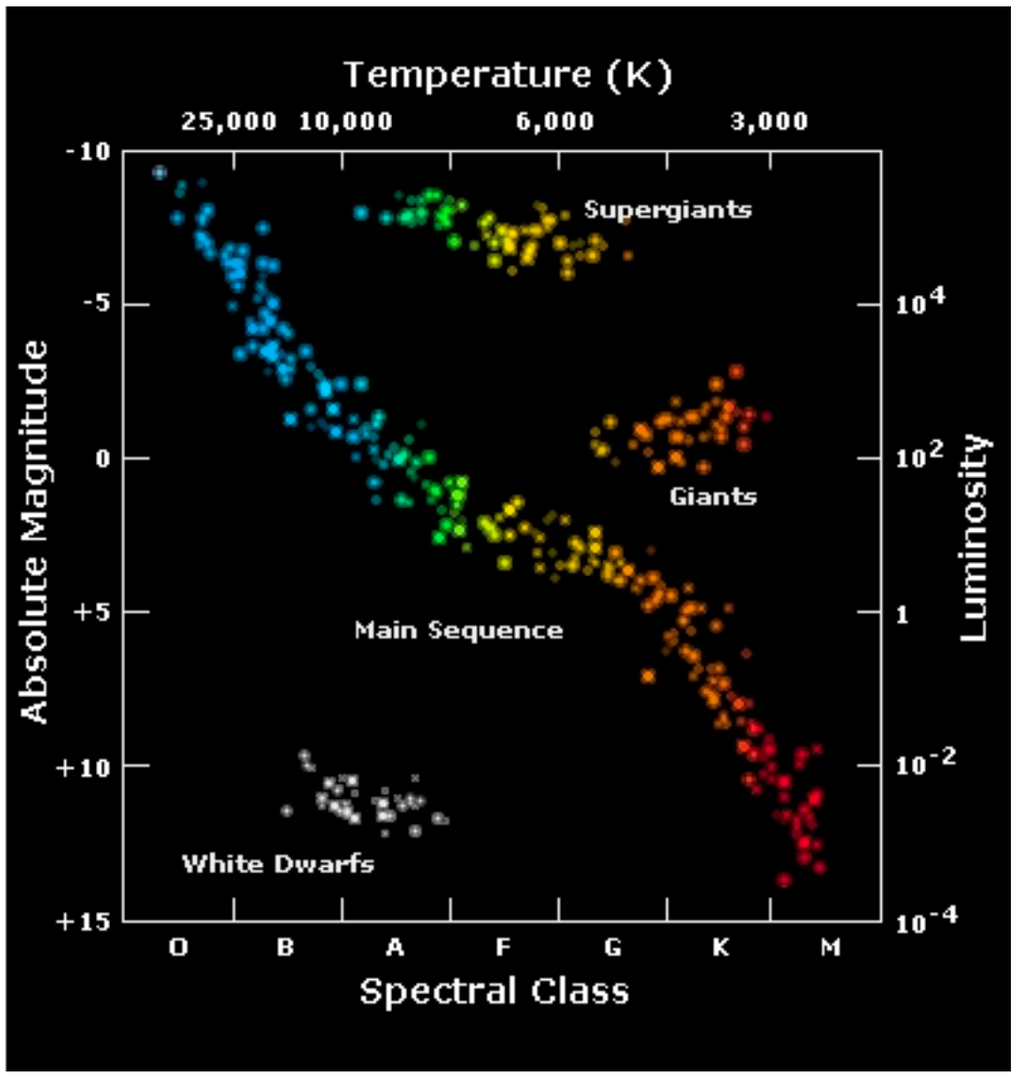
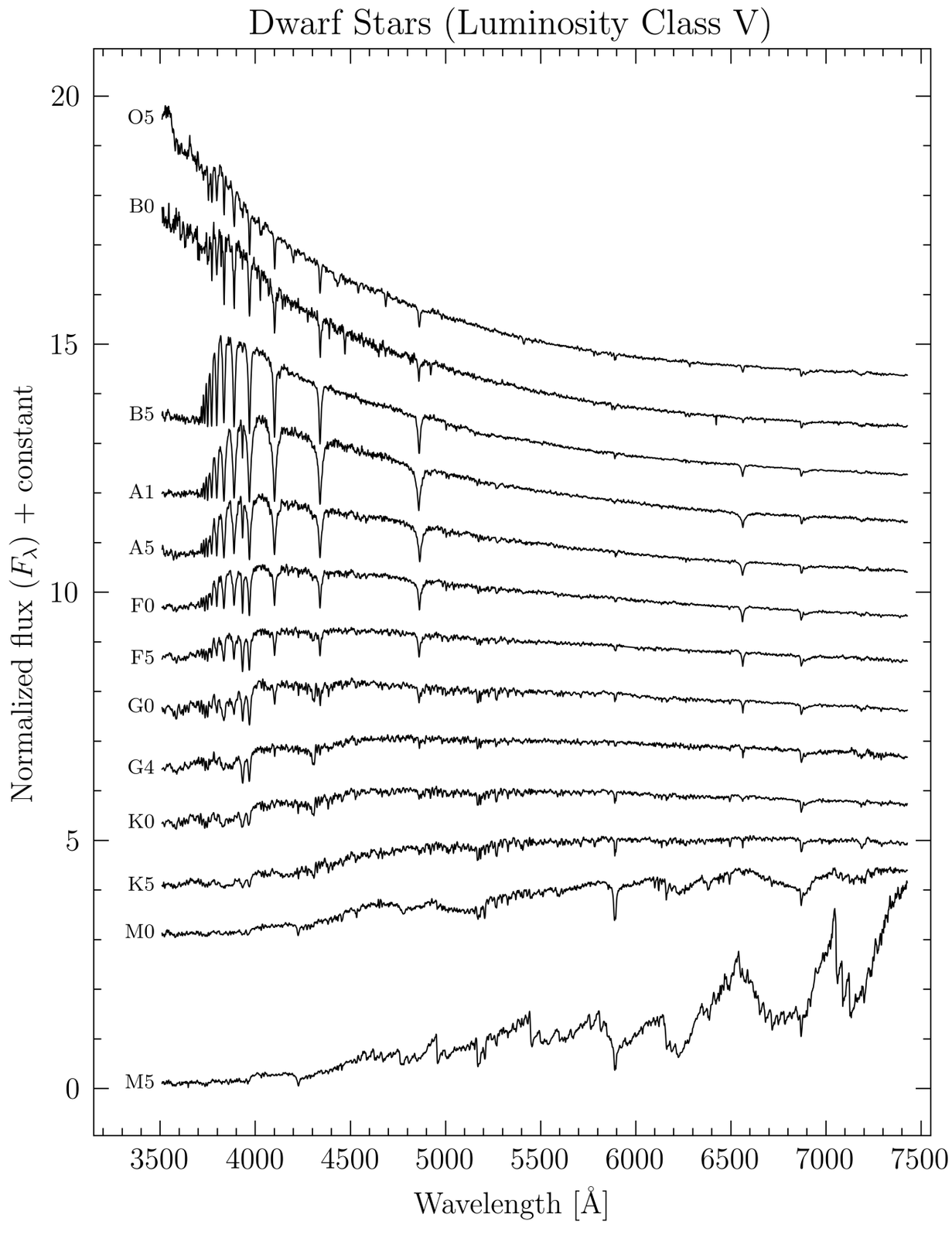
- Scientists, and in particular astronomers, have been doing cluster analysis well before they used programing or Machine Learning algorithms.

Clusters in astronomy

1. Stellar spectral classes

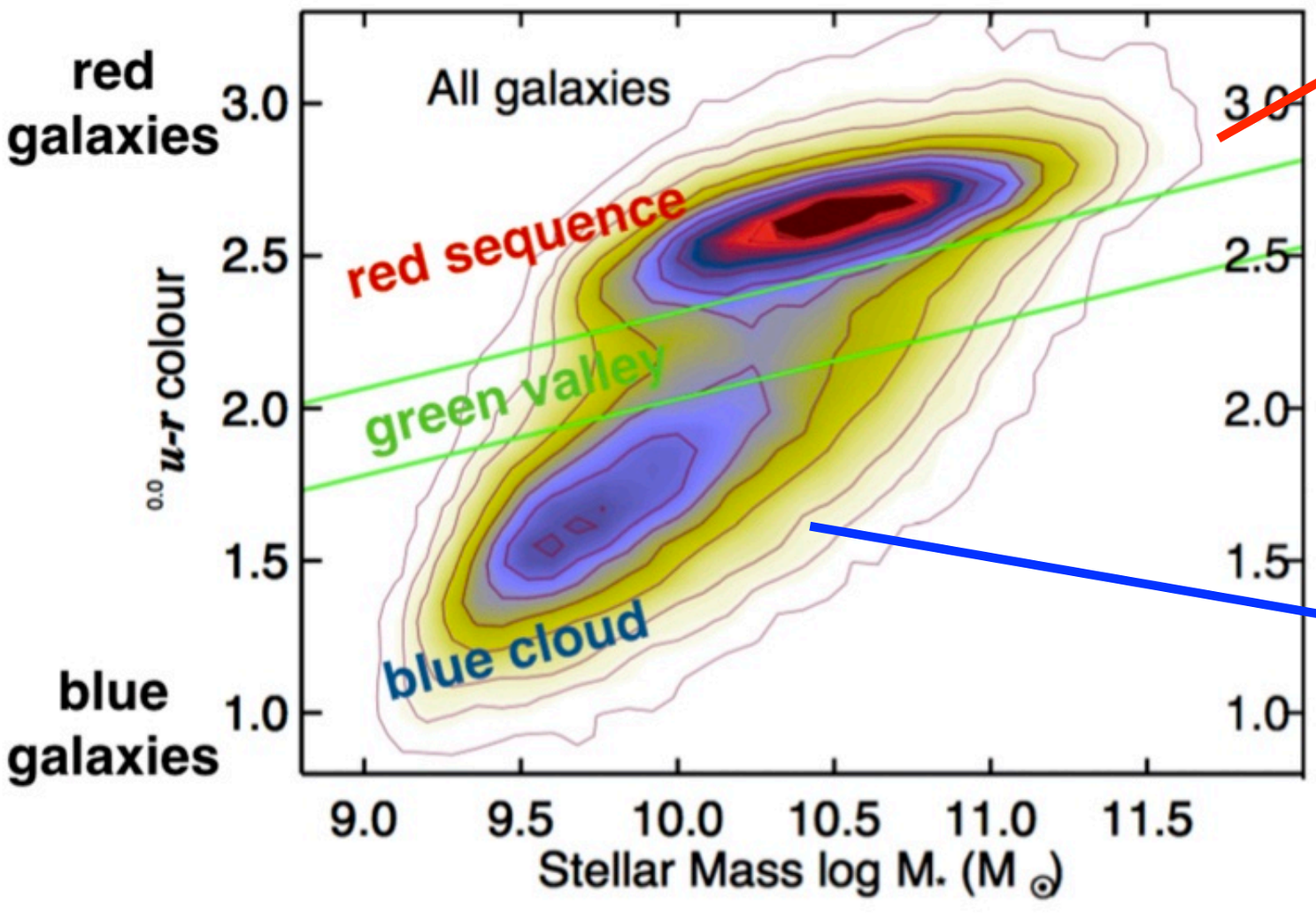


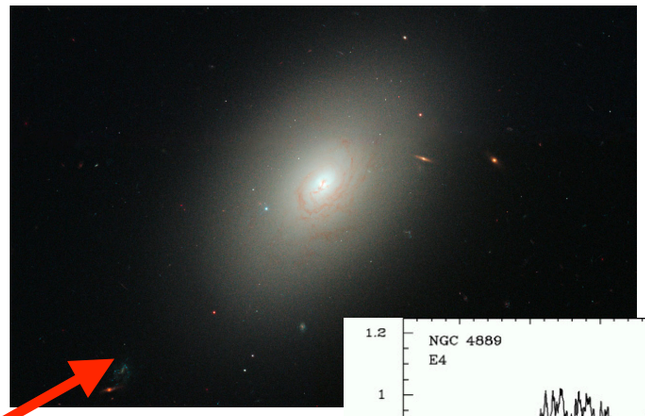


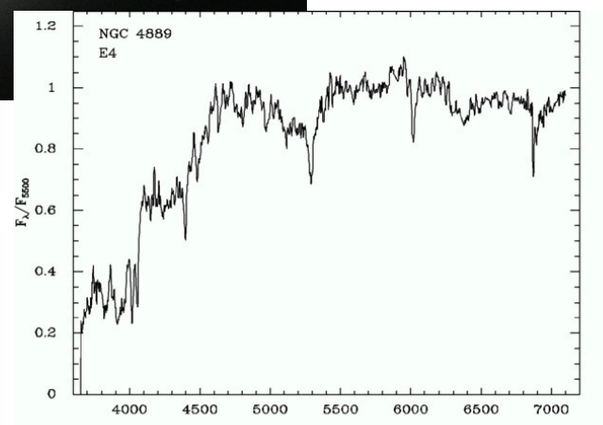
Clusters in astronomy

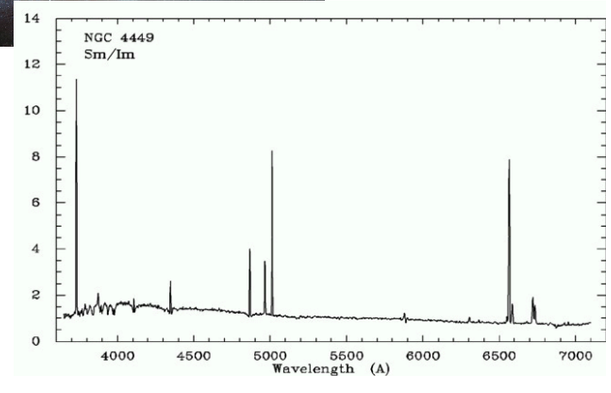
2. Galaxy bimodality

Taken from: Schawinski et al. (2014)



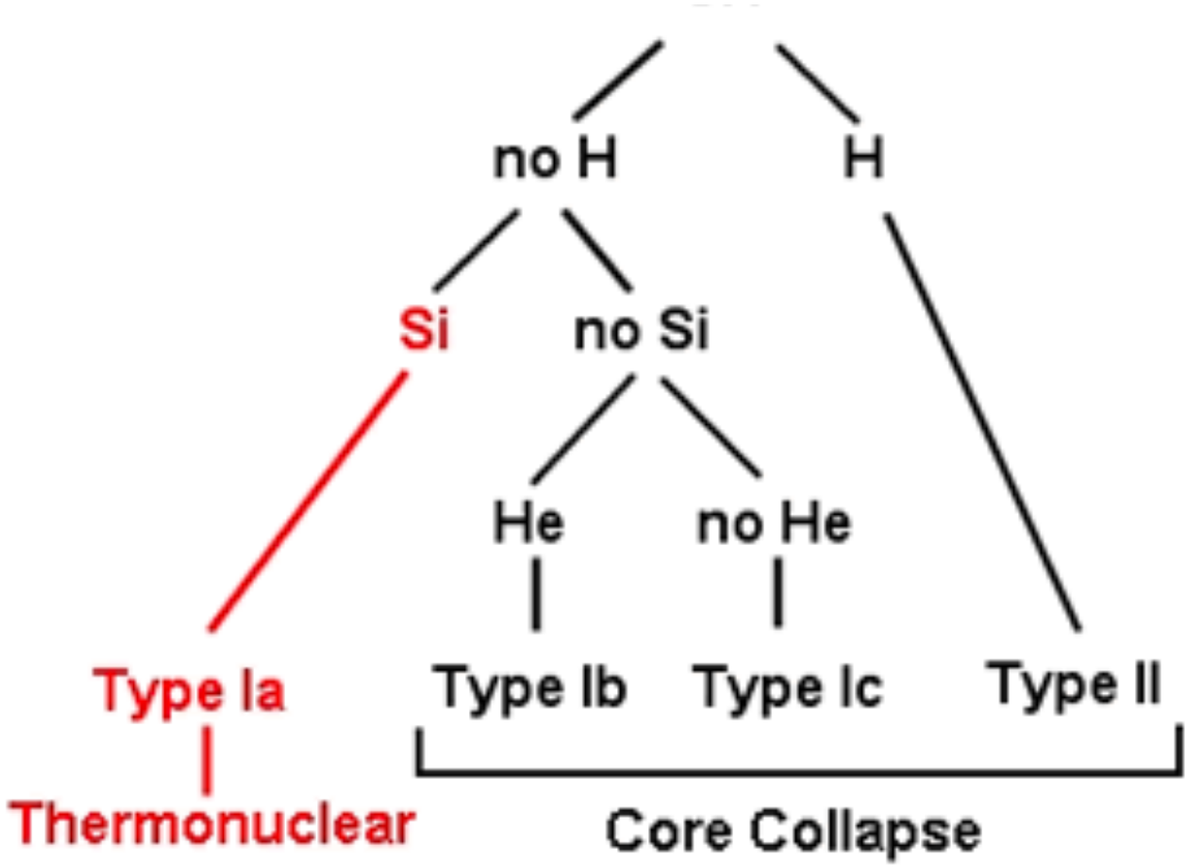


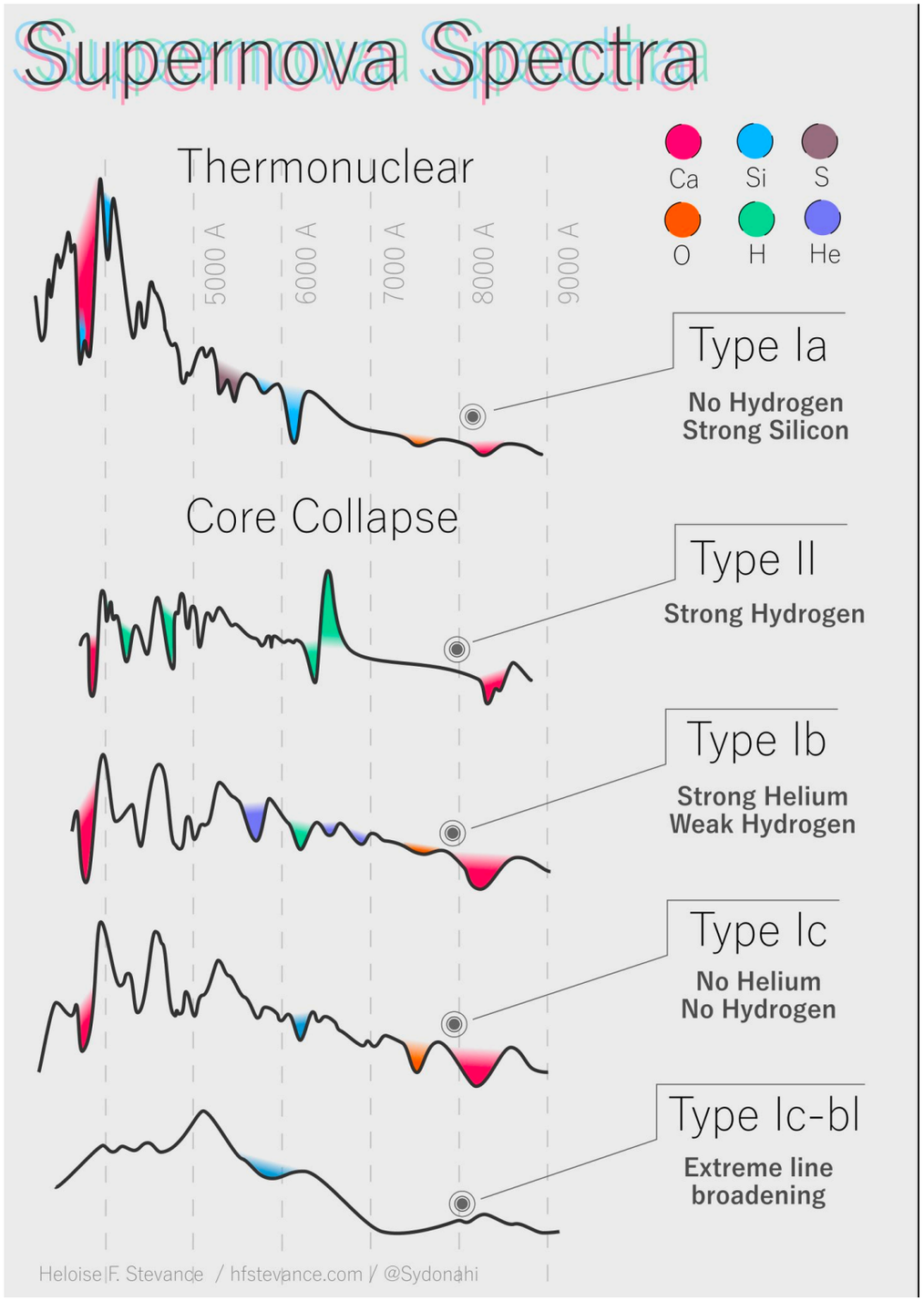




Clusters in astronomy

3. Supernova classes: type Ia and type II supernovae





By H. Stevance

What is fundamentally different now?

1. The volume and rate of information grows exponentially:

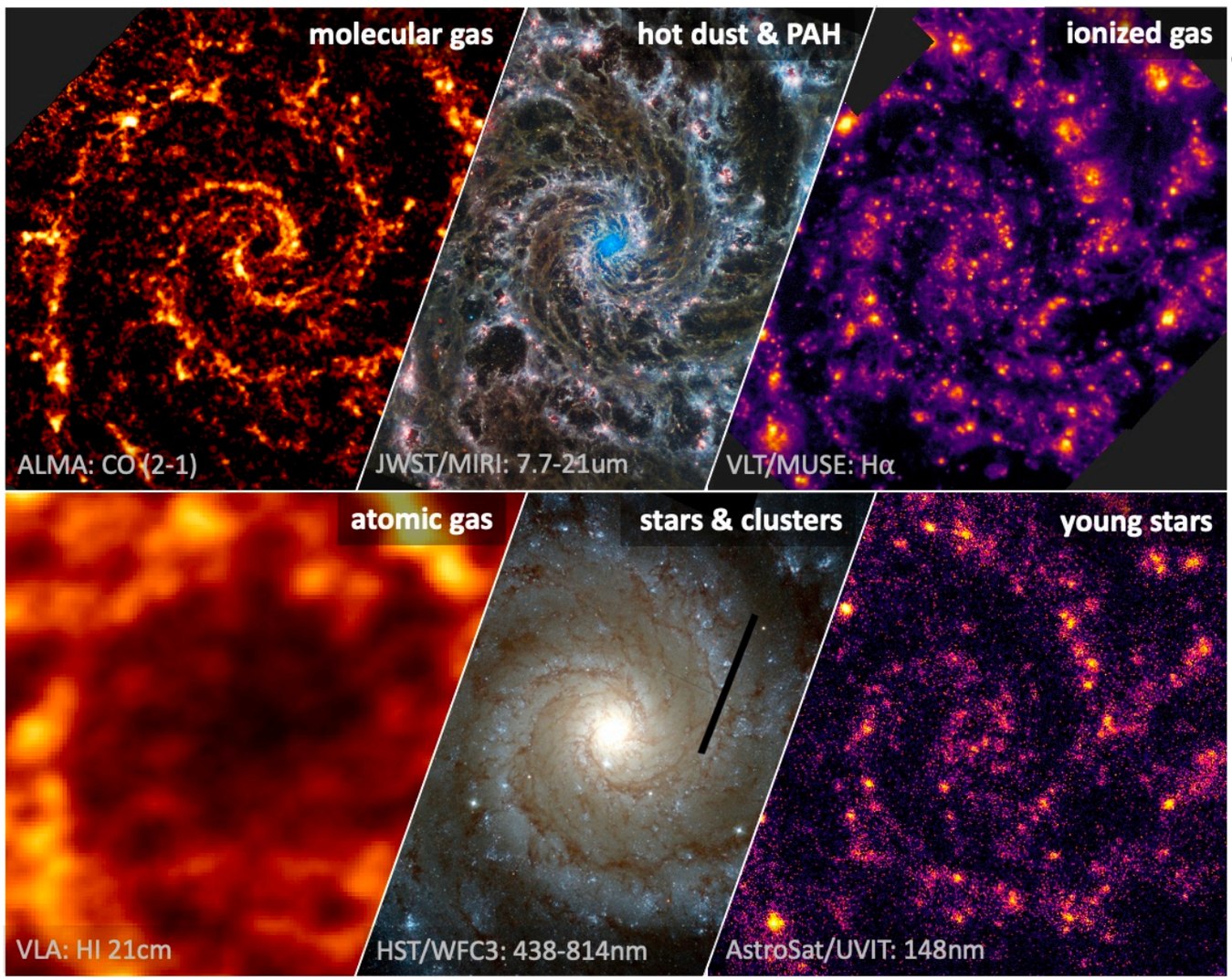
   - Sky survey now generate ~1 PB of data + derived products. Astronomical databases now routinely include $10^6 - 10^9$ objects.

