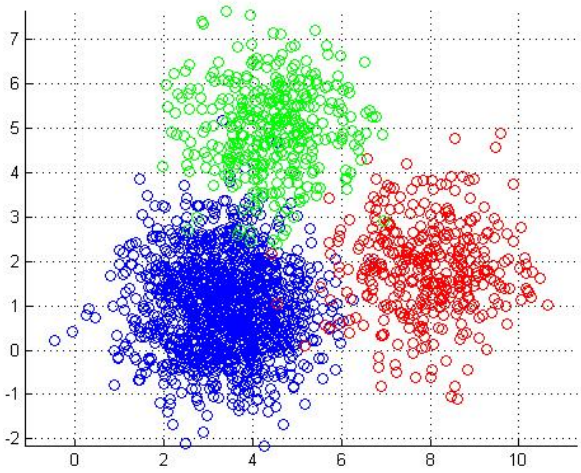
Clustering

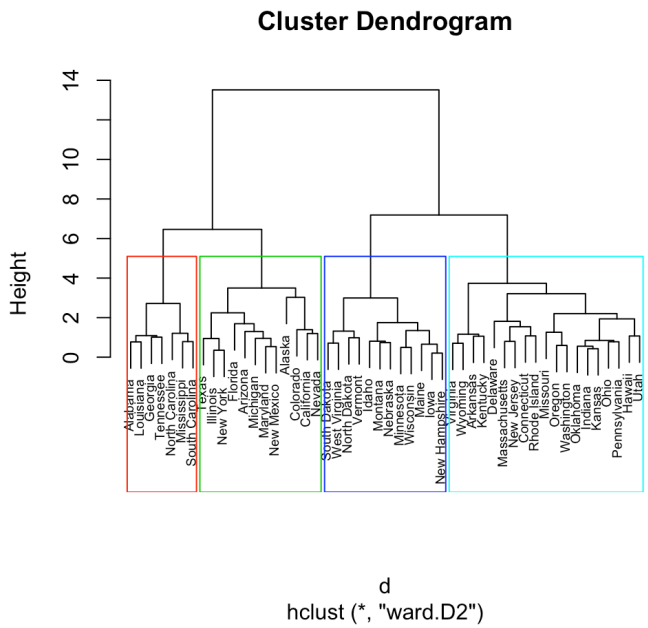
Clustering

- Broad set of techniques for finding **subgroups**.
- Observations **within groups are quite similar to each other** and observations in **different groups quite different from each other**.

Clustering methods

- Partitioning: **k-means** clustering
- Agglomerative/divisive: **hierarchical** clustering
- Model-based: mixture models





K-means clustering

- Simple approach to partitioning a data set into **K distinct, non-overlapping clusters**.
- **K is specified beforehand**.

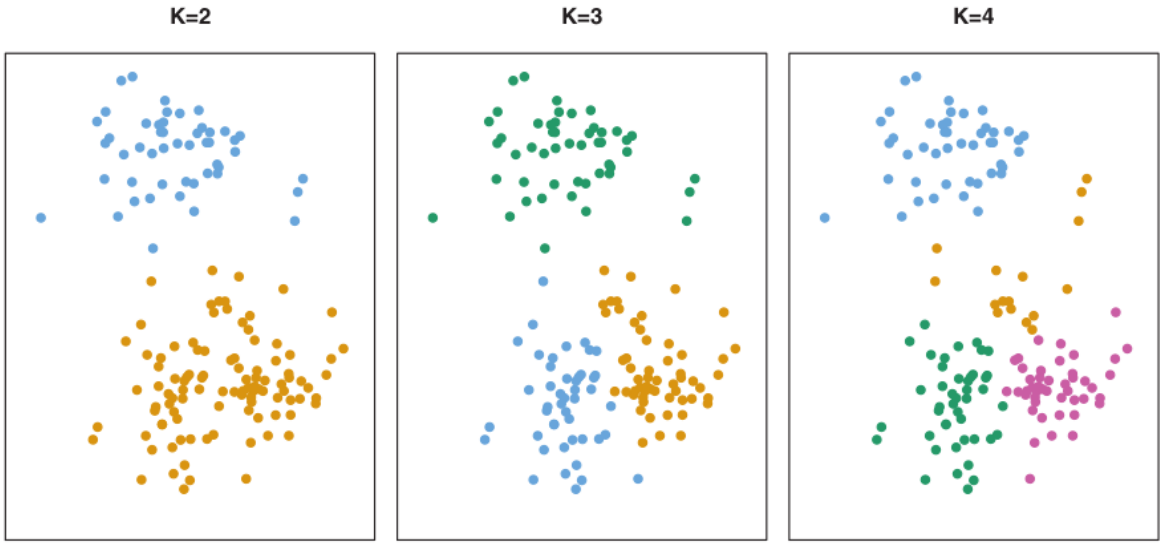


Figure 1: James et al. 2013

K-means algorithm

- K – number of clusters.

The process:

1. **Randomly** assign each observation to groups **1 to K**;
2. For each of K clusters, derive its **centroid** (midpoint);
3. **Reassign** each observation into a cluster whose centroid is the **closest**;
4. **Iterate** until stability in cluster assignments is reached (local vs global optima).

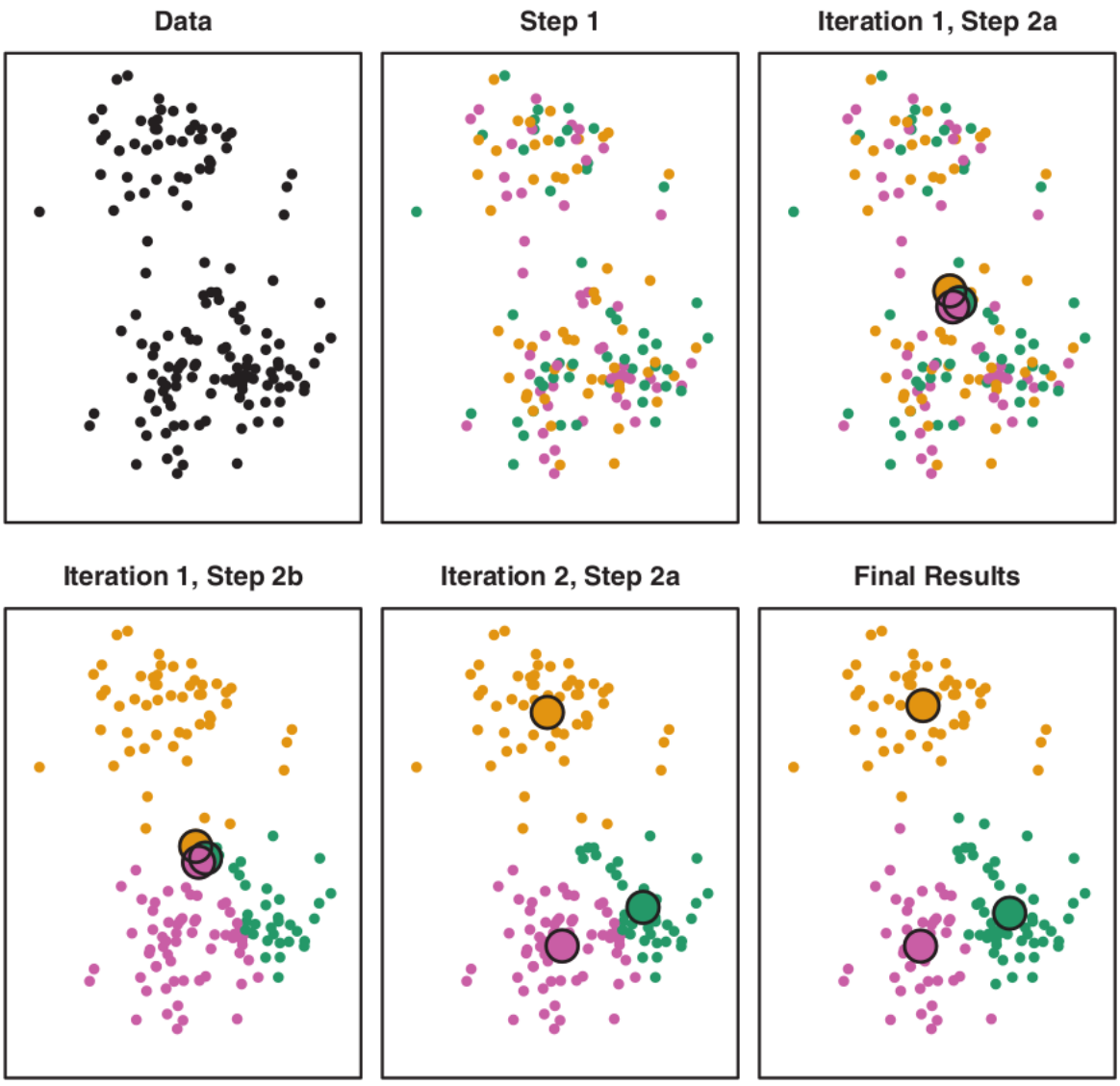
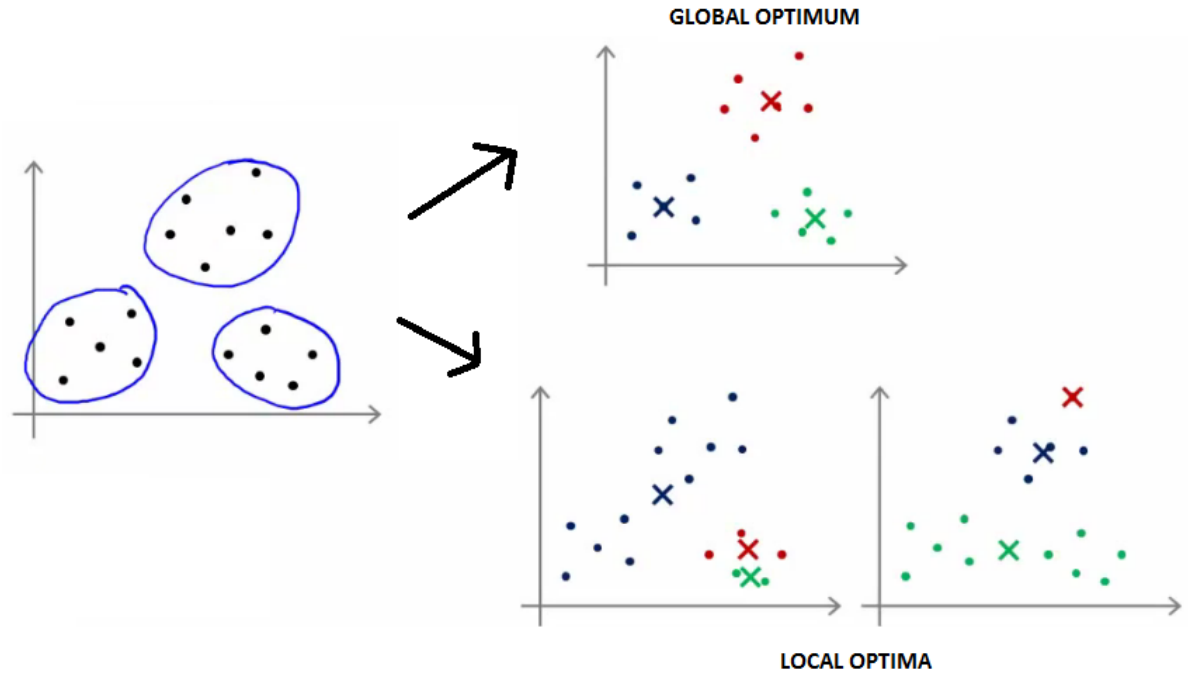