   - We can no longer manually-inspect all the data we collect.

What is fundamentally different now?

2. A great increase in data dimensionality and complexity:

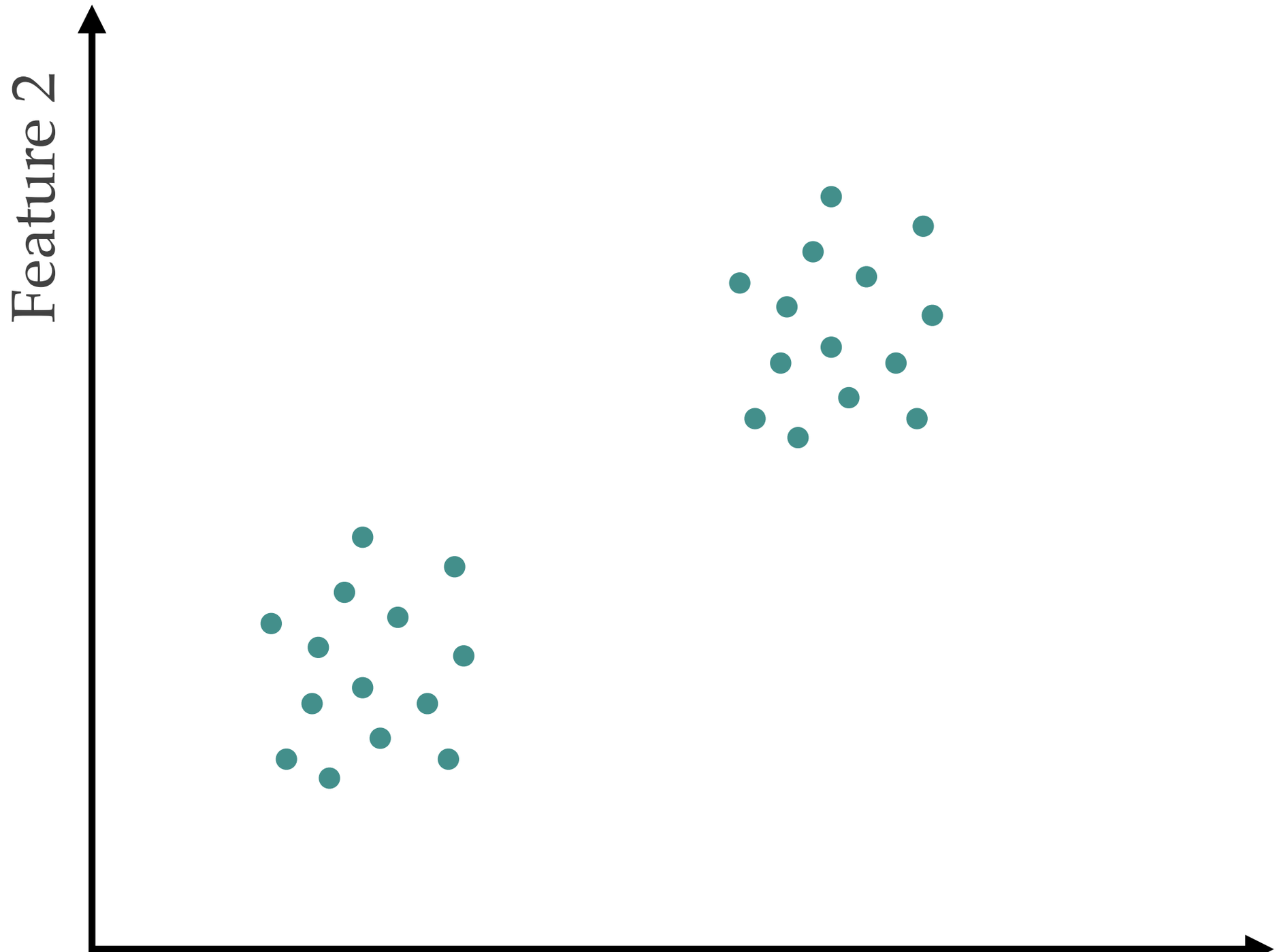
   - Data is heterogeneous and high-dimensional.
   - Patterns and correlations in the data can no longer be visualized in 3D.



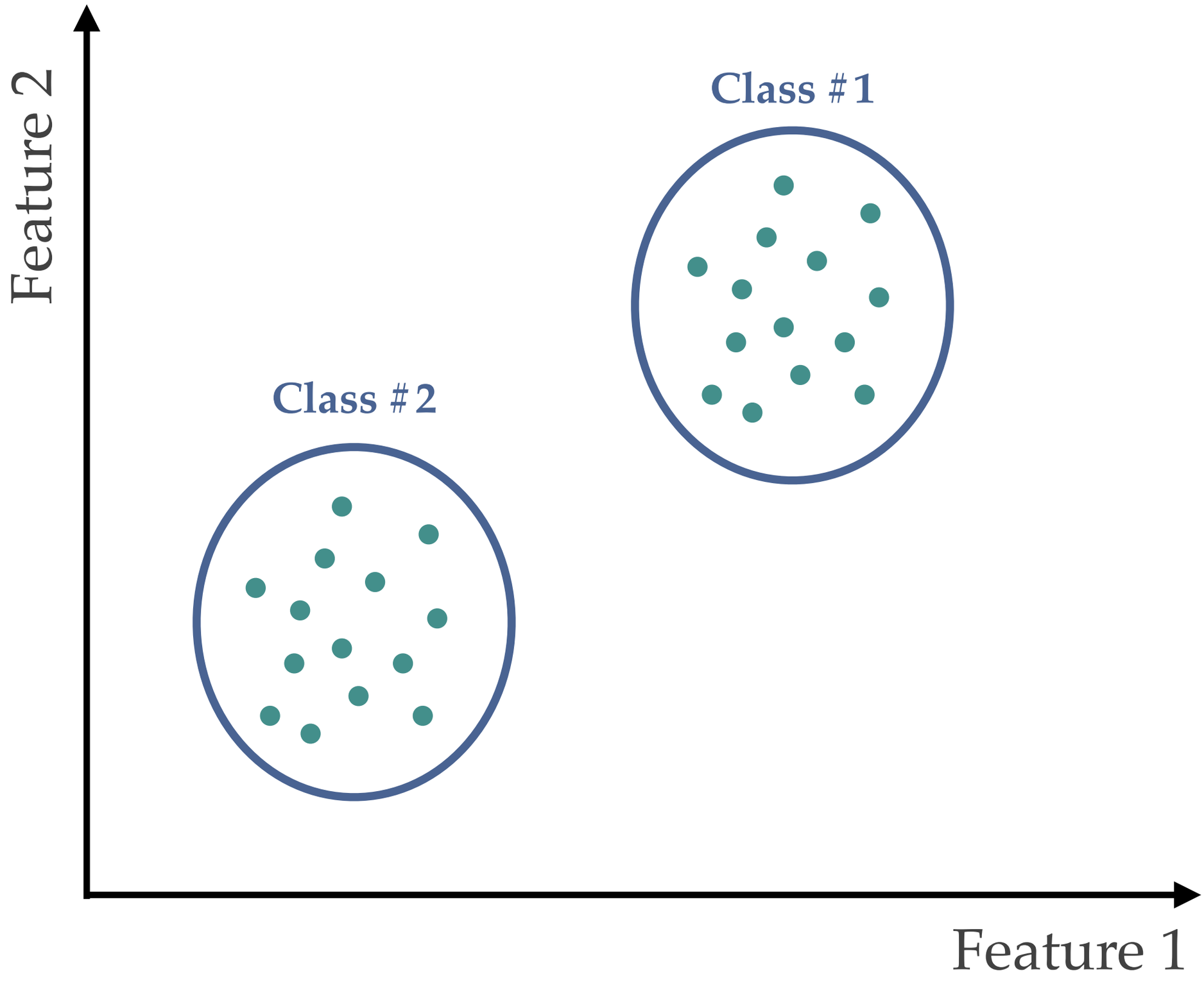
By J. Sun

Image by the PHANGS collaboration

Clustering



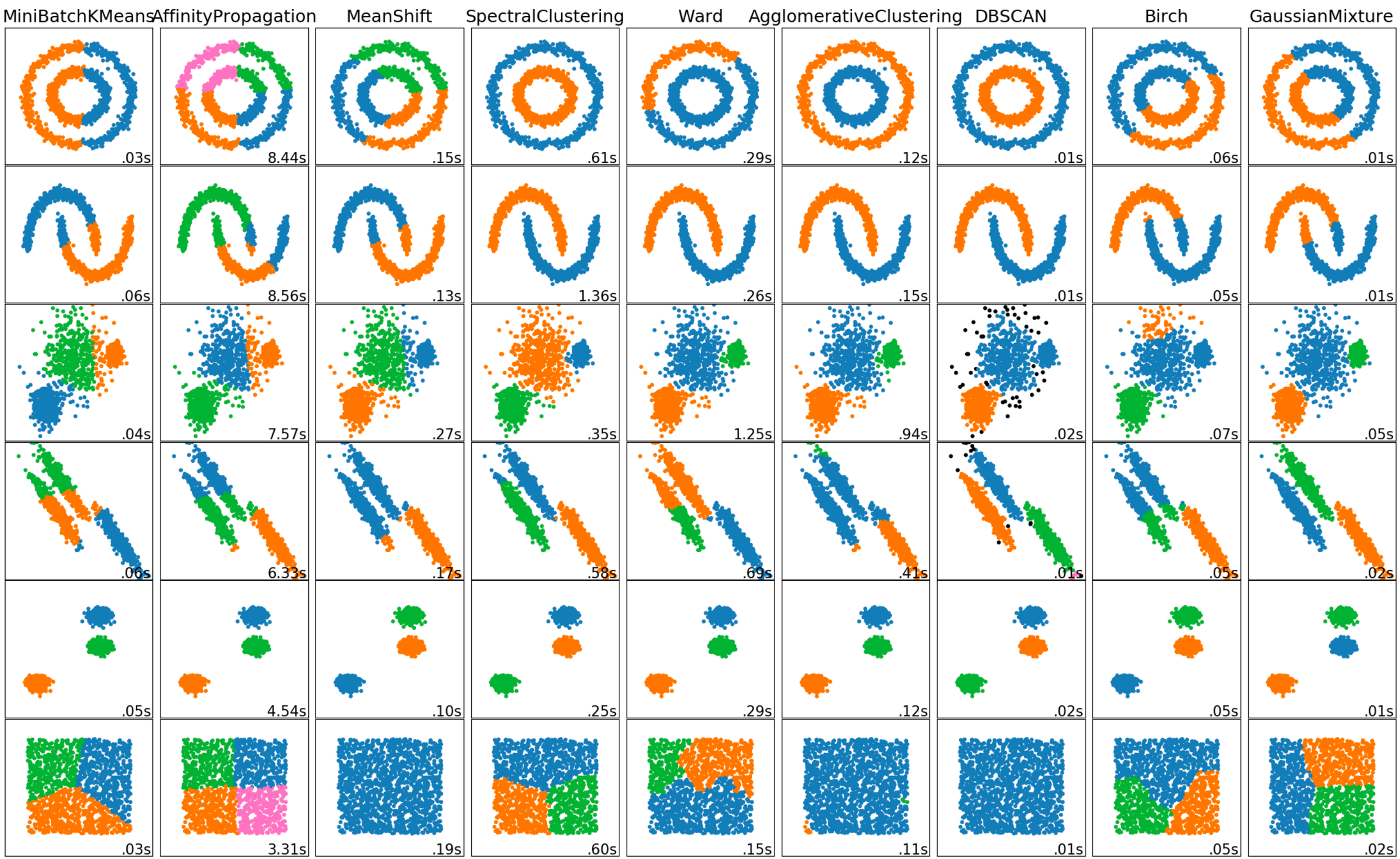
Clustering



Clustering

From Scikit-learn's example gallery:

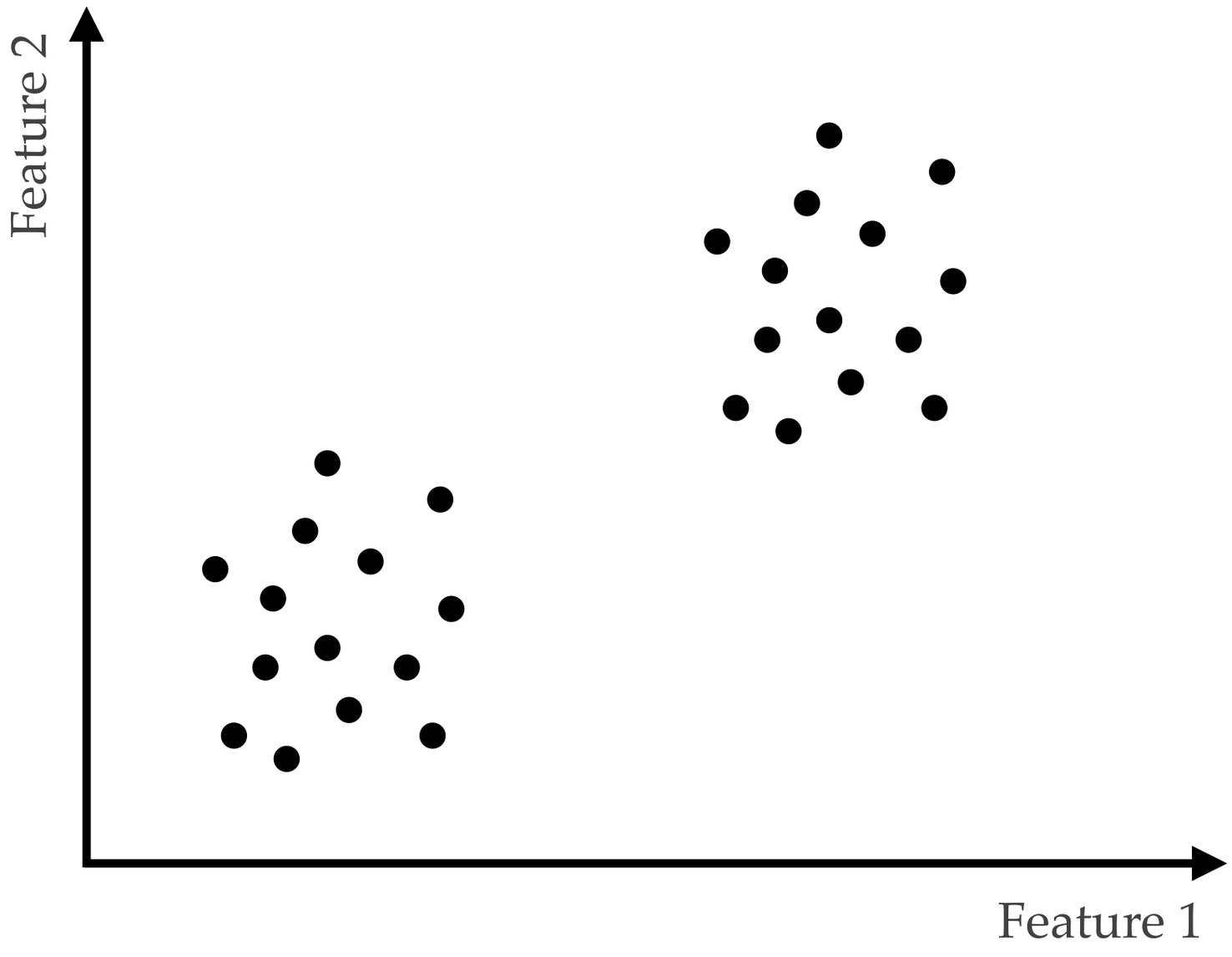
see this comparison between algorithms



K-means

Input: measured features, and the number of clusters, k.

The algorithm will classify all the objects in the sample into k clusters.



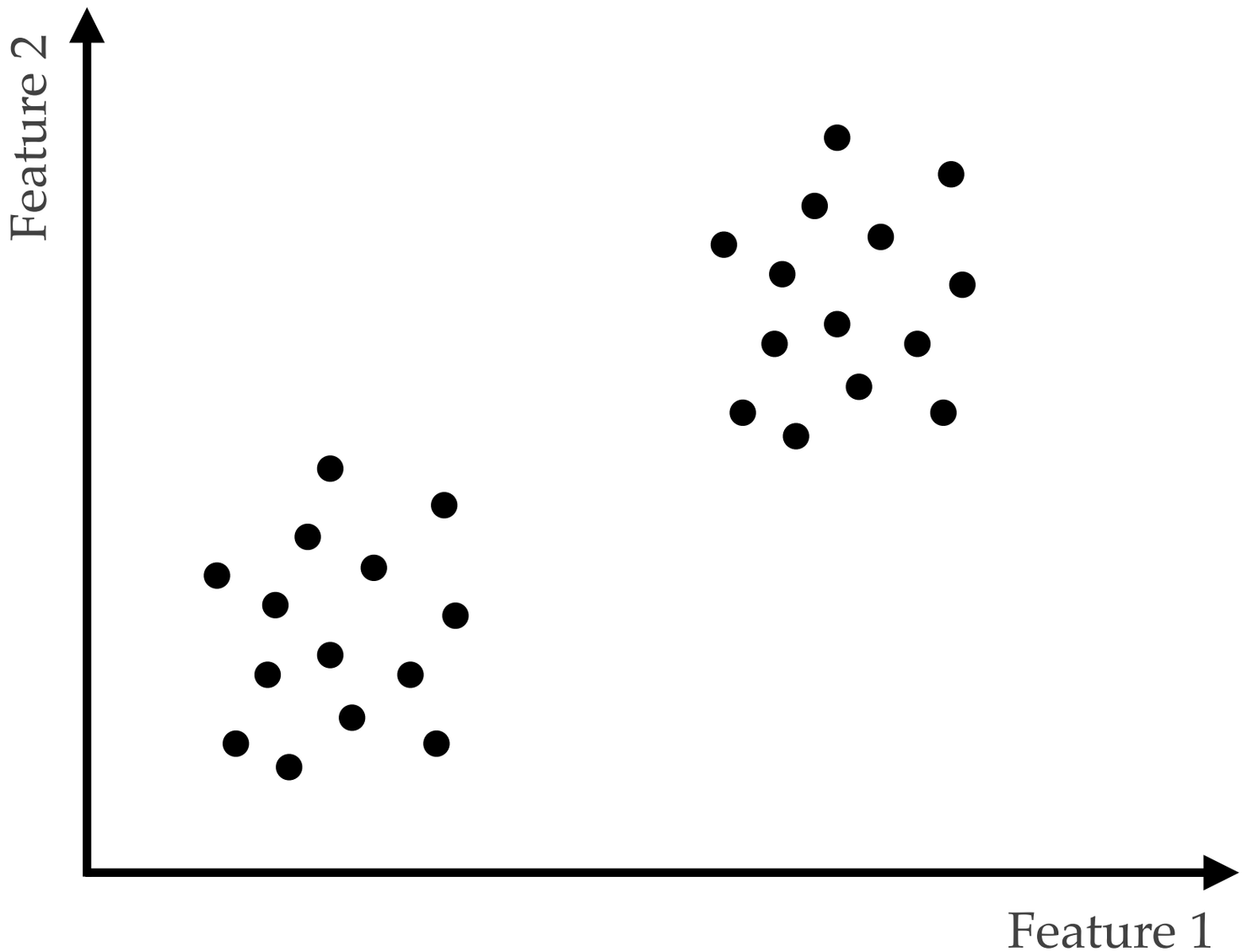
K-means

(I) Random assignment of **k** points that represent the centroids of the clusters.

Iterate:

(II) Associate each object with a single cluster, using the **distance** from the cluster centroid.

(III) Recalculate the cluster centroid according to the objects that are associated with it.



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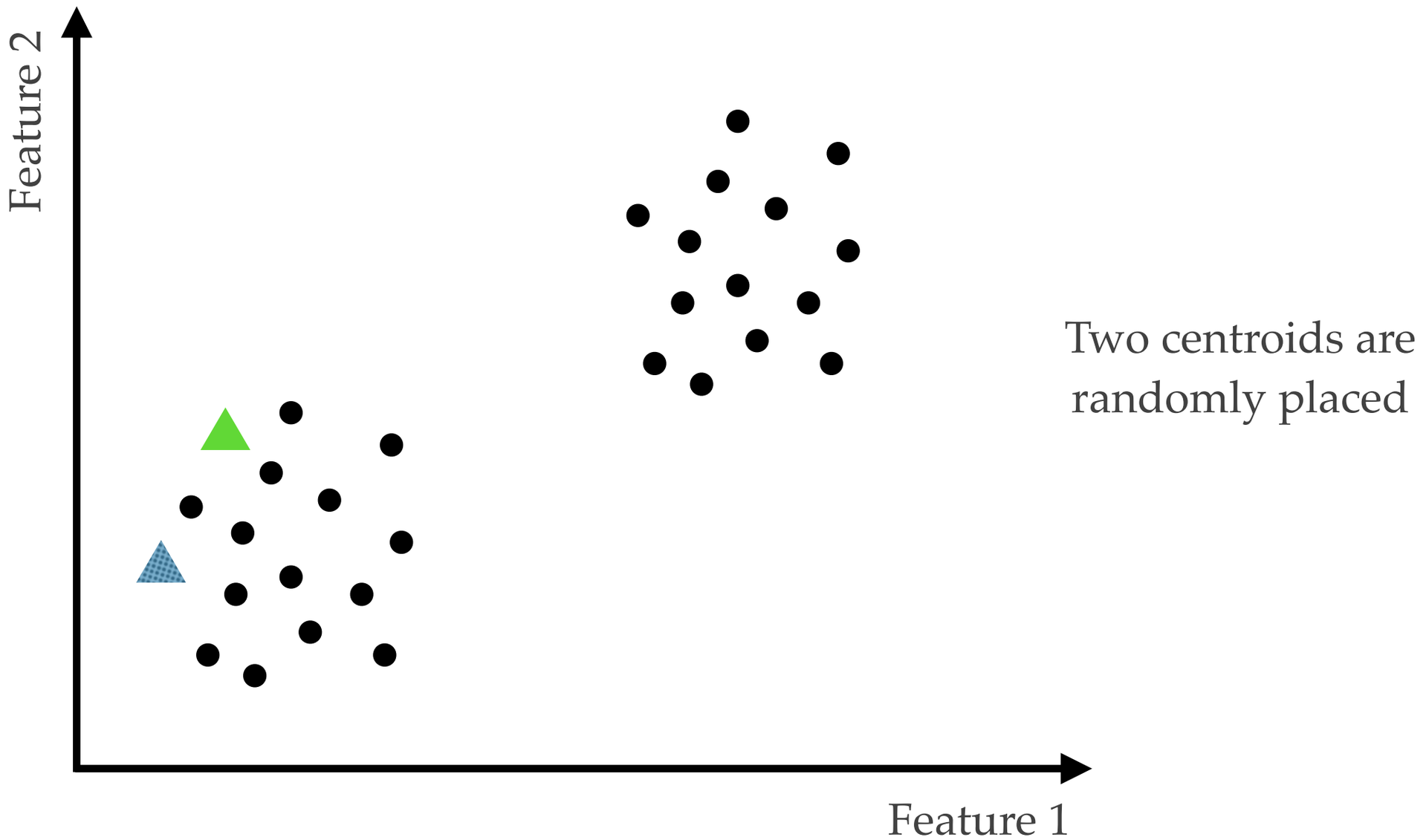

Two centroids are randomly placed

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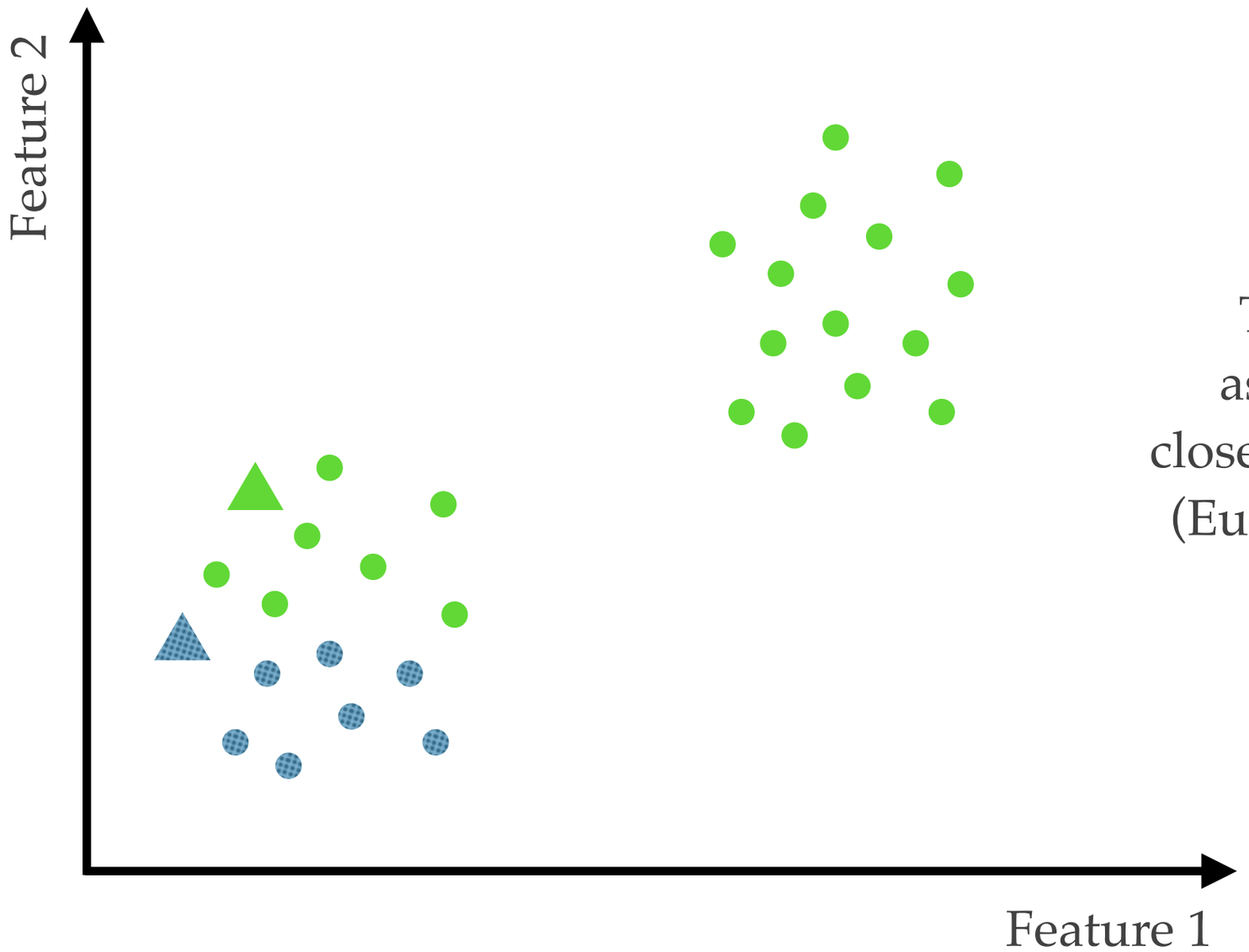

The objects are associated to the closest cluster centroid (Euclidean distance).

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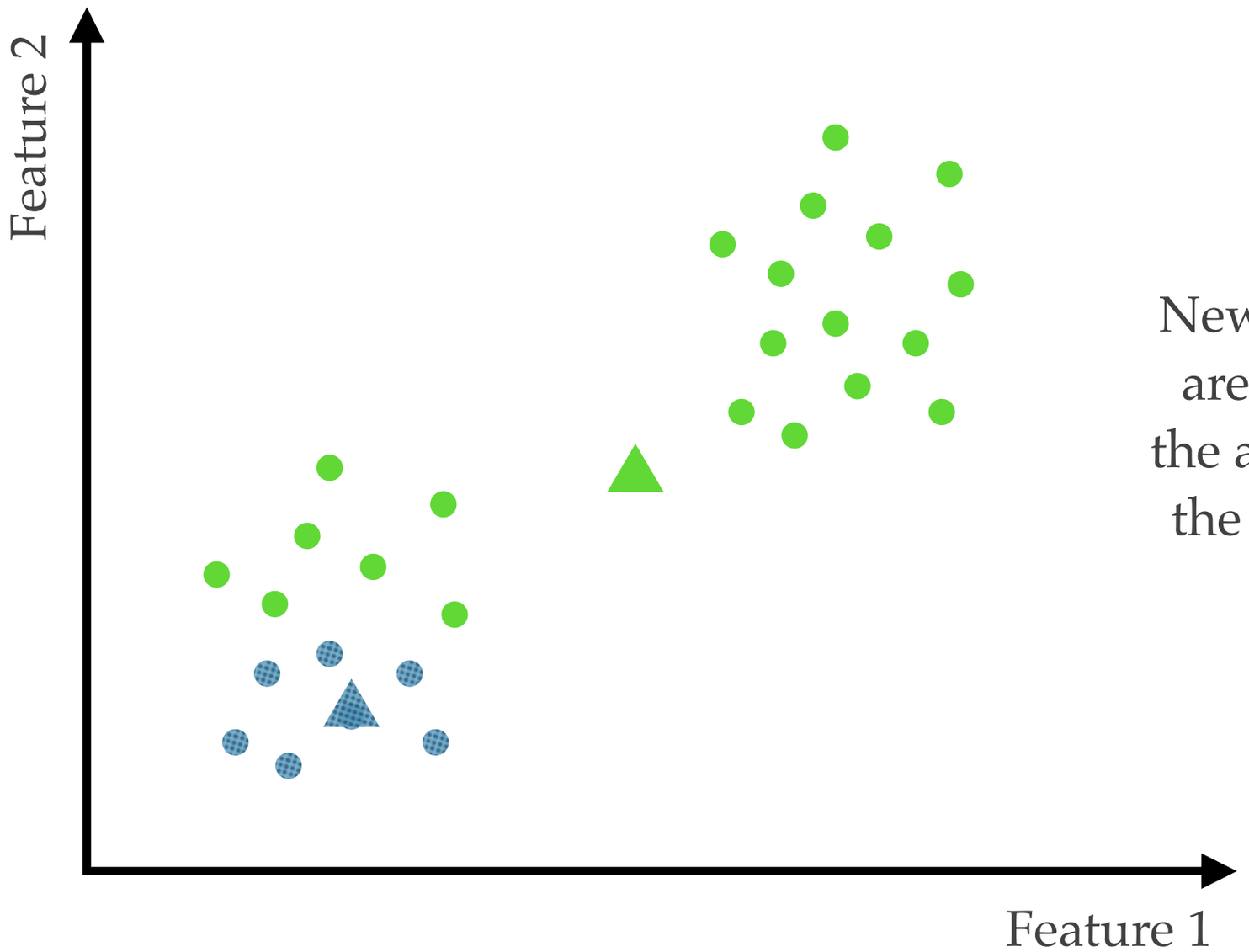

New cluster centroids are computed using the average location of the cluster members.

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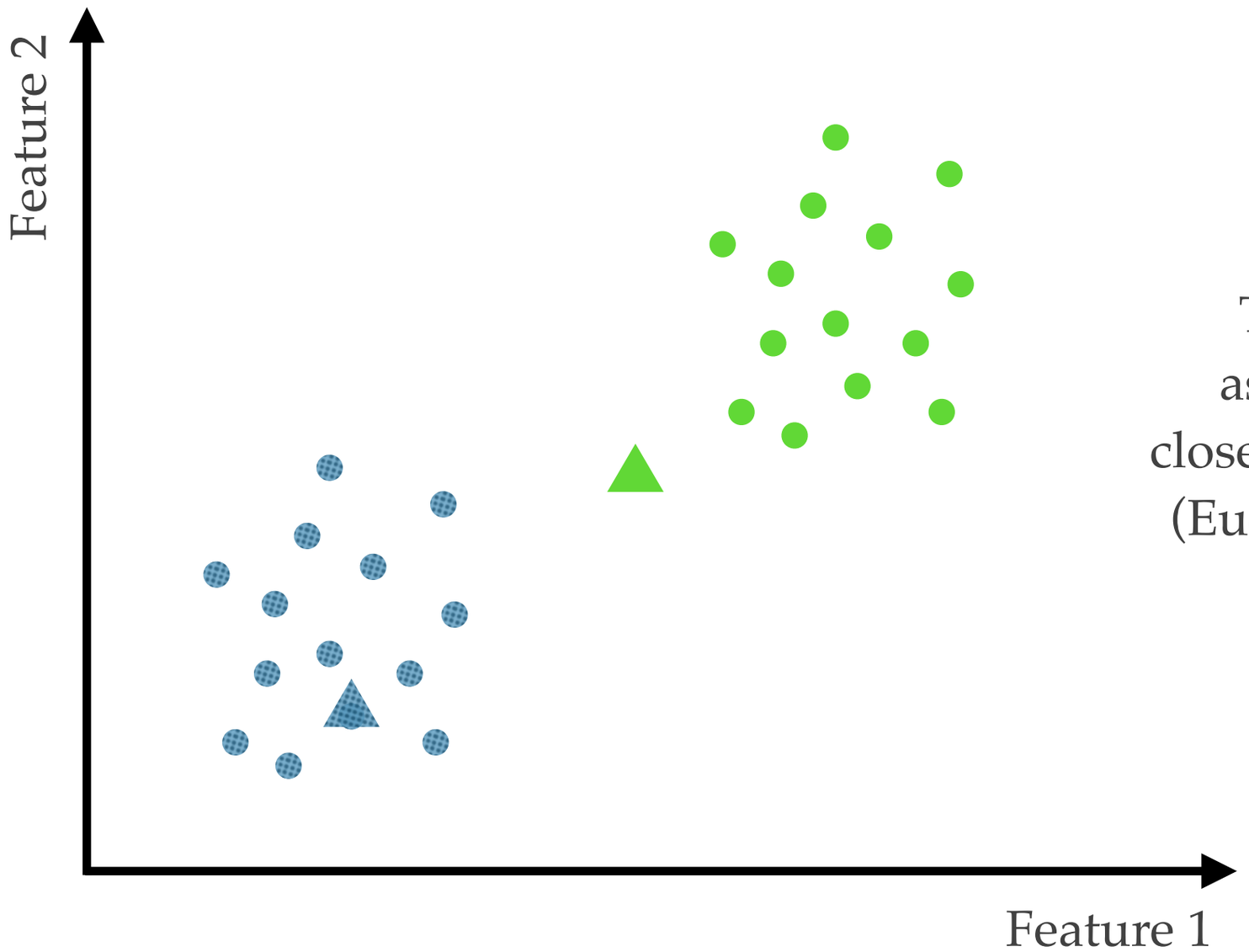

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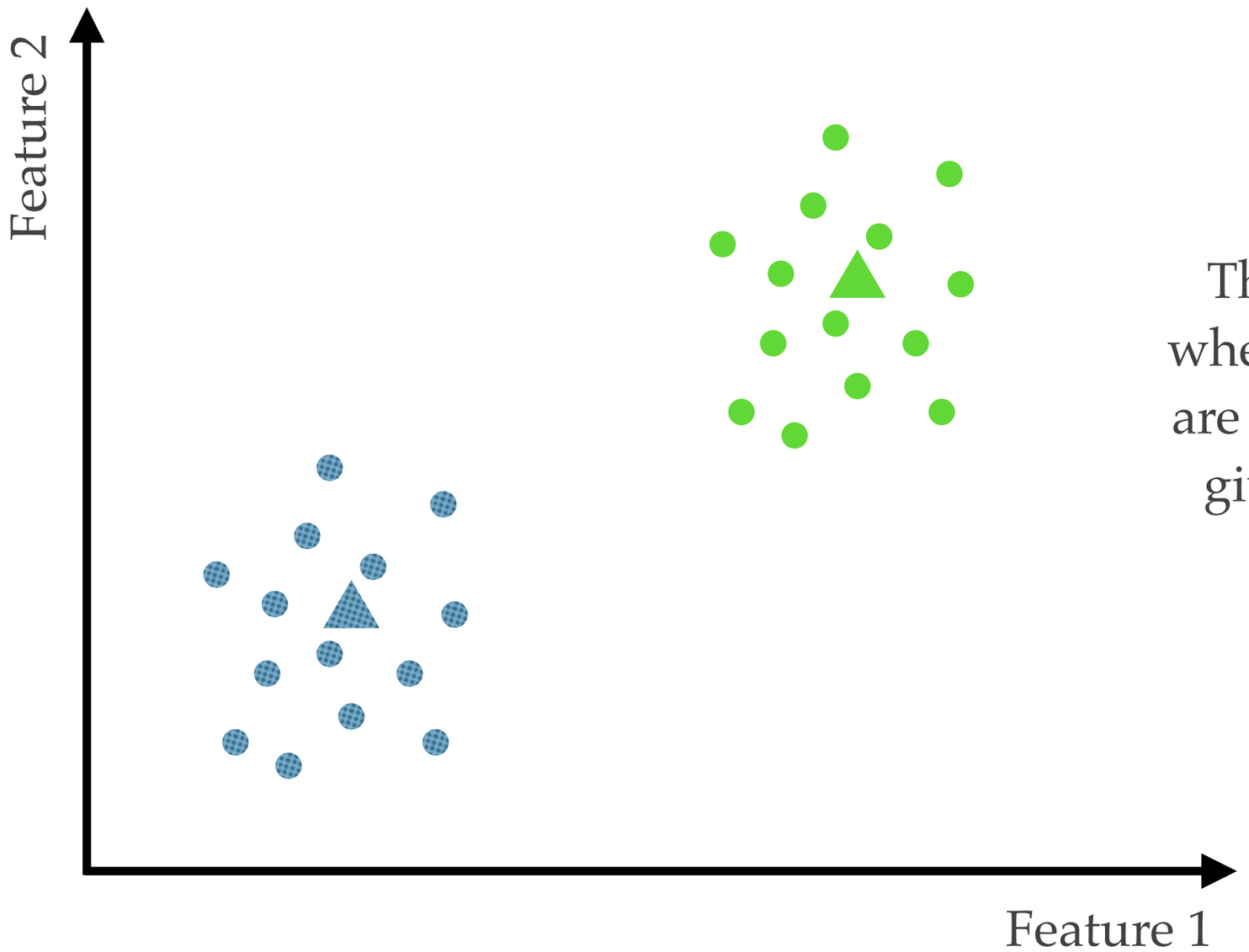

The process stops when the objects that are associated with a given class do not change.

The anatomy of K-means

$$f(\overrightarrow{X}, \{a_1, a_2, ...\}) = \overrightarrow{y}$$

Internal choices and/or internal cost function:

(I) Initial centroids are randomly selected from the set of examples.

(II) The global cost function that is minimized by K-means:

$$J = \sum_{k=1}^{K} \sum_{i \in C_k} ||x_i - \mu_k||^2$$

cluster centroids

Euclidean distance

cluster members

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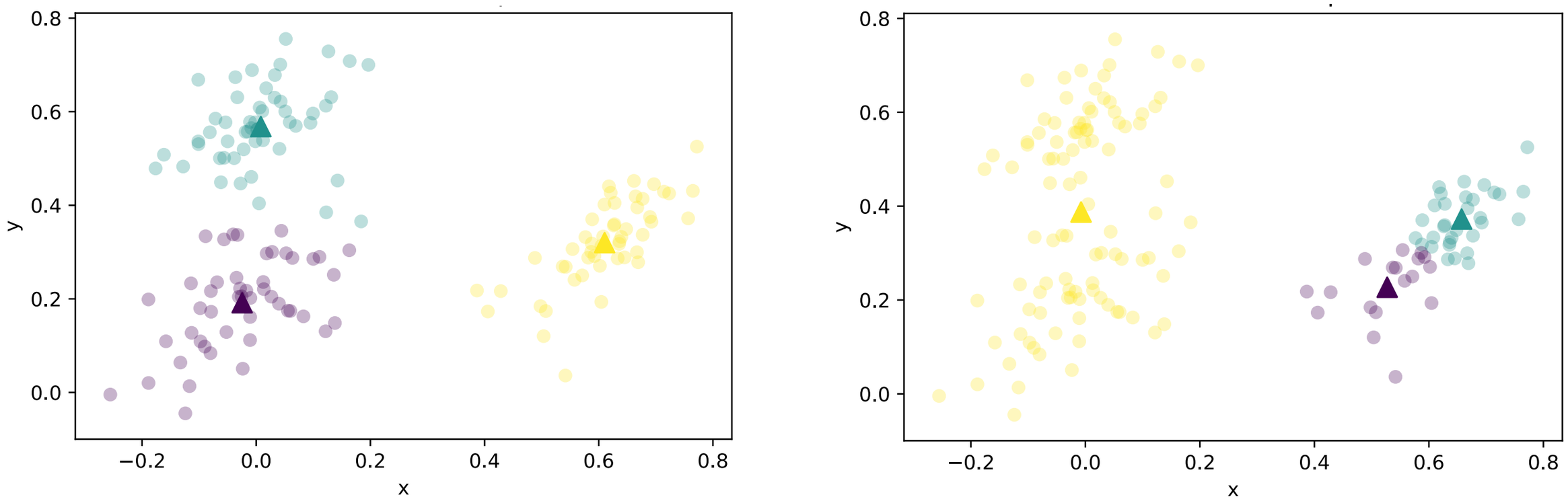
k=3, and two different random placements of centroids



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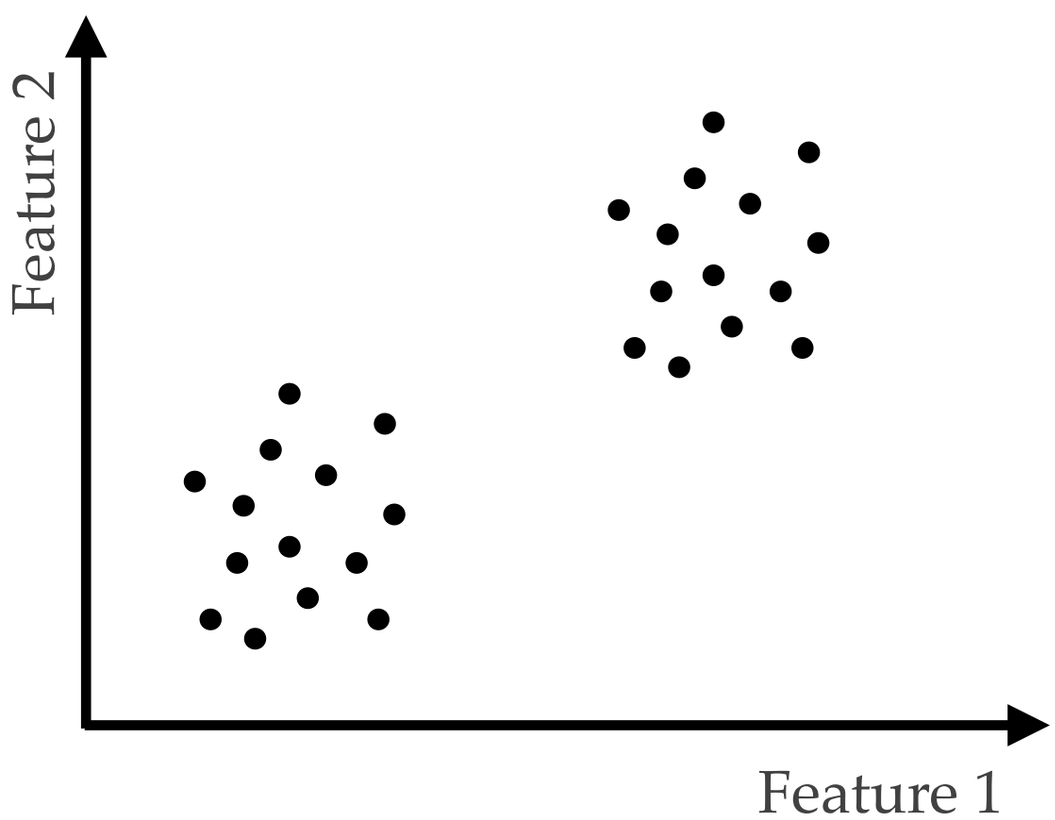
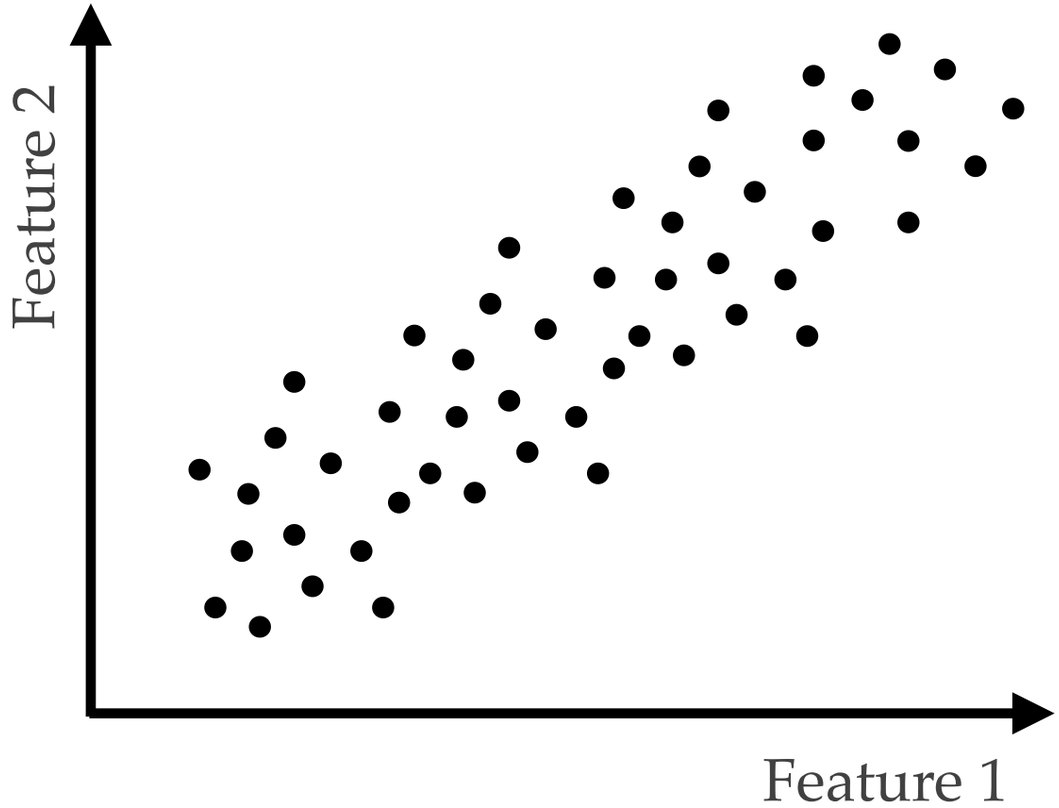
Input dataset: a list of objects with measured features.

For which datasets should we use K-means?





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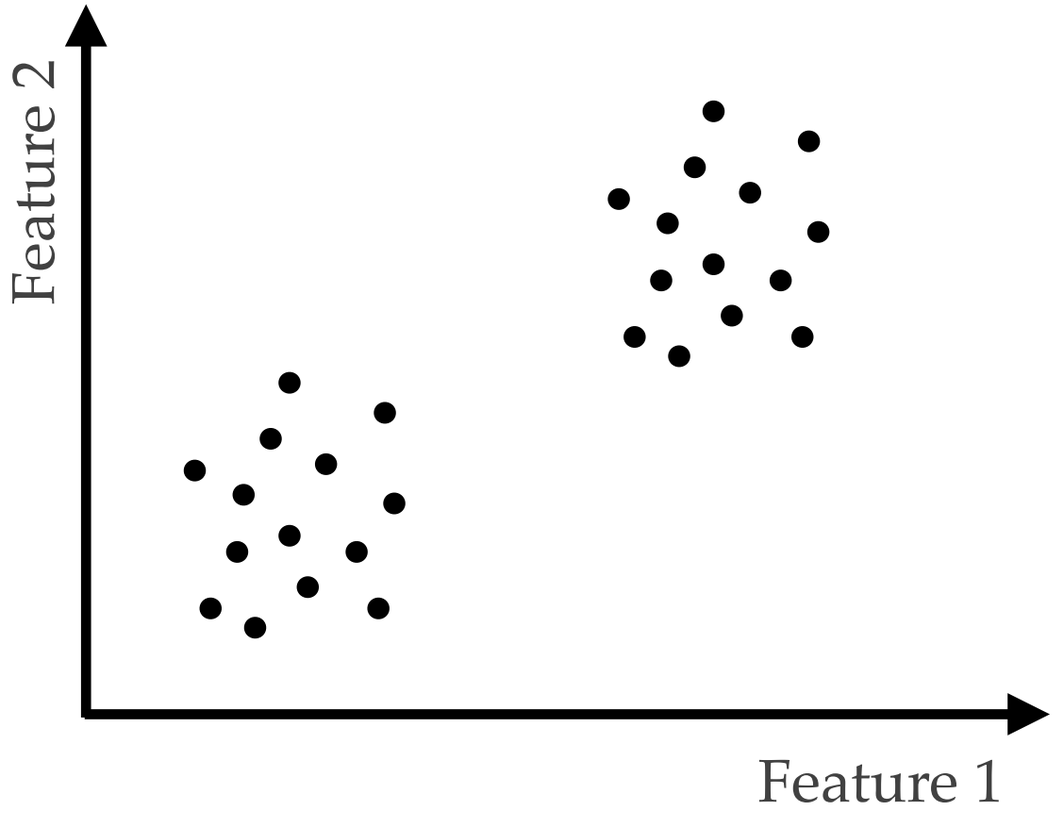
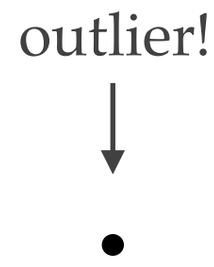
What happens when we have an outlier in the dataset?