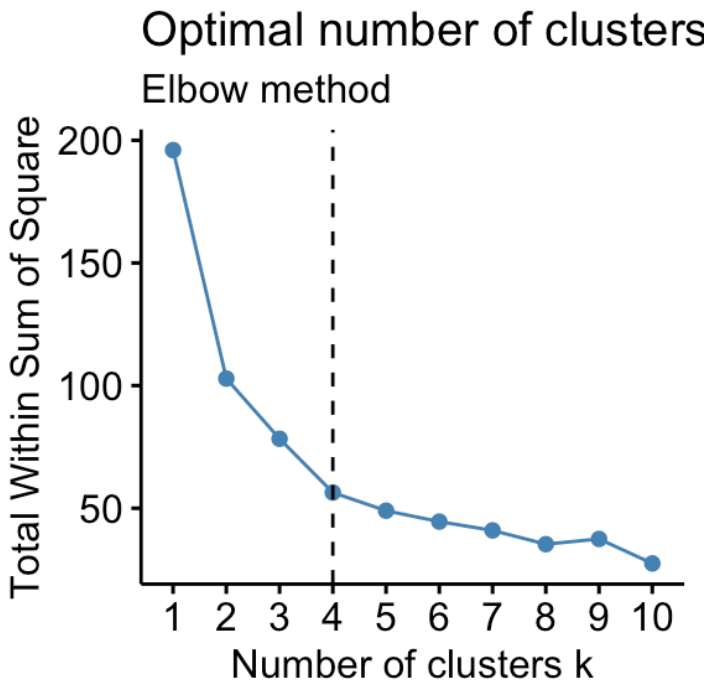
Figure 2: James et al. 2013

Some properties of K-means partitioning

- Standard algorithm for k-means clustering is using **Euclidean distance** (distances are calculated using *Pythagorean theorem*).
- Different **local optima** (stability) can be reached.