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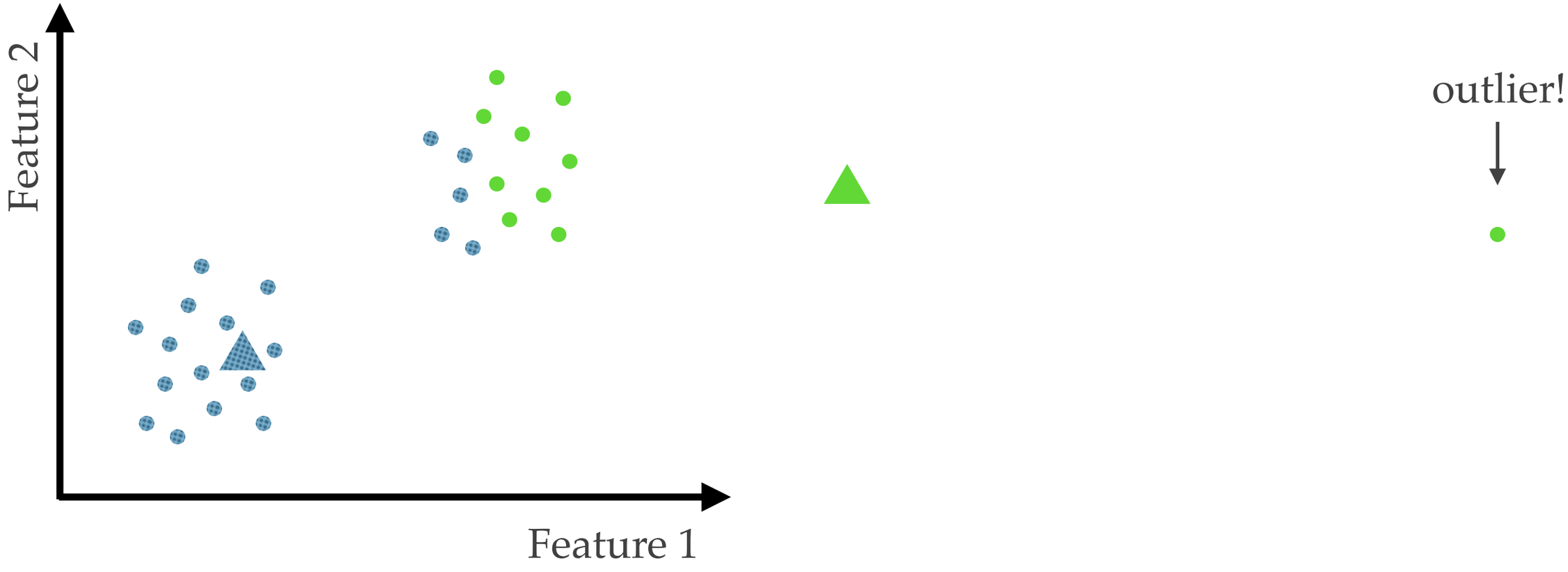

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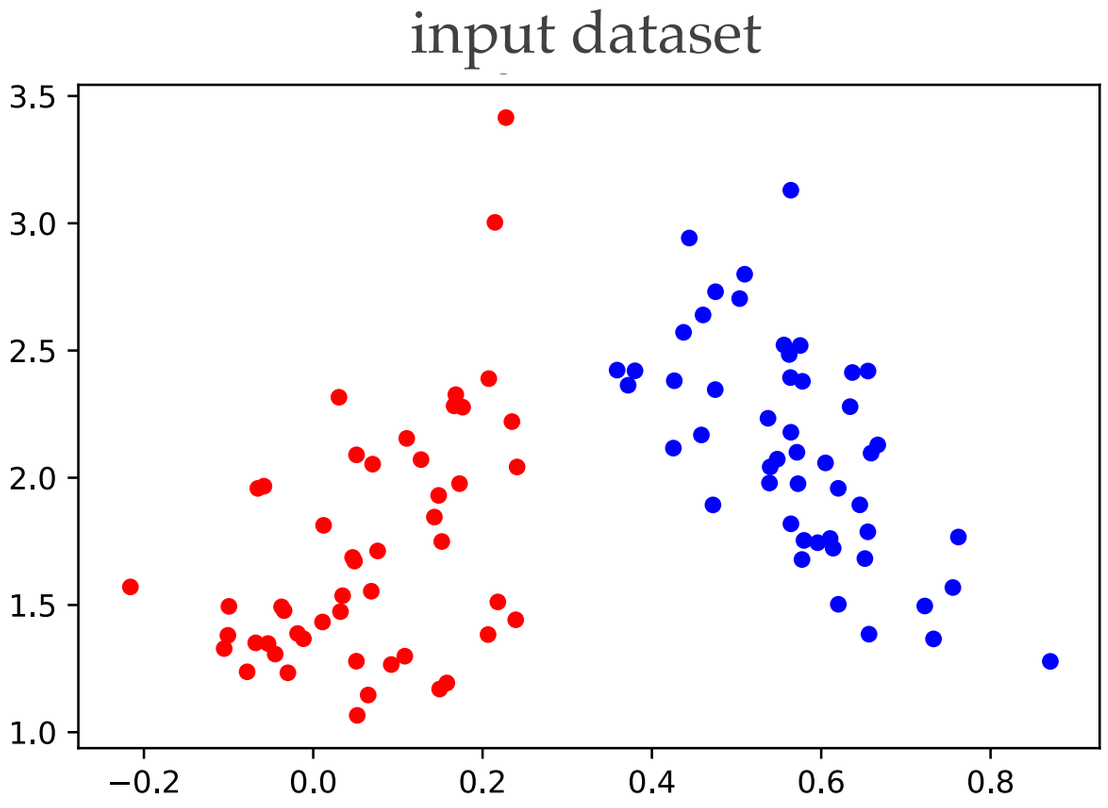
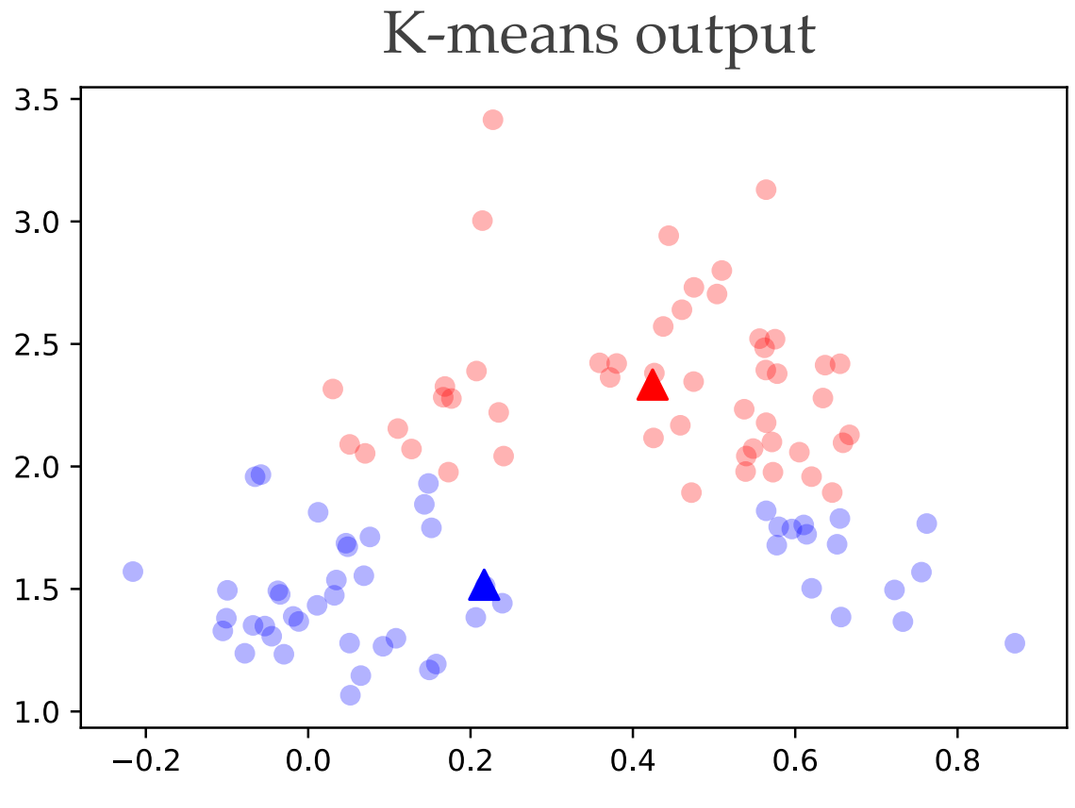
What happens when the features have different physical units?



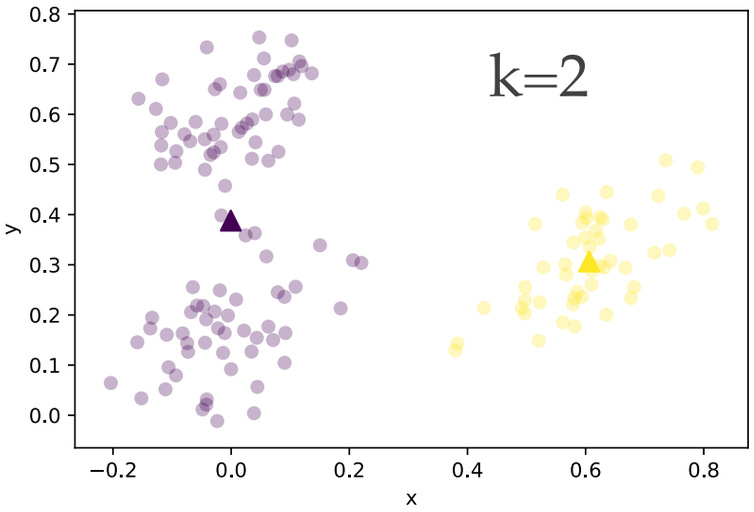


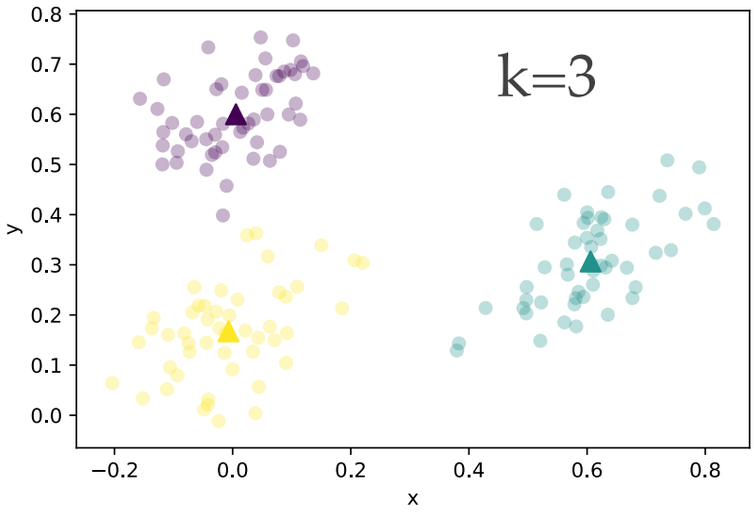
The anatomy of K-means

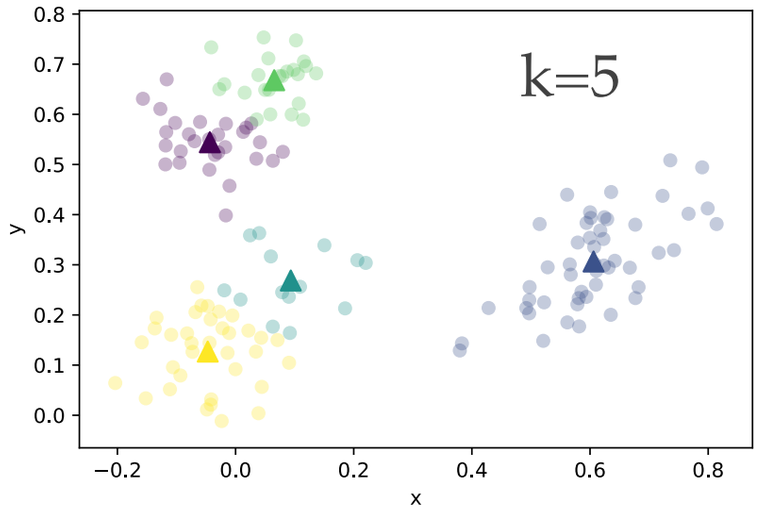
$$f(\vec{X}, \{a_1, a_2, ...\}) = \vec{y}$$

Hyper-parameters: the number of clusters, k.

Can we find the optimal k using the cost function?







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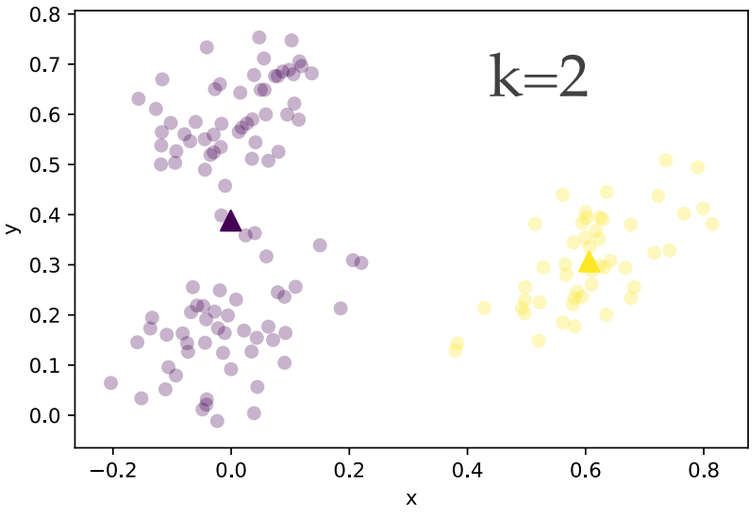
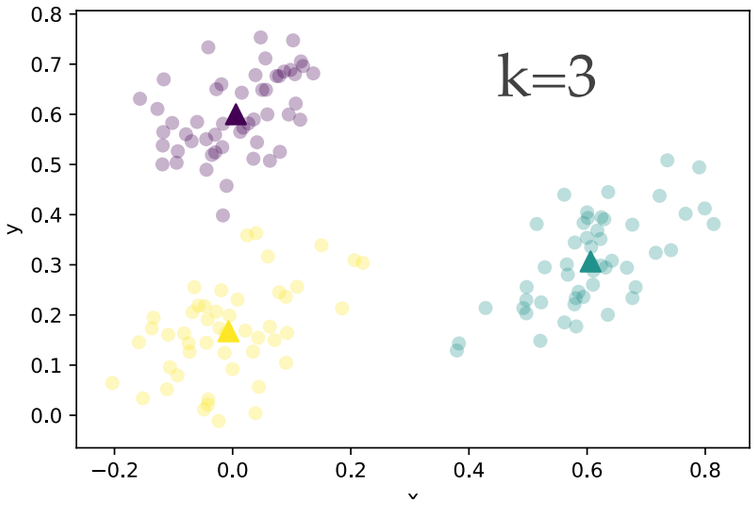
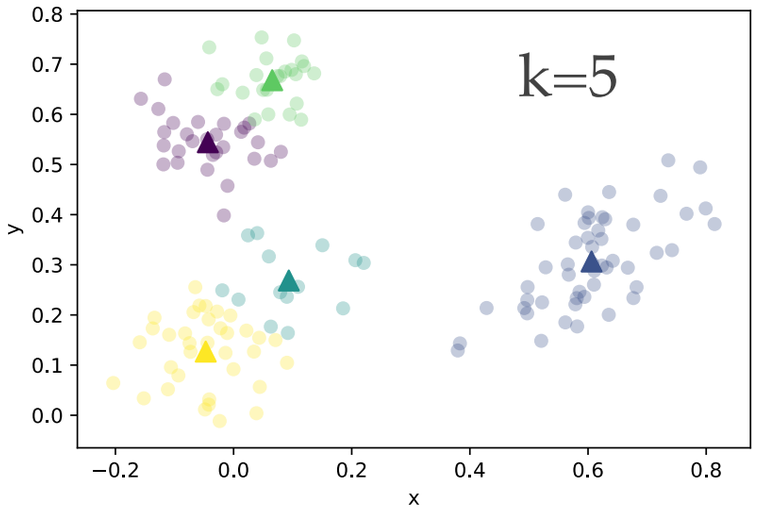
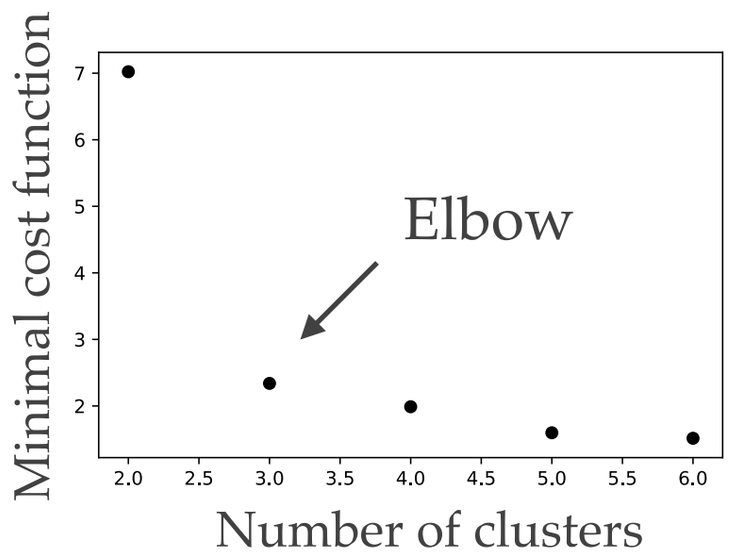




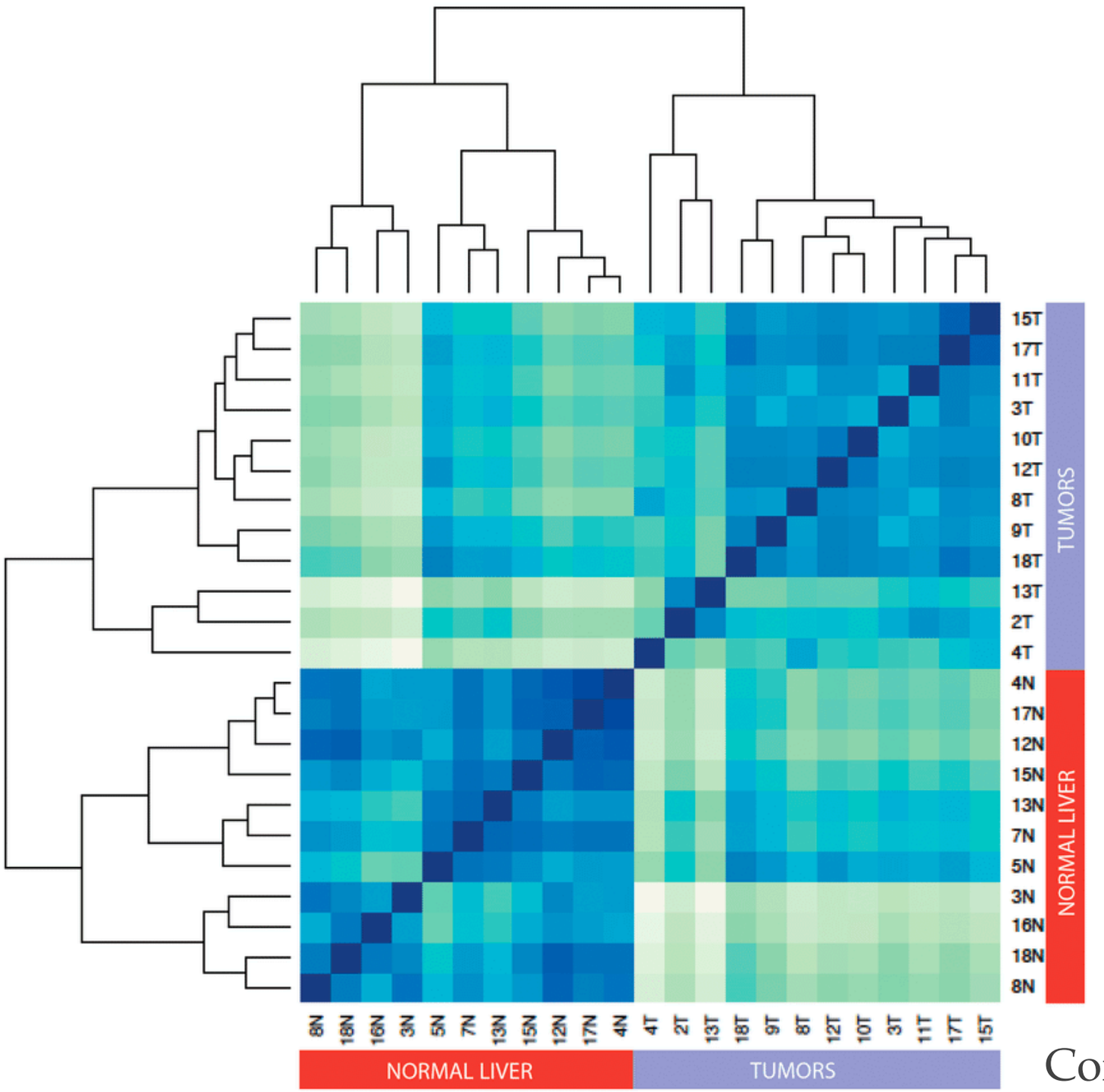




Questions?

Hierarchal Clustering

or, how to visualize complicated similarity measures

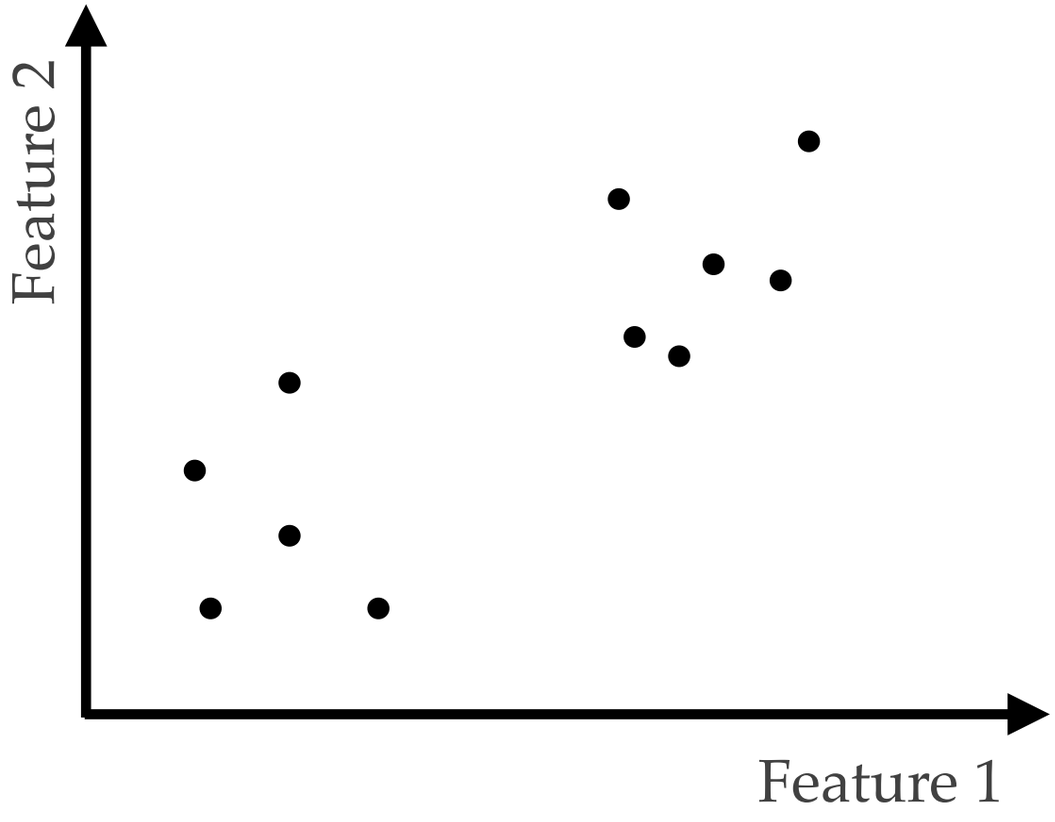


Correa-Gallego+ 2016

Hierarchal Clustering

Input: measured features, or a distance matrix that represents the pair-wise distances between the objects. Also, we must specify a linkage method.

Initialization: each object is a cluster of size 1.



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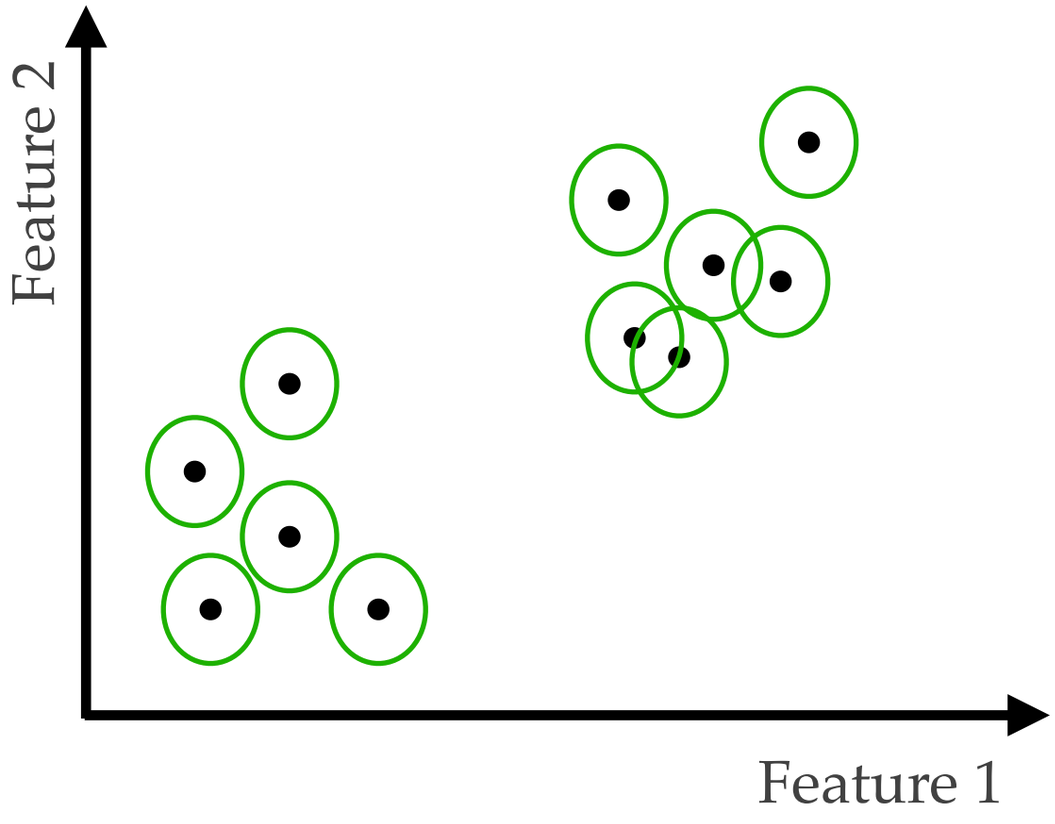

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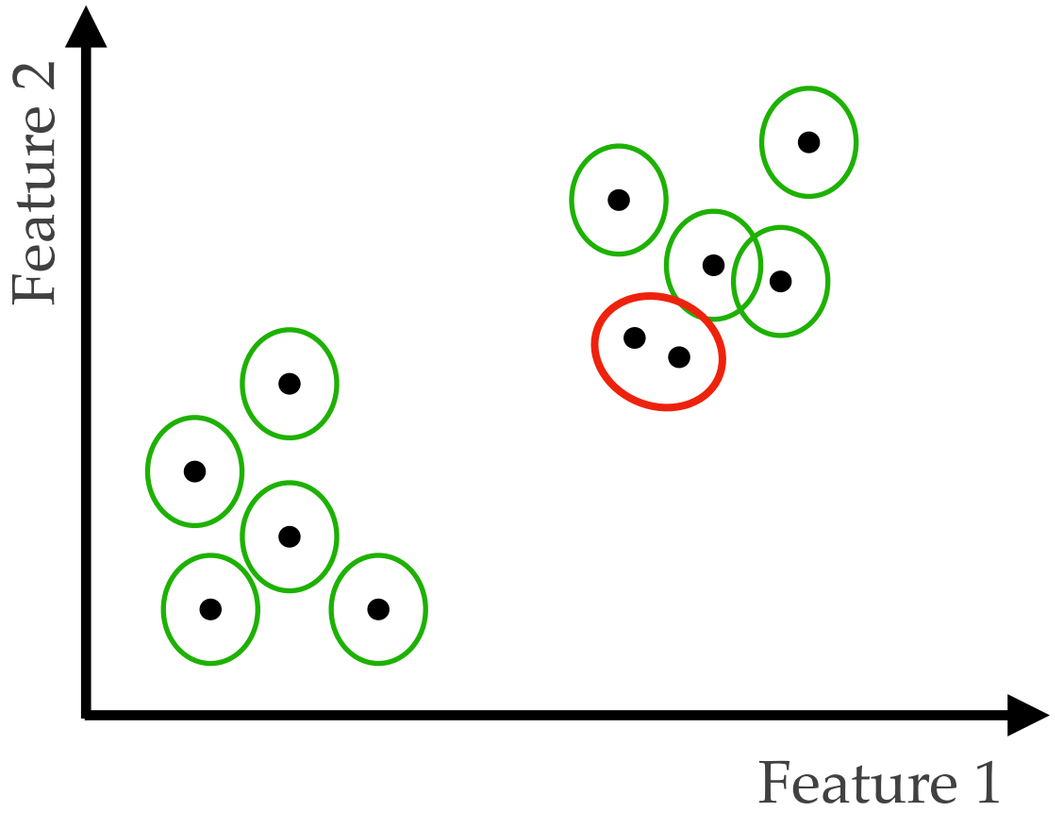

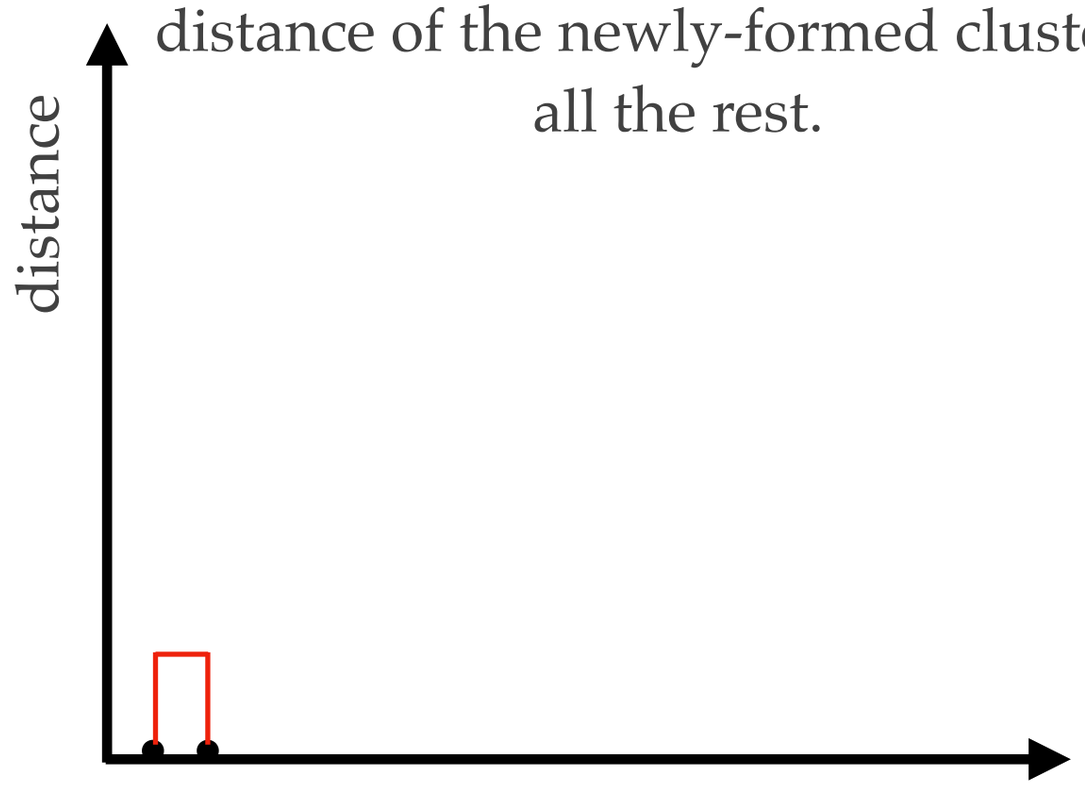

Dendrogram

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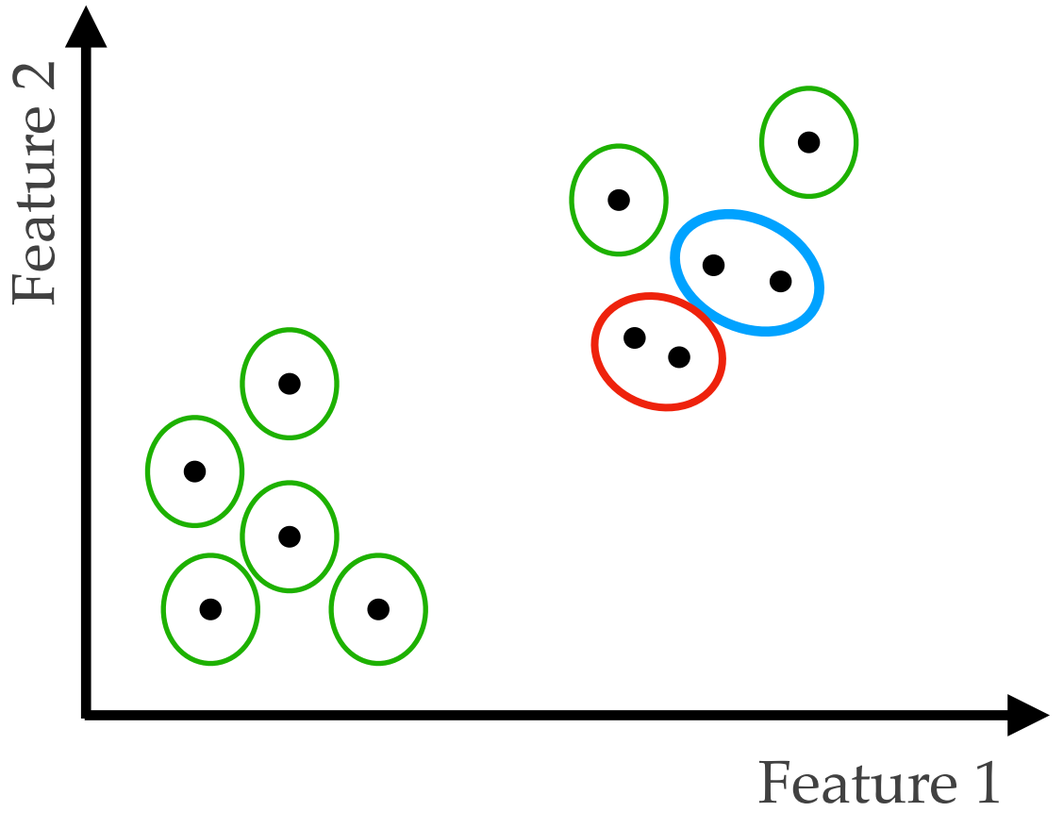

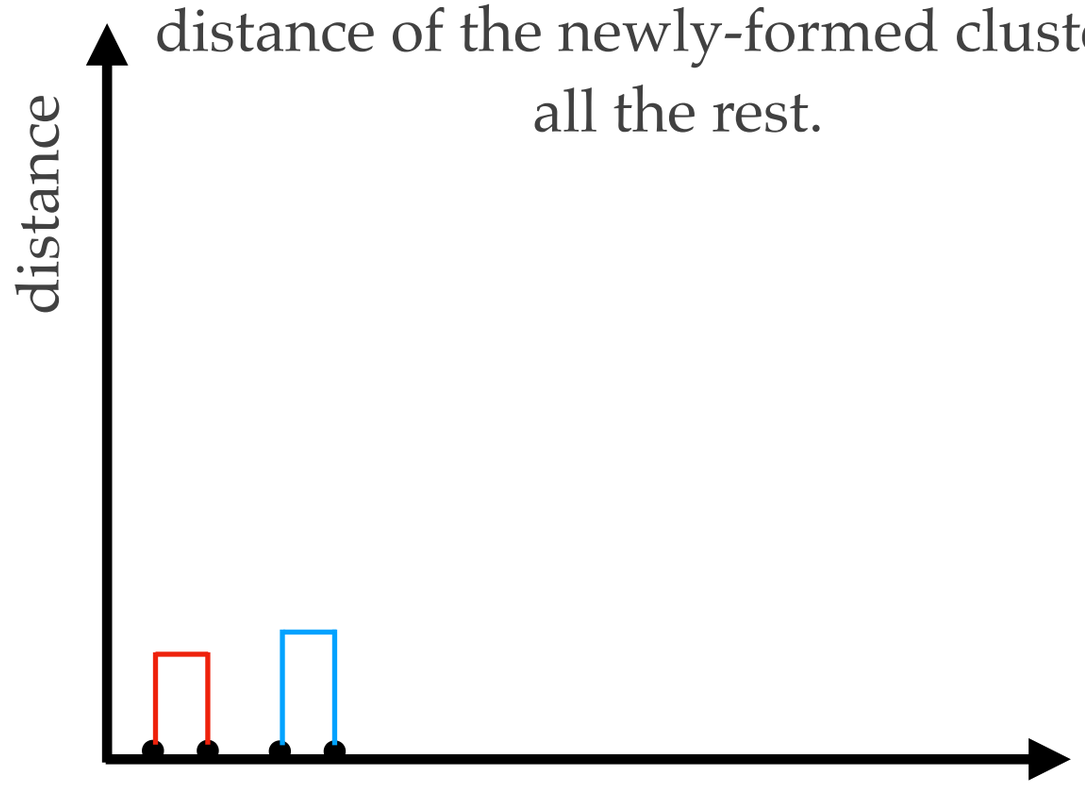

Dendrogram

Hierarchal Clustering

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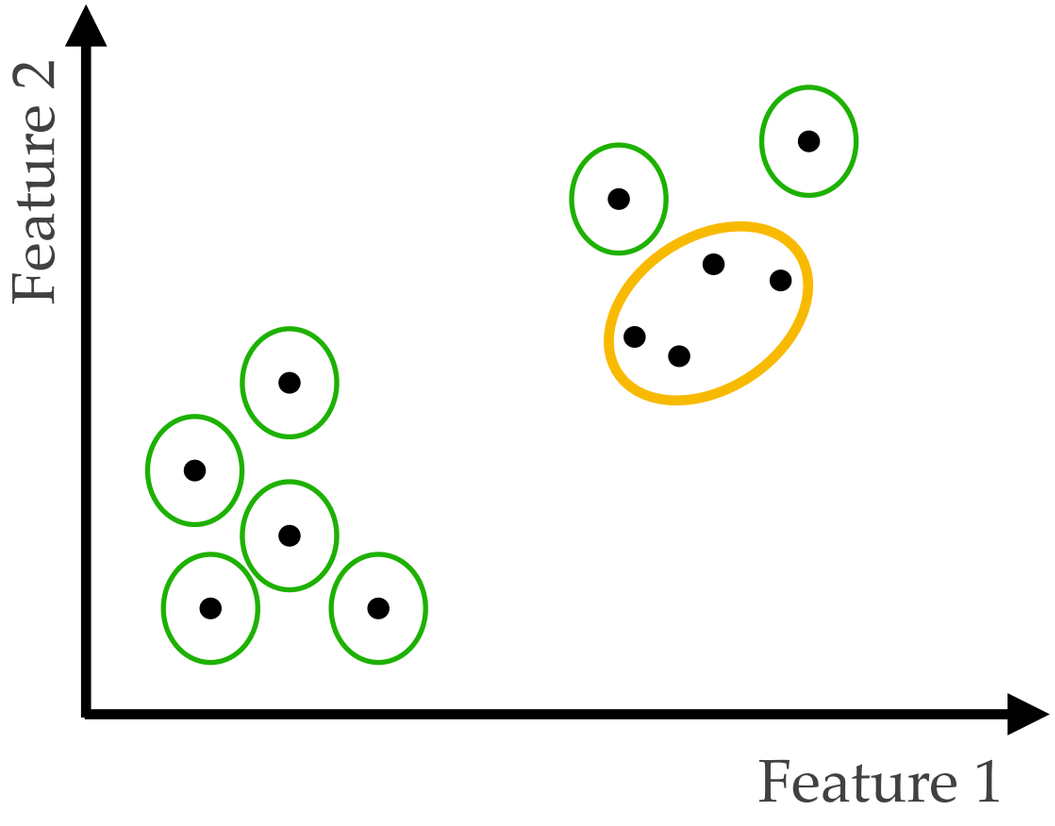

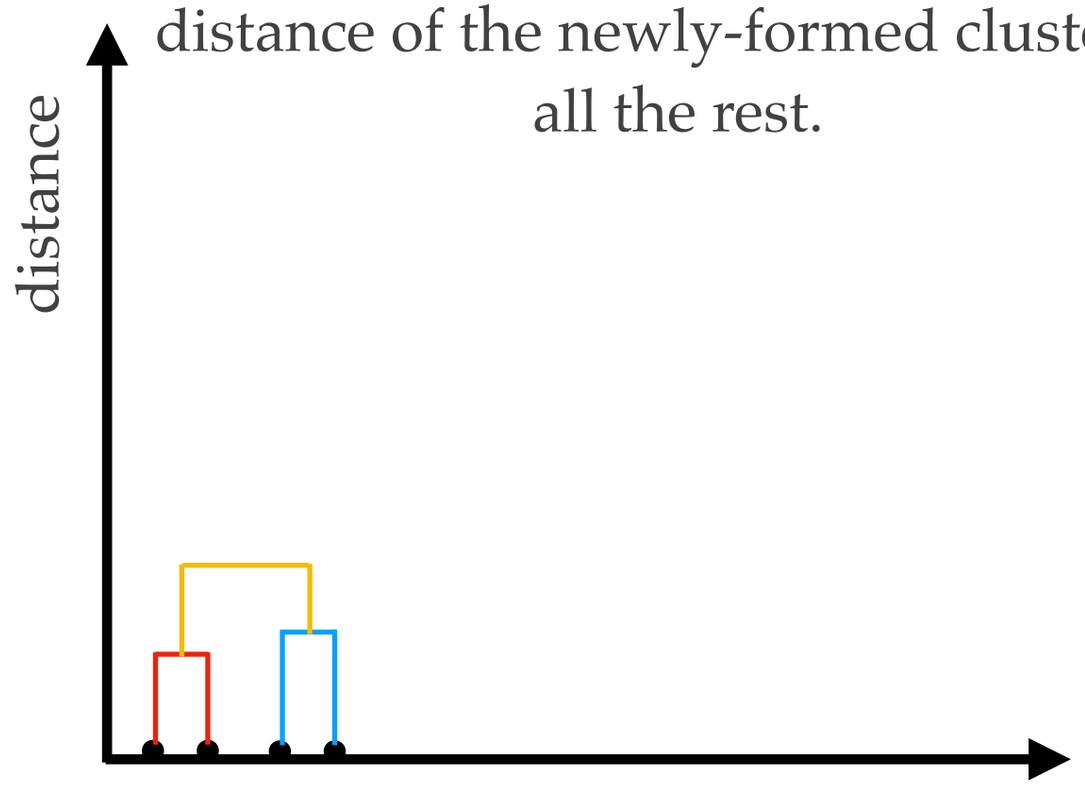

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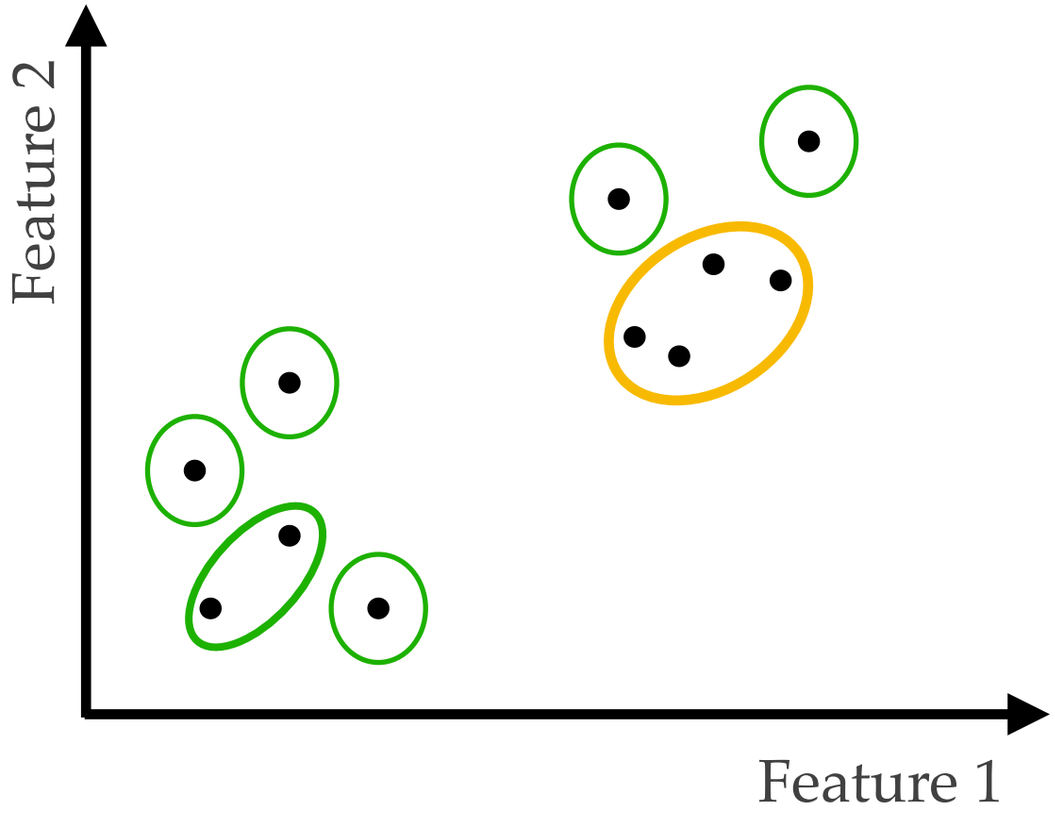