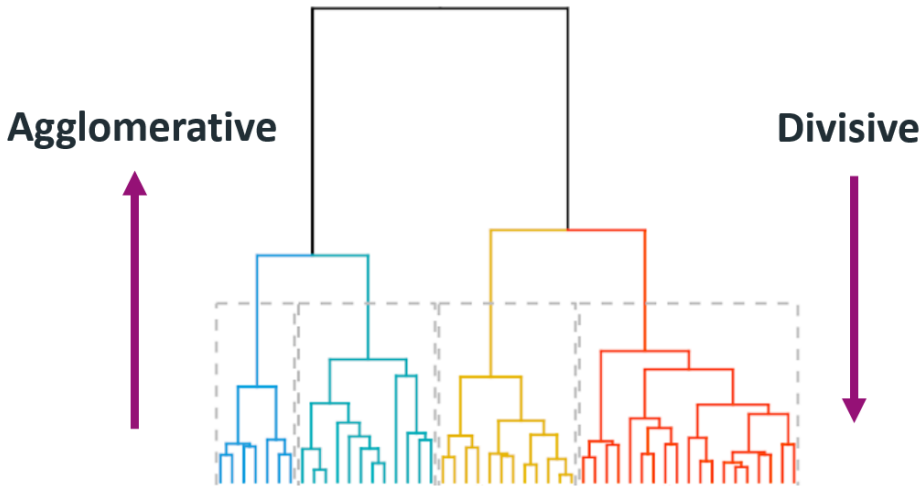


- **Number of clusters** ***K*** must be specified in advance
- How to determine **optimal** number of clusters?
  - Elbow method,
  - Silhouette method



Hierarchical clustering

- The number of clusters is **not specified beforehand**.
- Output is a **dendrogram** – a hierarchical structure visualizing the cluster growth.
- Starts with a **distance matrix**.



Agglomerative

- Builds the hierarchy of clusters from **bottom-up** until a **single cluster is reached**.

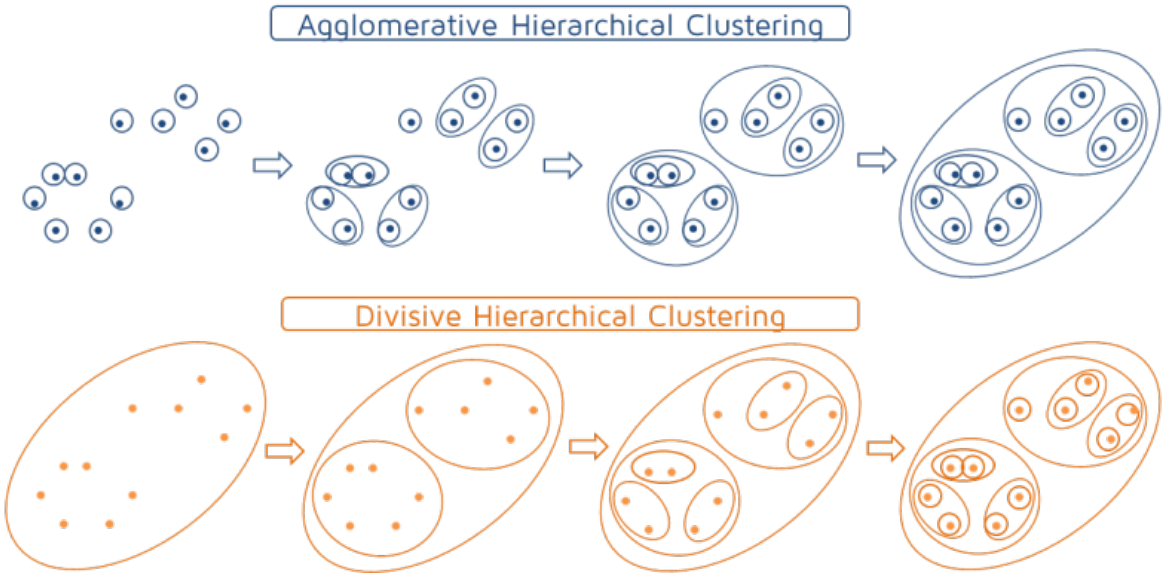
1. Put each object in its own cluster;
2. Join the clusters that are the closest;
3. Iterate until a single cluster encompassing all objects is reached.