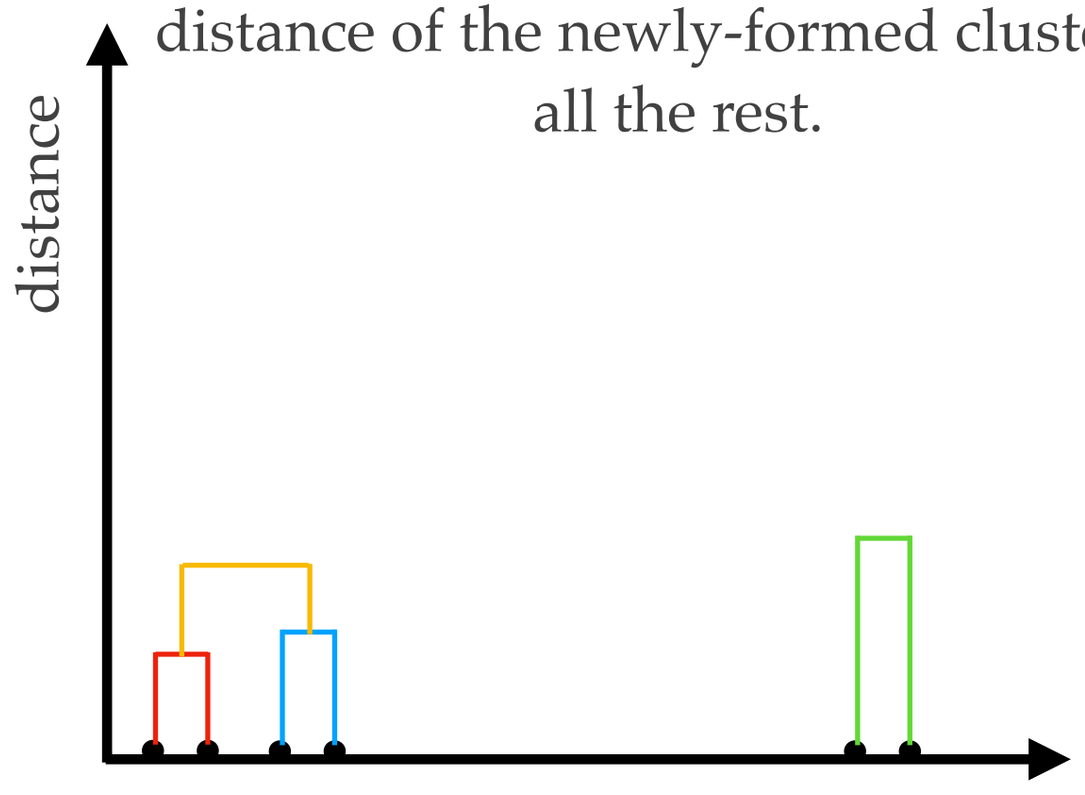

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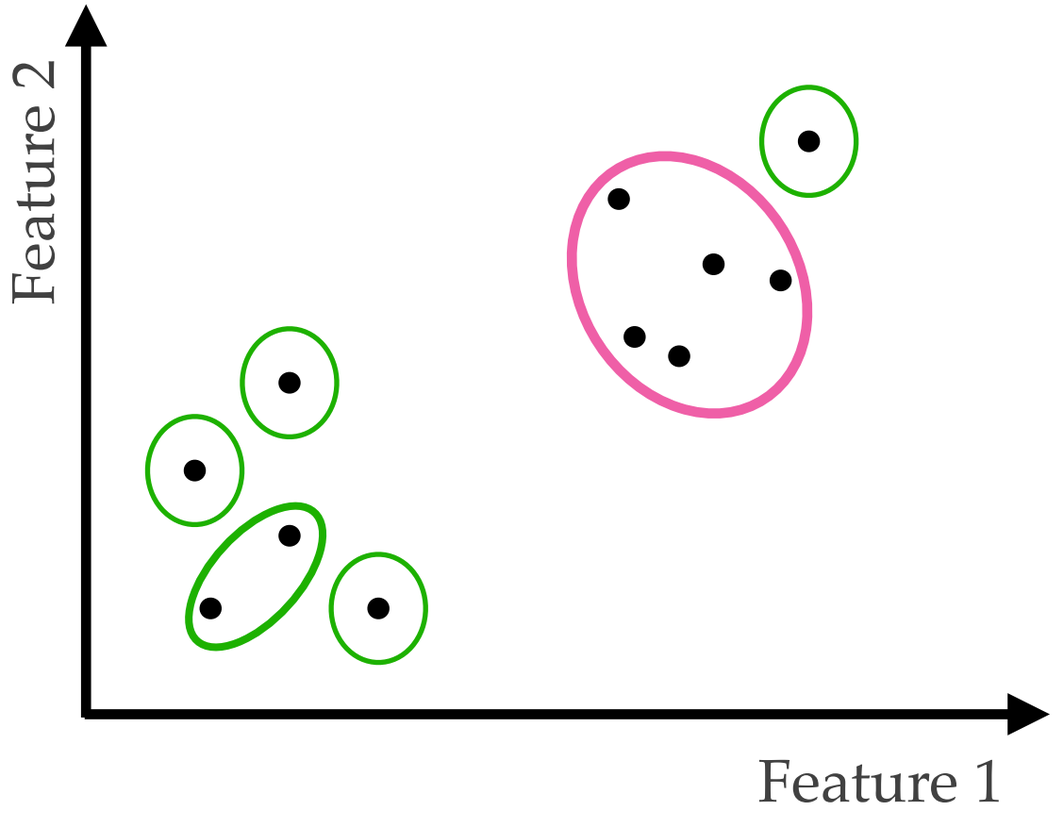

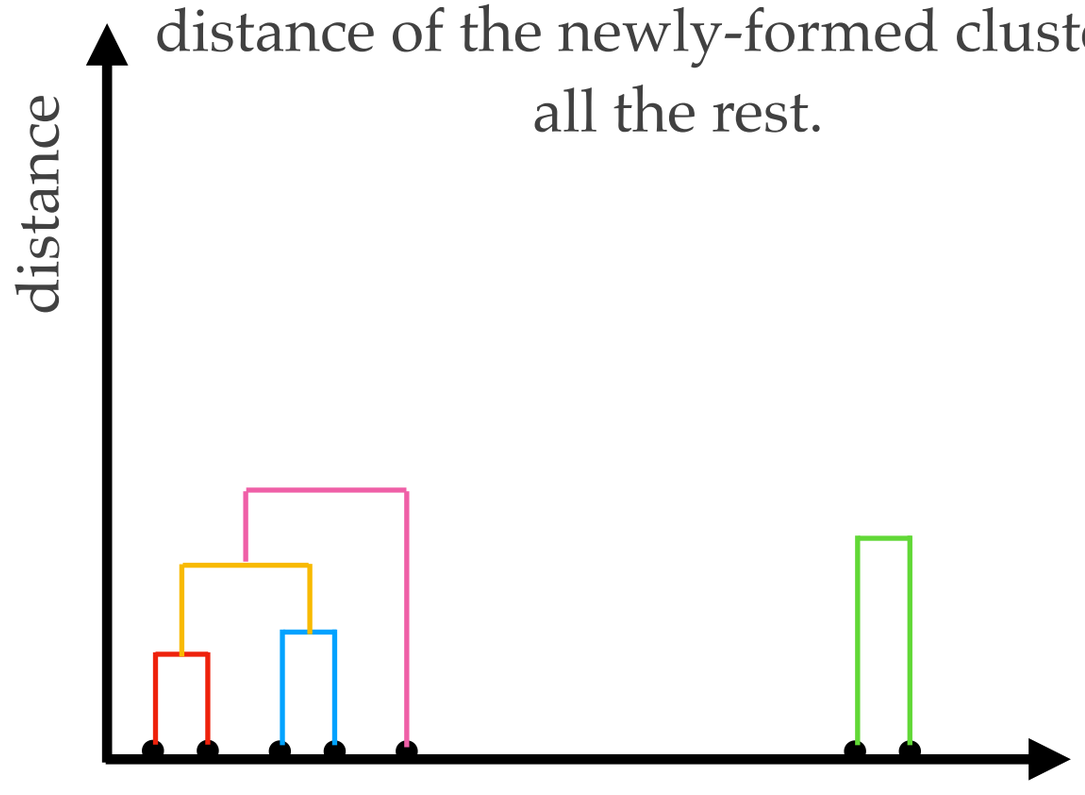

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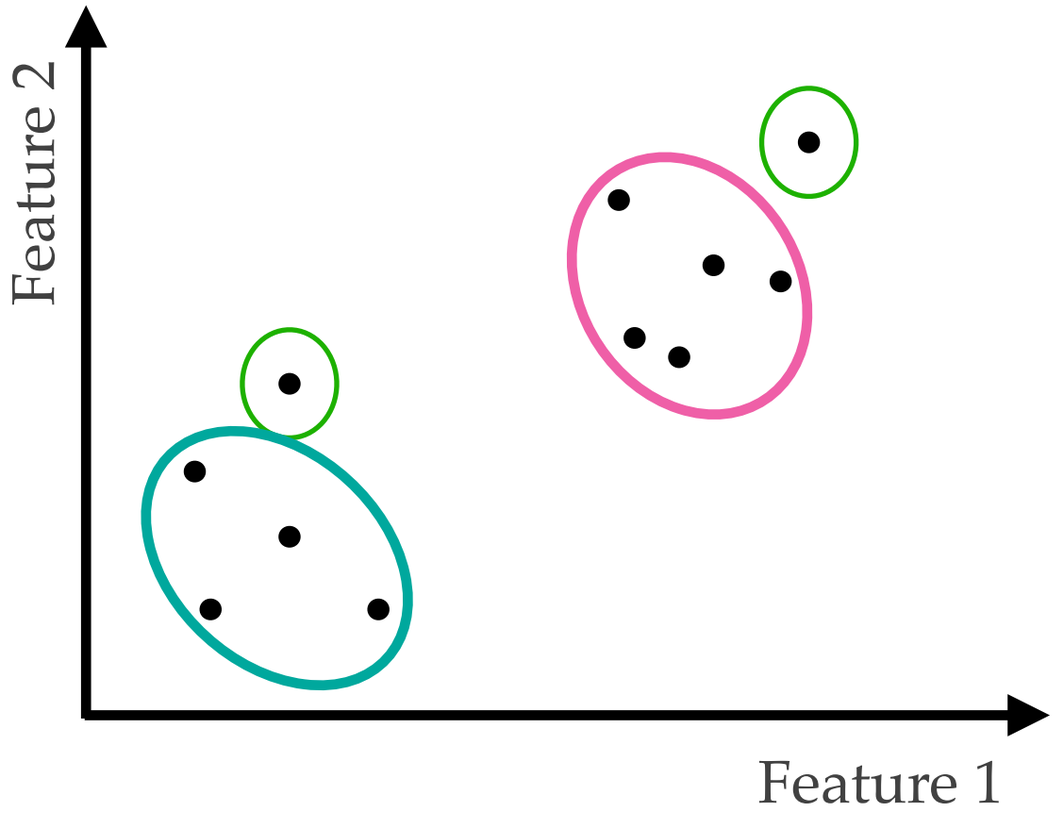

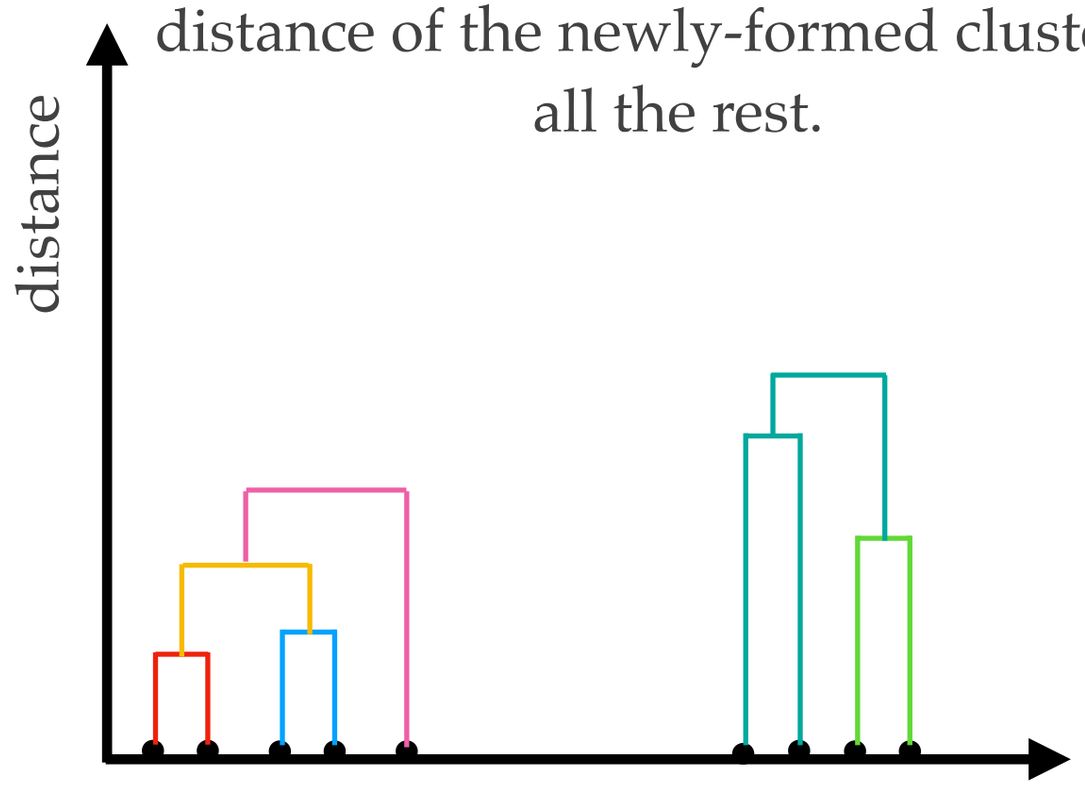

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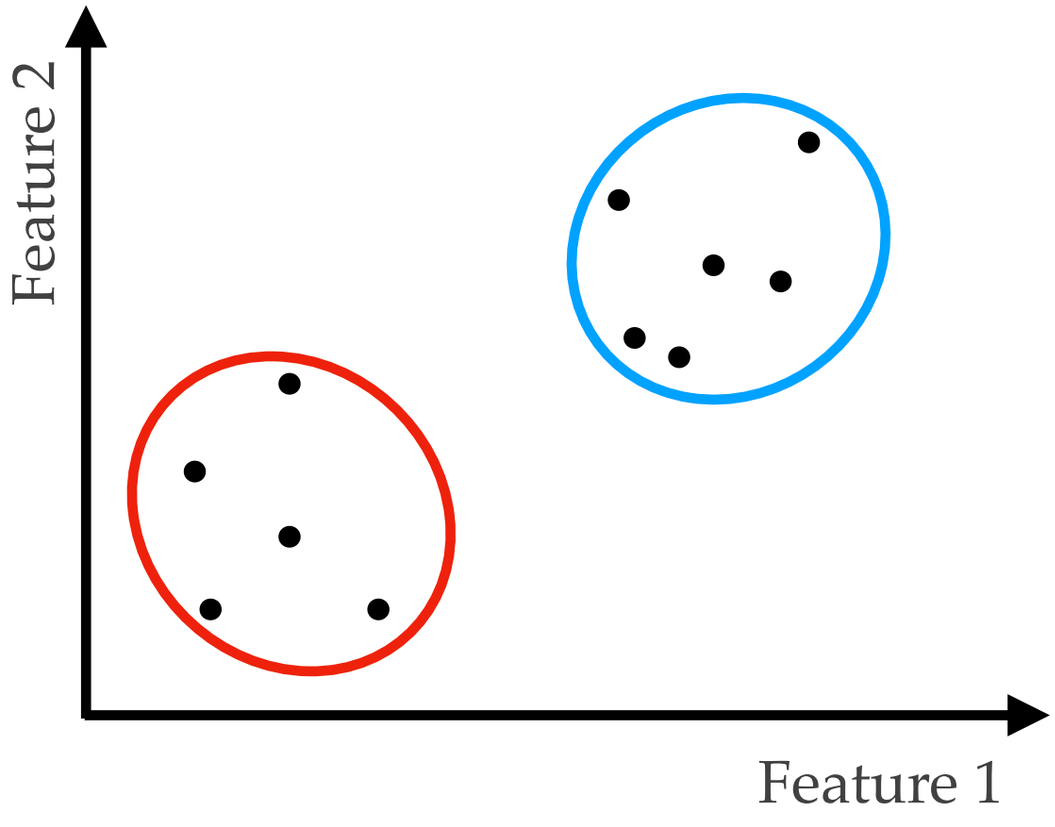

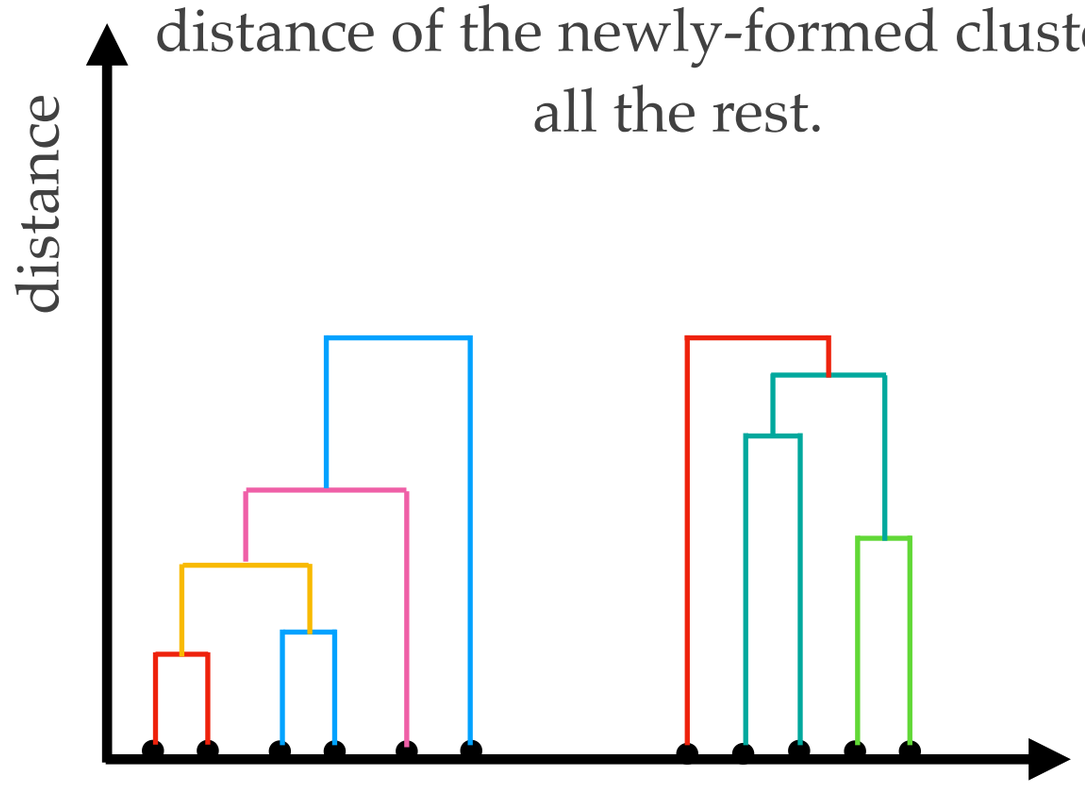

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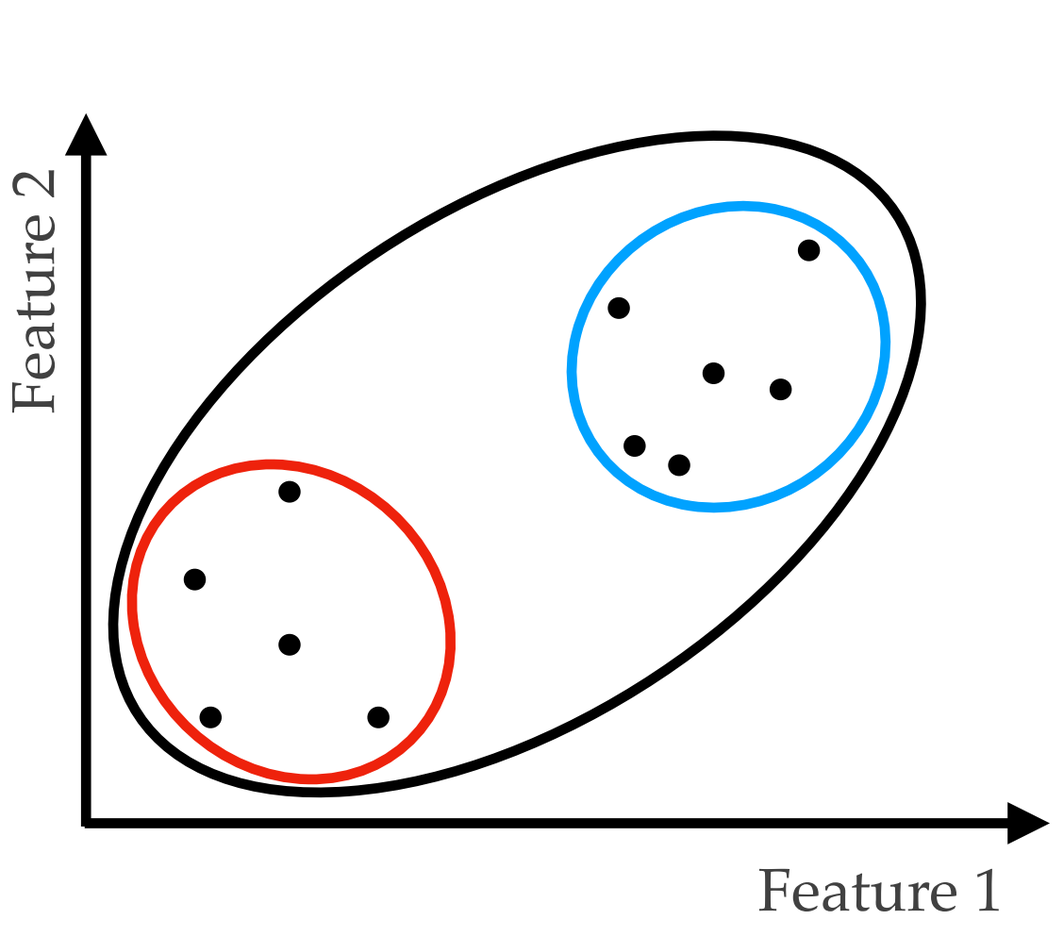
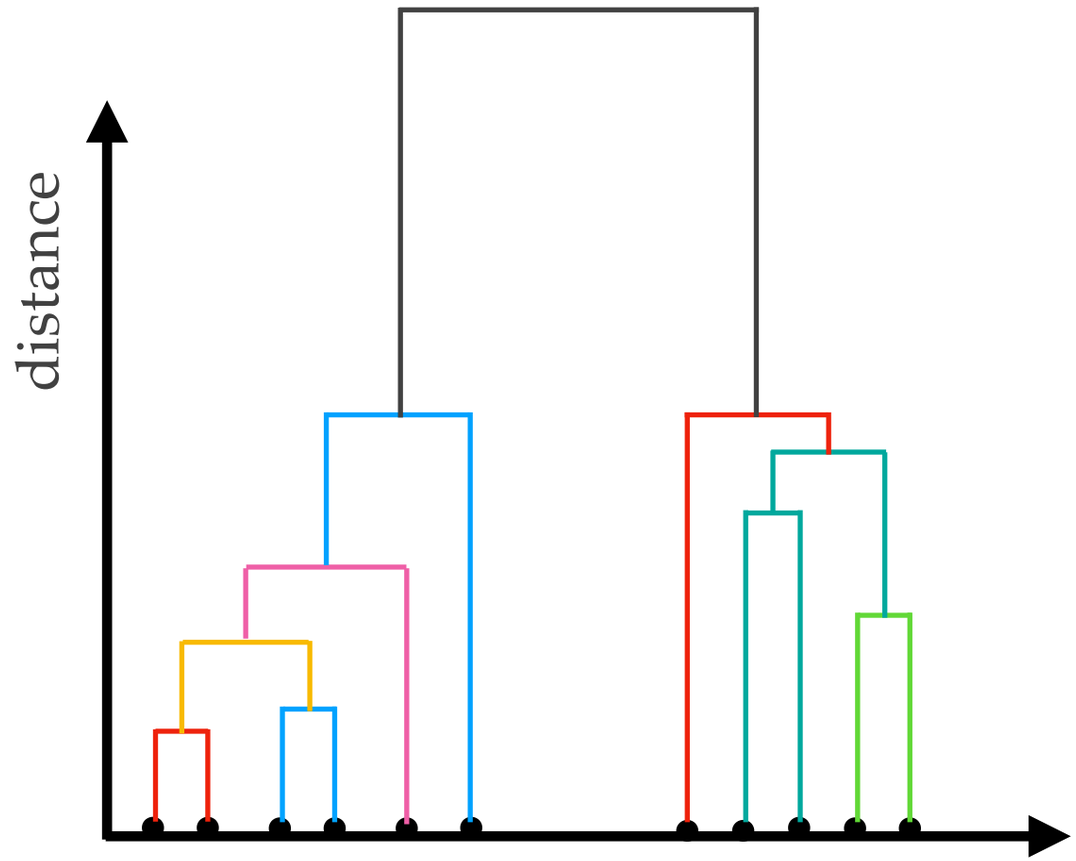
The process stops when all the objects are merged into a single cluster





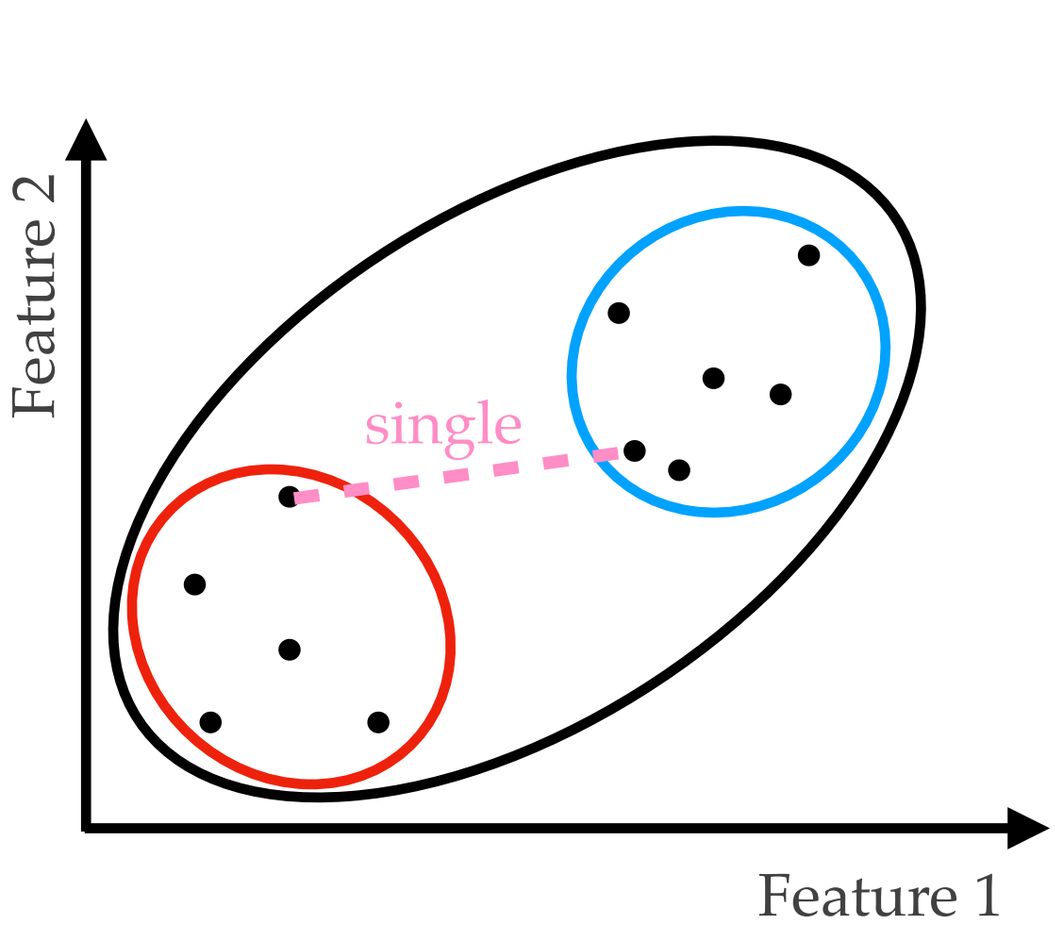
Dendrogram

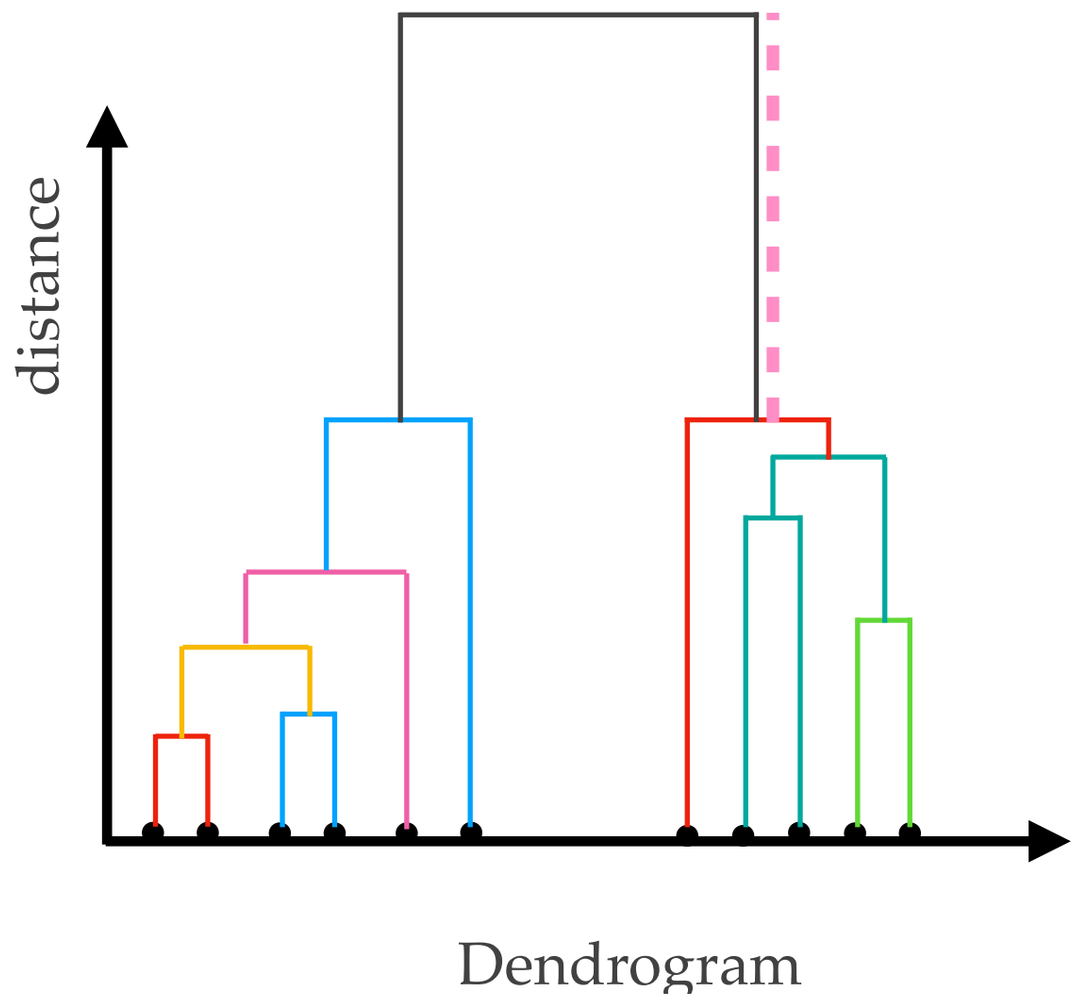
The anatomy of Hierarchal Clustering

$$f(\vec{X}, \{a_1, a_2, ...\}) = \vec{y}$$

Internal choices and/or internal cost function:

The linkage method is used to define a distance between two newly formed clusters.
Methods include: single (minimal), complete (maximal), average, etc.





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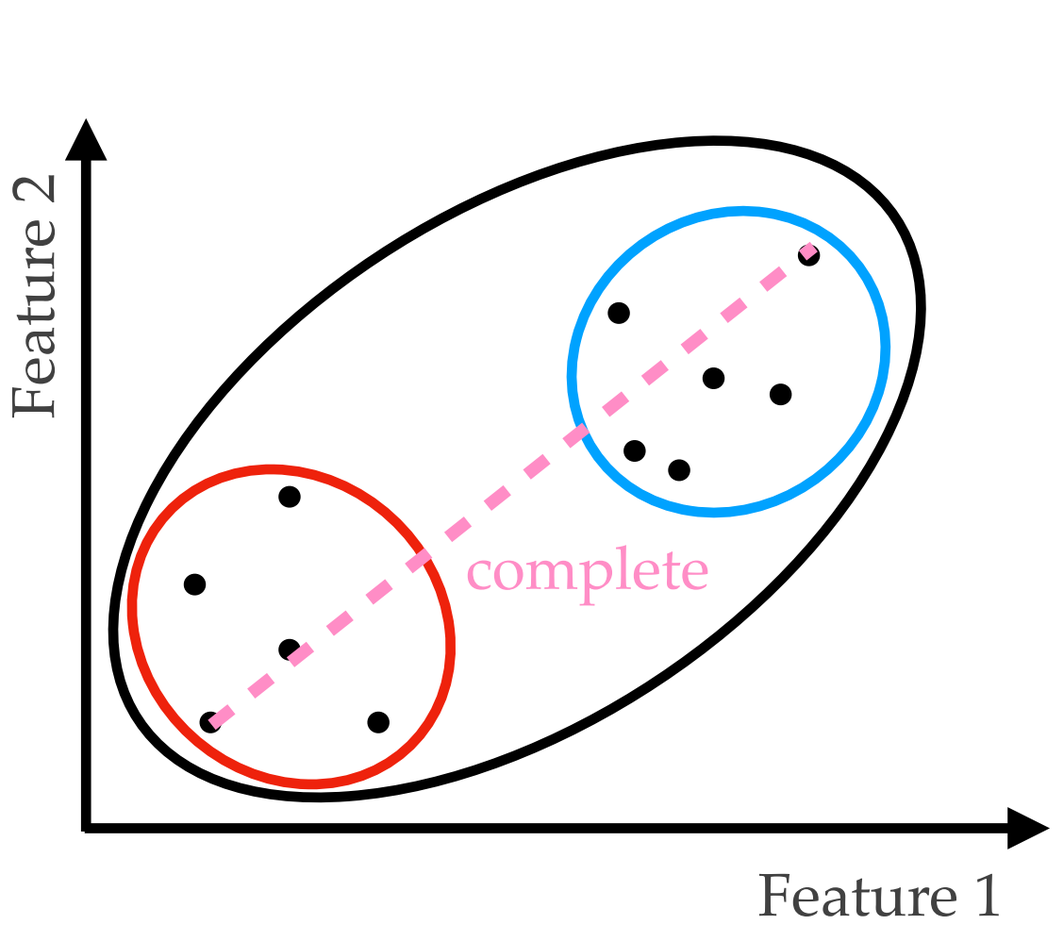

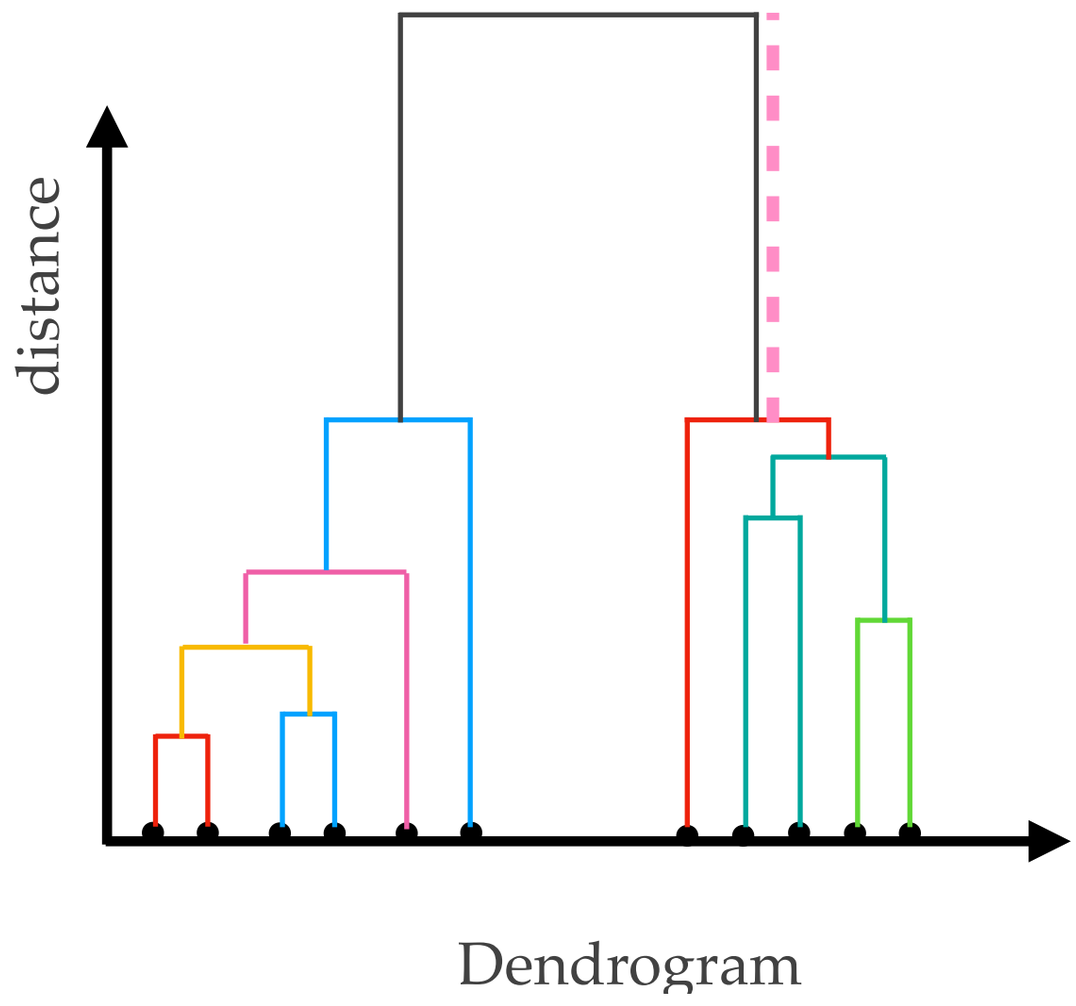

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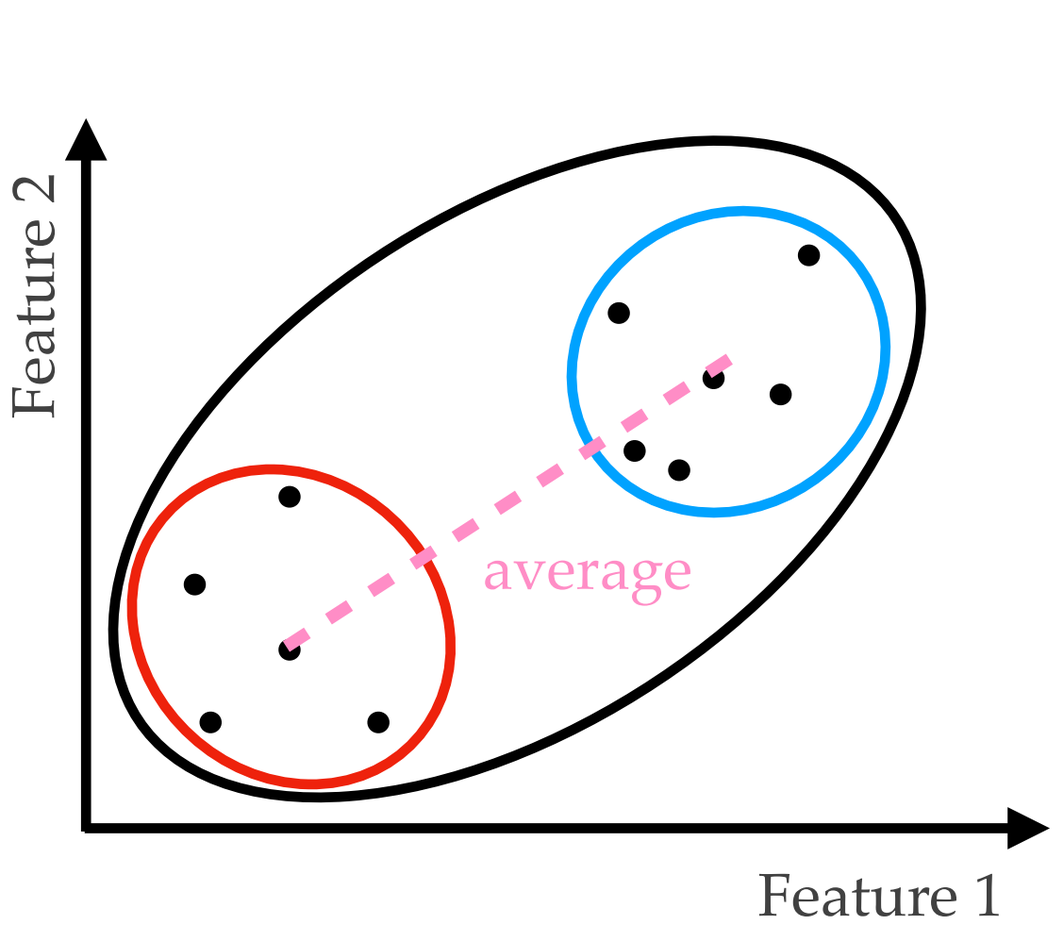
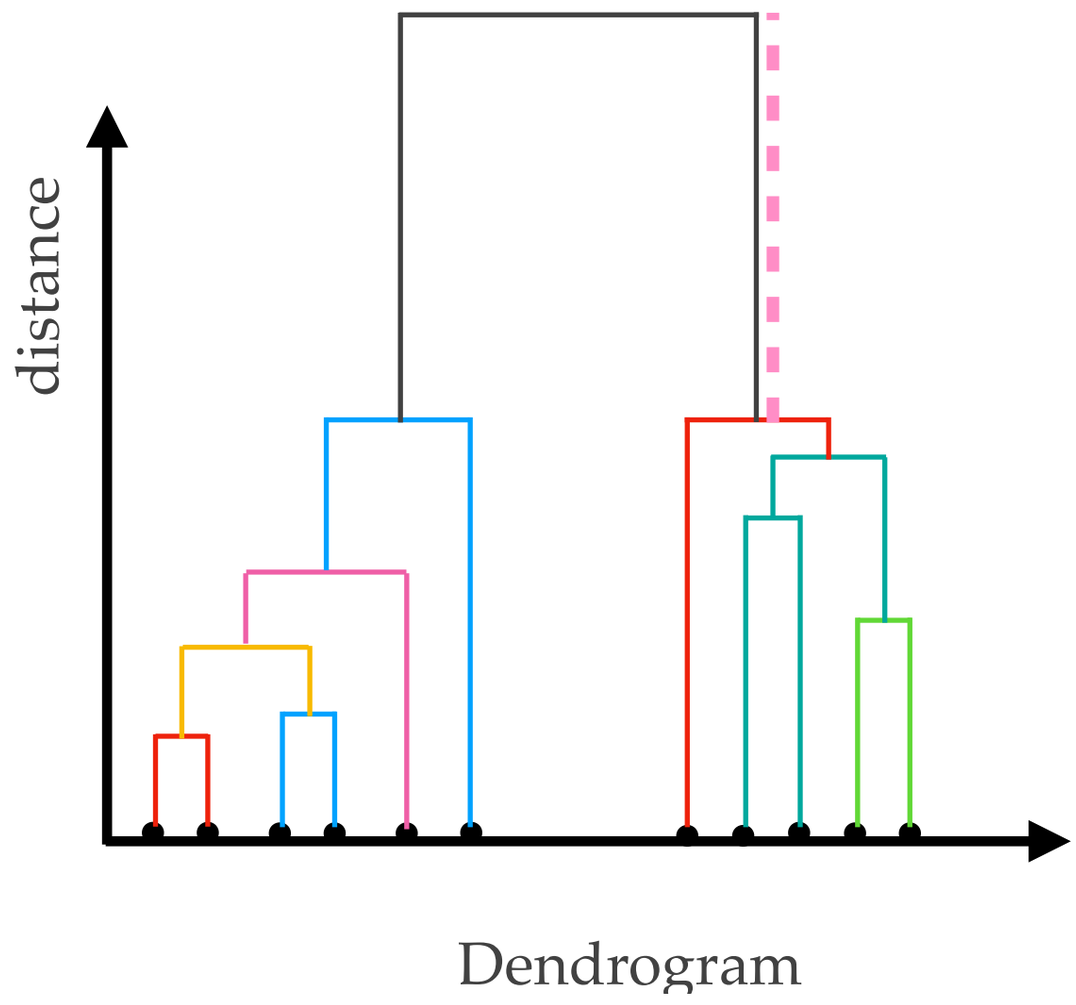
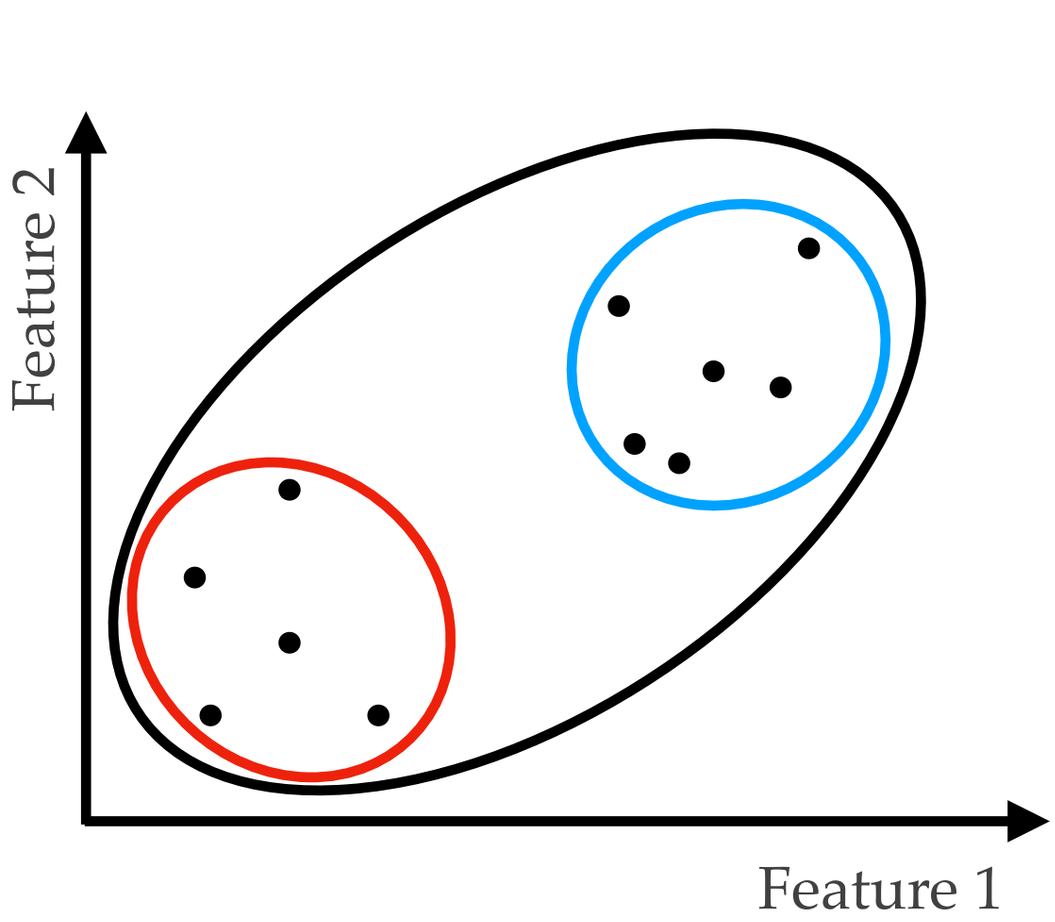


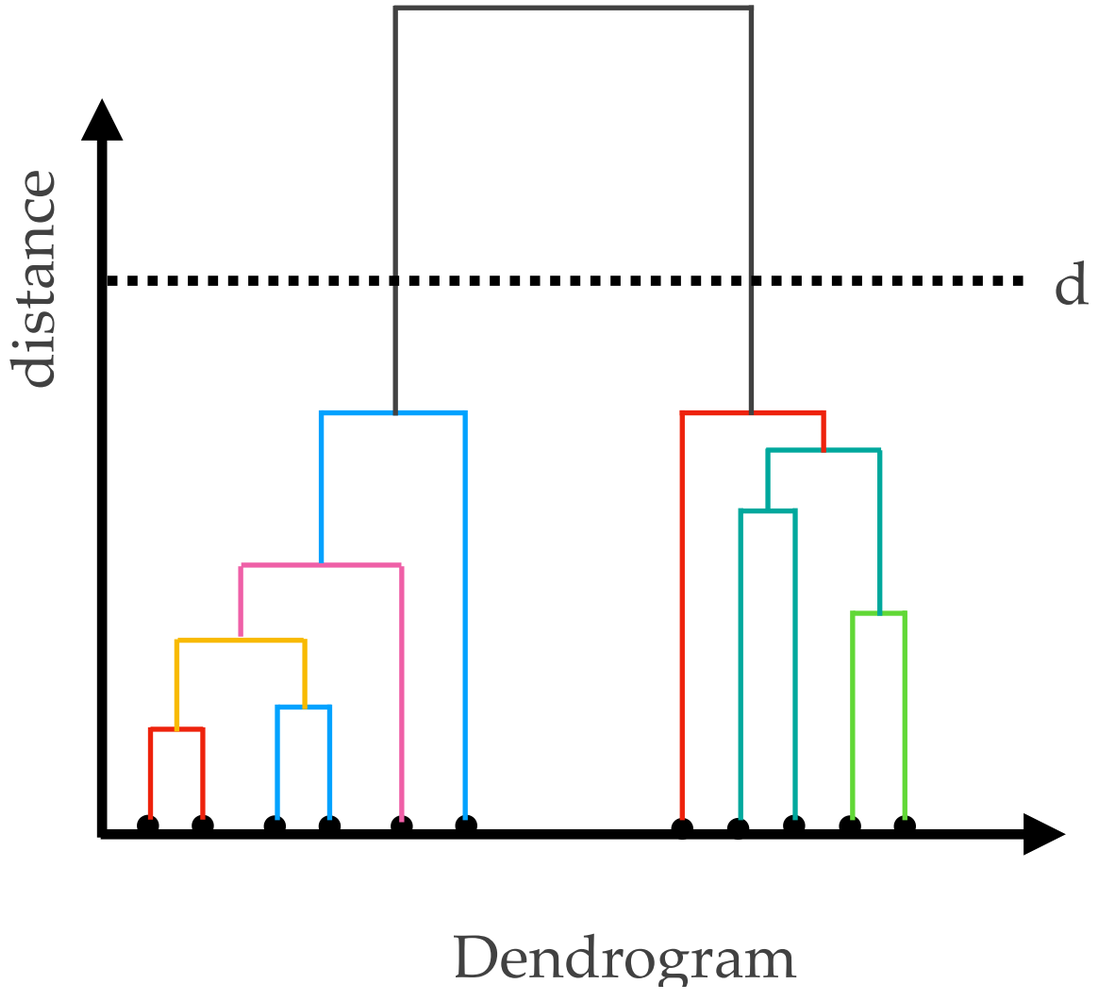


The anatomy of Hierarchal Clustering

$$f(\overrightarrow{X}, \{a_1, a_2, ...\}) = \overrightarrow{y}$$

Hyper-parameters: clusters are defined beneath a threshold d. Alternatively, we can select a threshold d that corresponds to the desired number of clusters, k.