Divisive

- **Divides** a single large cluster into **individual objects** (top-down).

1. Put all objects into a single cluster;
2. Divide the cluster into subclusters at a similar distance;
3. Iterate util all objects are in their own clusters.

Hierarchical clustering algorithms

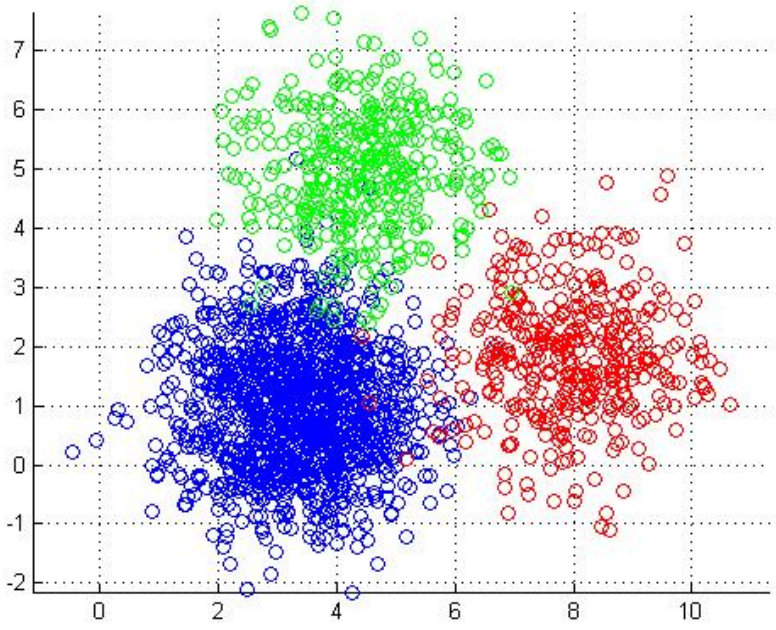


Clustering methods comparison

K-means partitioning

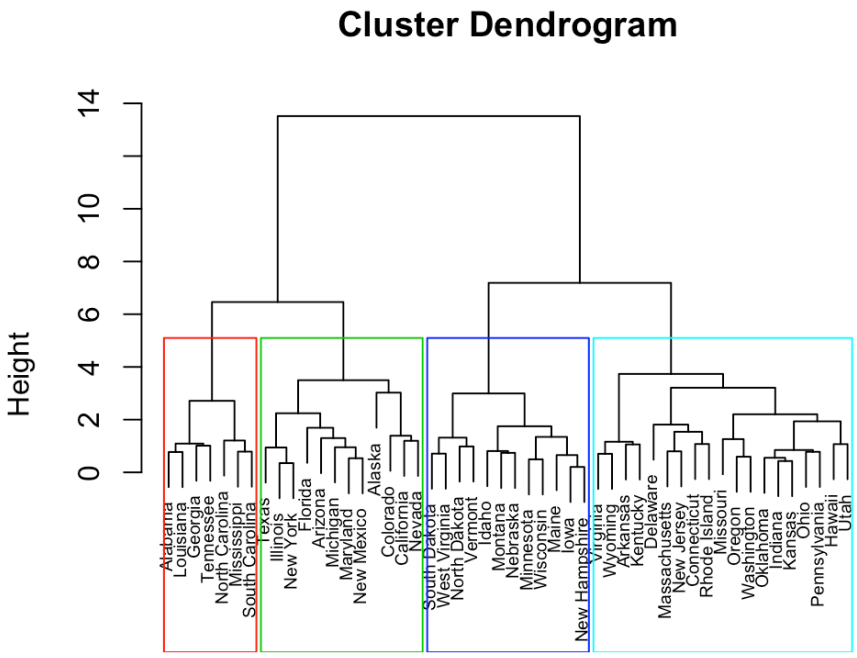
- Pre-specified number of clusters.
- Clusters may vary (different local optima).

- Best when groups in data are (hyper)spheres.



Hierarchical clustering

- Variable cluster numbers.
- Clusters are stable.
- Any shape of data distribution.



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