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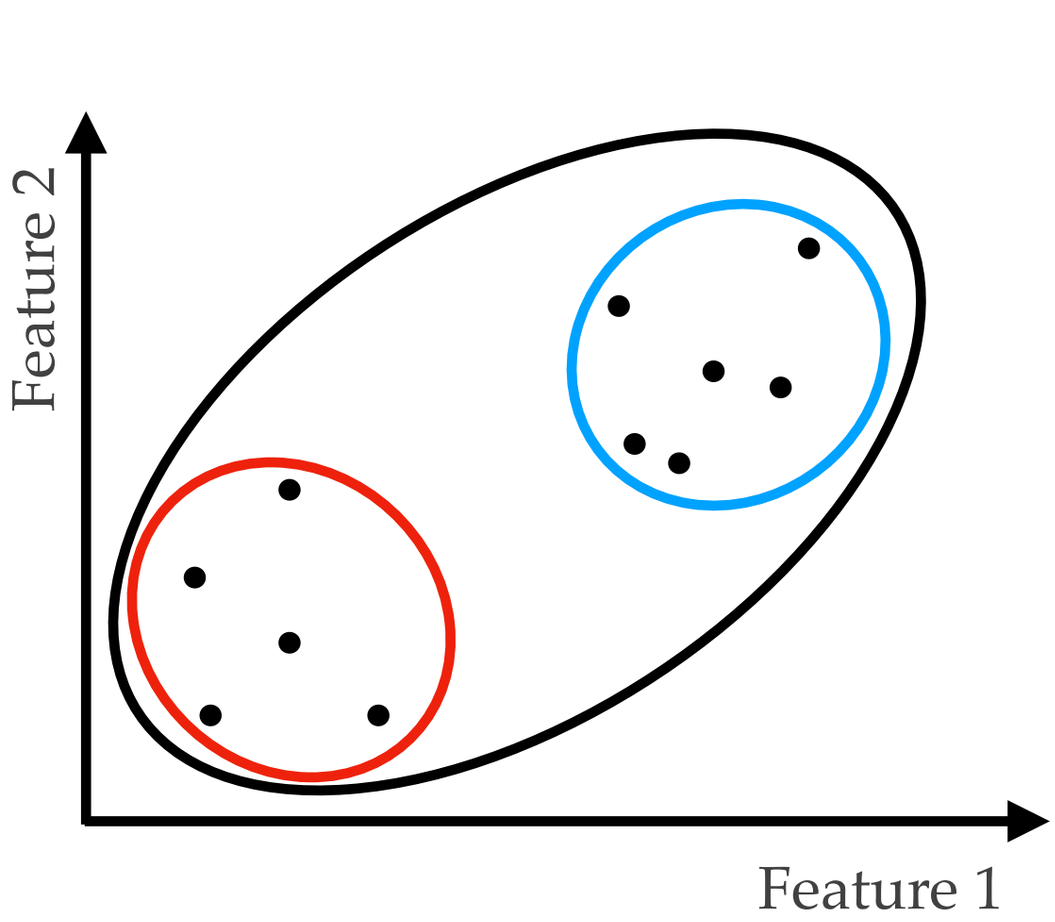
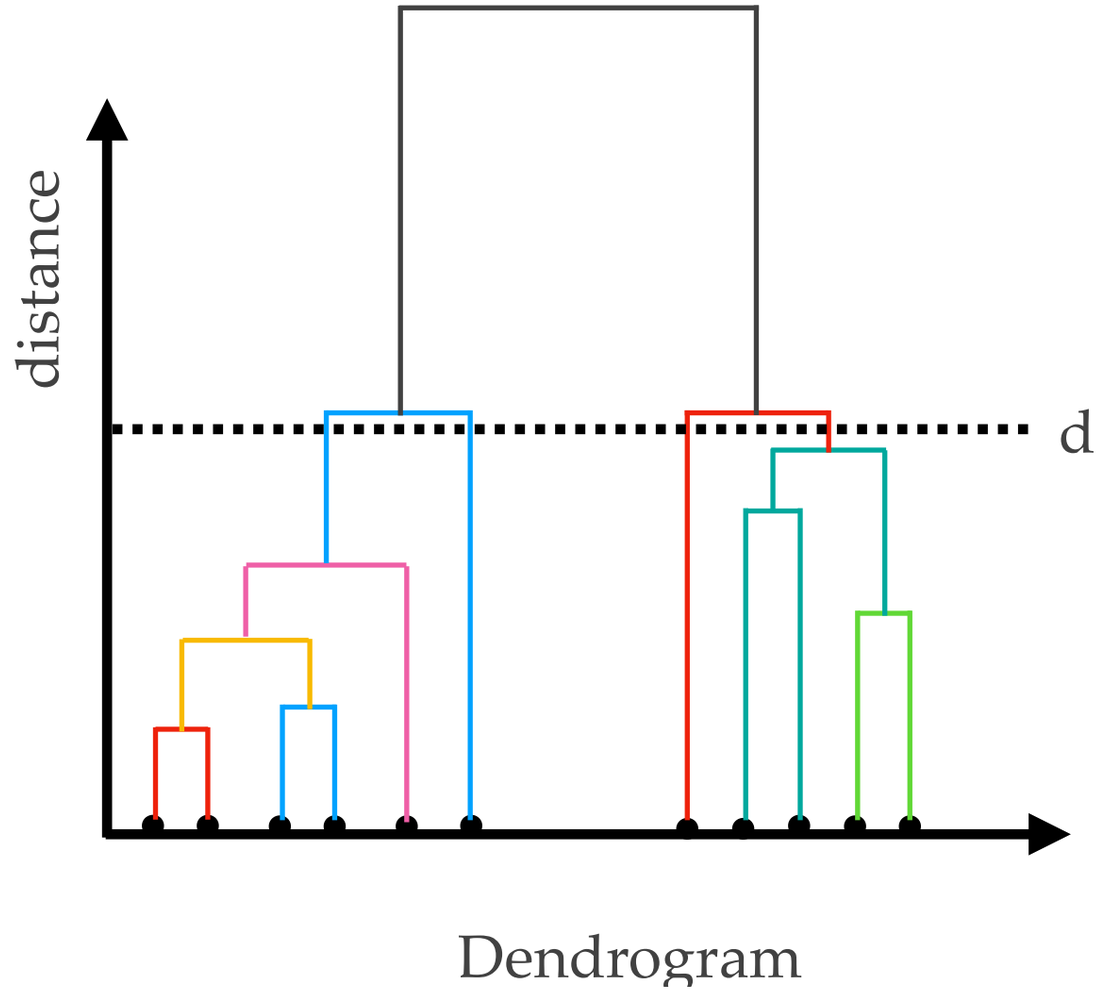


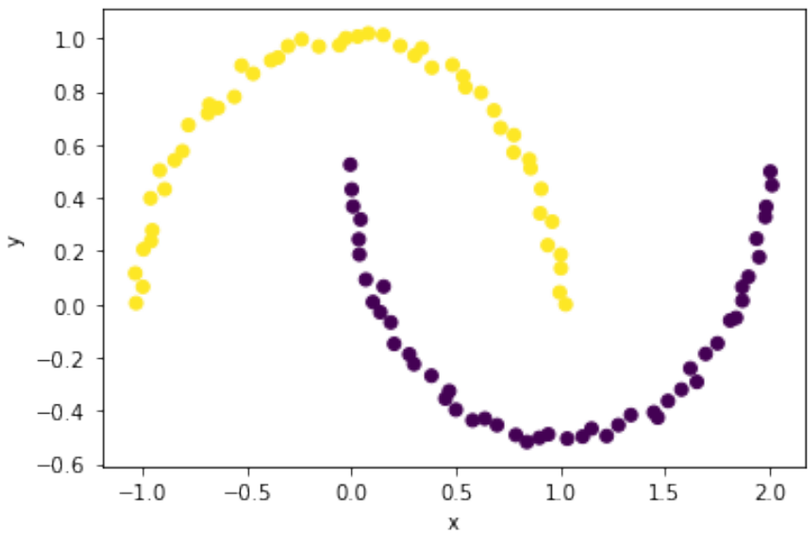


The anatomy of Hierarchal Clustering

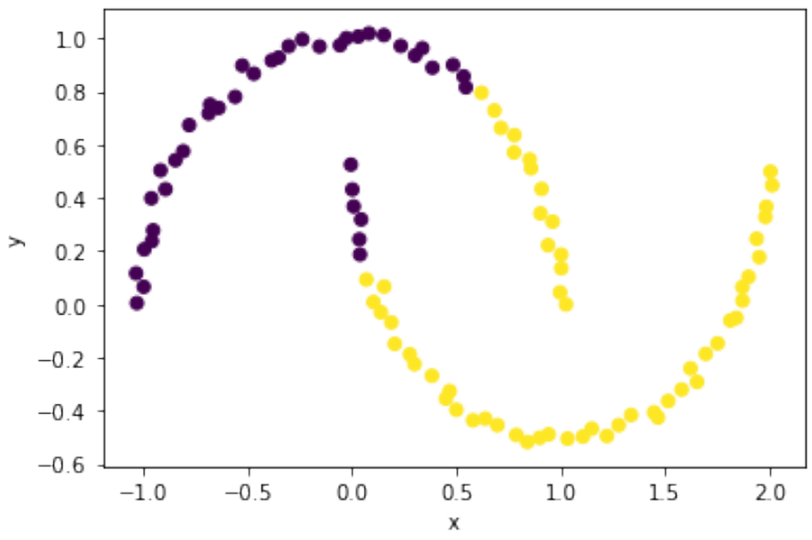
$$f(\overrightarrow{X}, \{a_1, a_2, ...\}) = \overrightarrow{y}$$

Hyper-parameters: the linkage method is essentially a hyper-parameter of the algorithm. Different linkages will result in a different output.

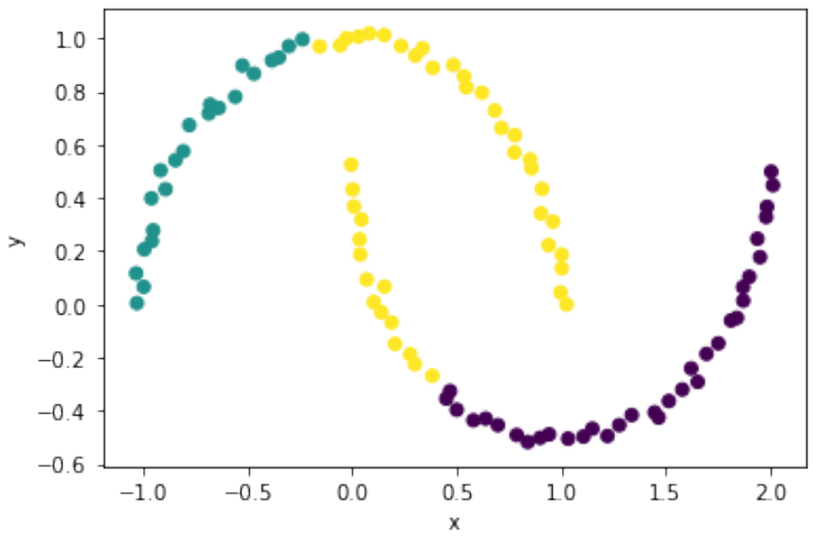
single linkage



complete linkage



average linkage



The anatomy of Hierarchal Clustering

$$f(\overrightarrow{X}, \{a_1, a_2, ...\}) = \overrightarrow{y}$$

Input dataset: can either be a list of objects with measured properties, or a distance matrix that represents pair-wise distances between objects.

What happens if we have an outlier in the dataset?

The anatomy of Hierarchal Clustering

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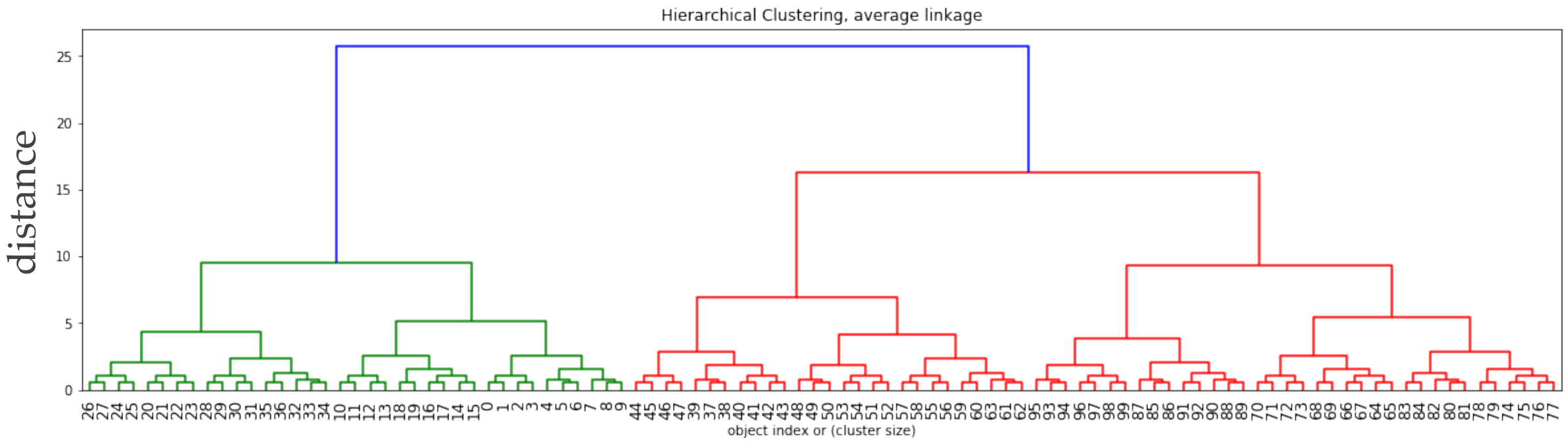
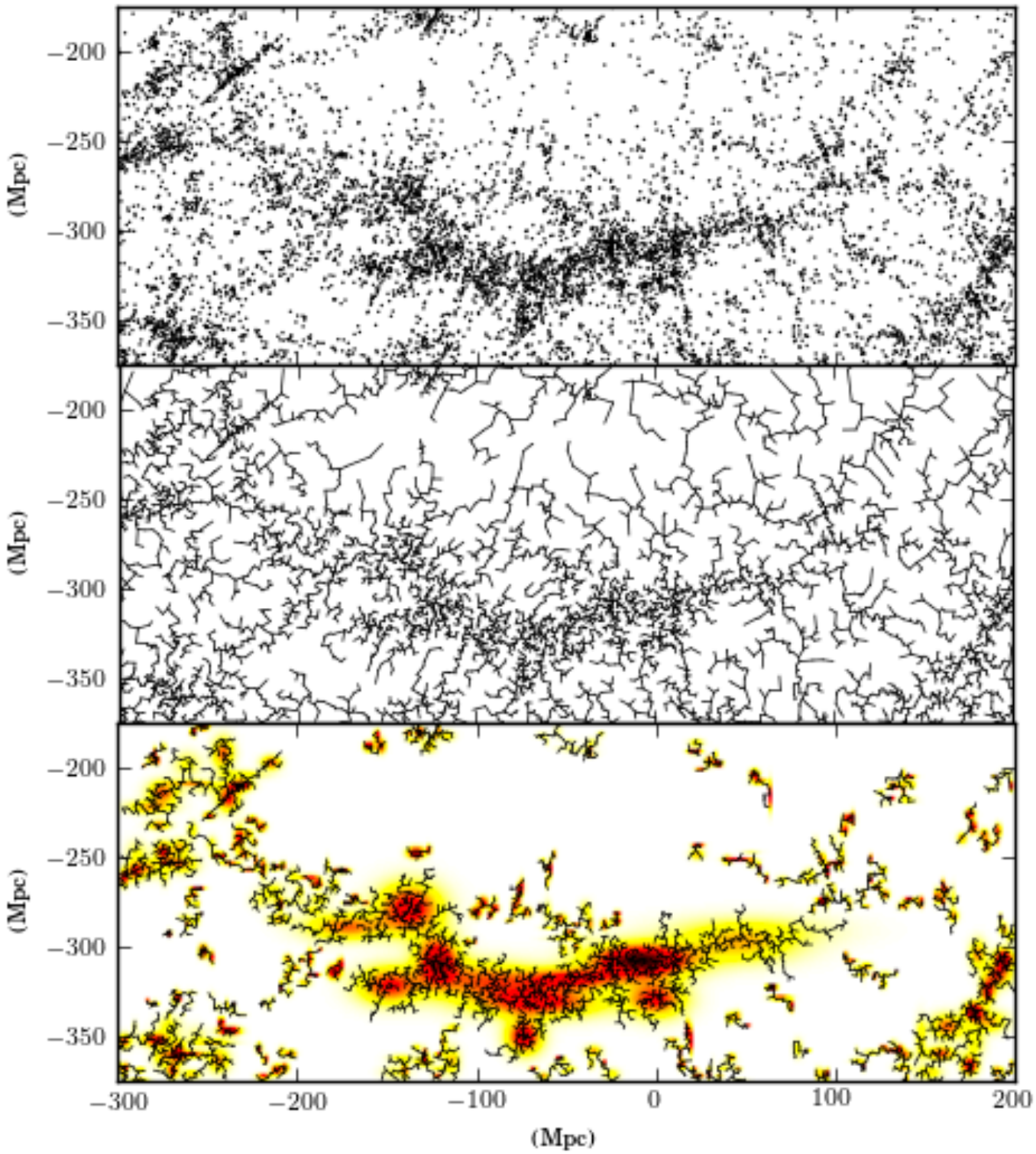
What happens if the dataset does not have clear clusters?



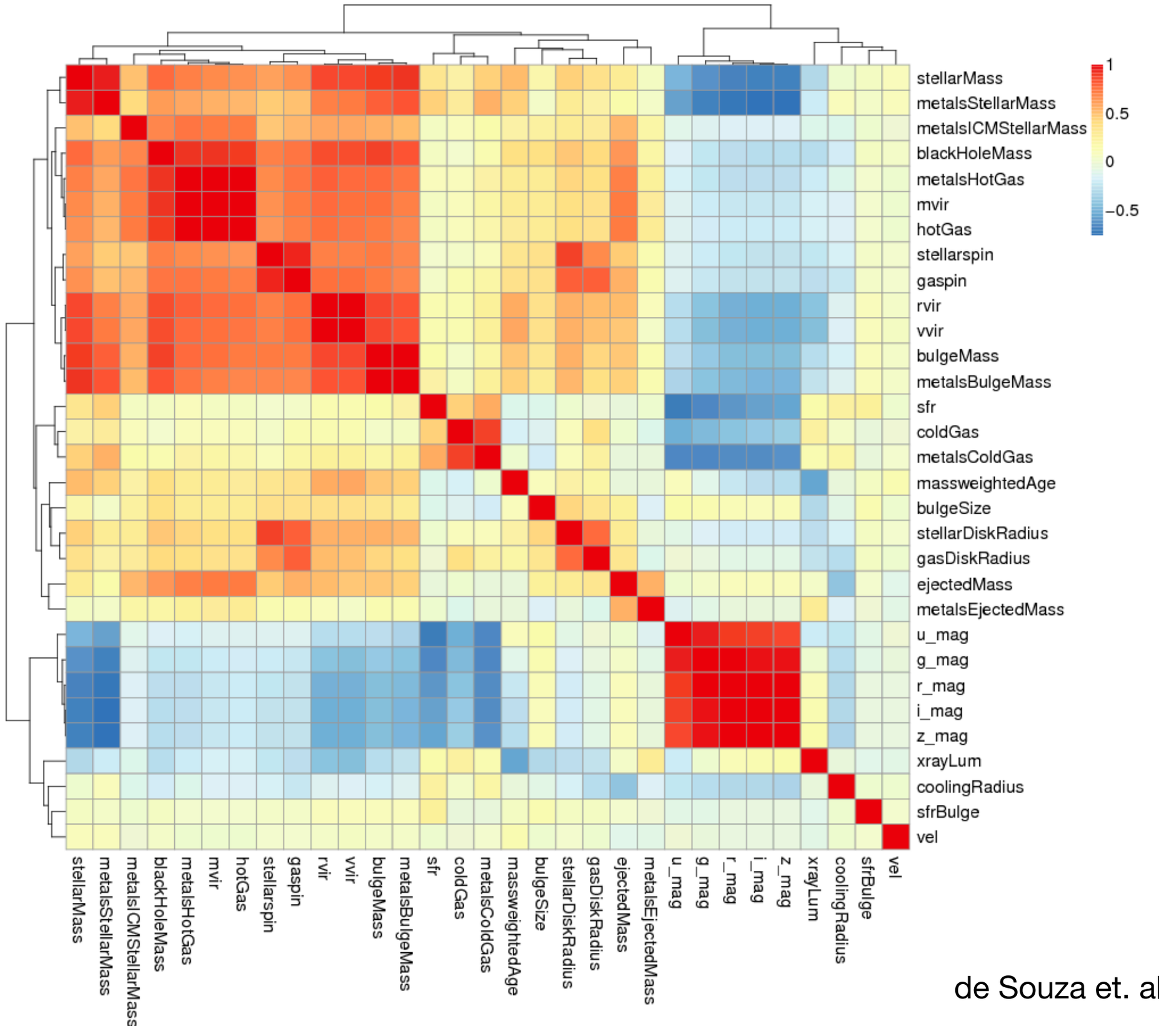
Spatial clustering: example



See code here.

"Statistics, Data Mining, and Machine Learning in Astronomy", by Ivezic, Connolly, Vanderplas, and Gray (2013).

Visualizing correlations with Hierarchical Clustering



de Souza et. al 2015

Questions?