Introduction to Machine Learning

Clustering

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Hierarchical Clustering

HIERARCHICAL CLUSTERING

Hierarchical clustering is a recursive process that builds a hierarchy of clusters. We distinguish between:

1. Agglomerative (or bottom-up) clustering:
   - Start: Each observations is an *individual cluster*.
   - Repeat: Merge the two closest clusters.
   - Stop when there is only one cluster left.
2. Divisive (or top-down) clustering:
   - Start: All observations are within *one* cluster.
   - Repeat: Divide the cluster that results in two clusters with biggest distance.
   - Stop when each observation is an individual cluster.

HIERARCHICAL CLUSTERING

Let $\left\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\right\}$ be n observations of p features (dimensions), where $\mathbf{x}^{(i)} = \left(x_1^{(i)}, \ldots, x_p^{(i)}\right)^T$. A data set $\mathcal{D}$ is a ($n \times p$)-matrix of the form:

	feature 1	...	...	feature p
$\mathbf{x}^{(1)}$	$x_1^{(1)}$	...	...	$x_p^{(1)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\mathbf{x}^{(n)}$	$x_1^{(n)}$	...	...	$x_p^{(n)}$

HIERARCHICAL CLUSTERING

For hierarchical clustering, we need a definition for

- distances $d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ between two observations $\mathbf{x}^{(i)}$ and $\mathbf{x}^{(j)}$:
  - manhattan distance:

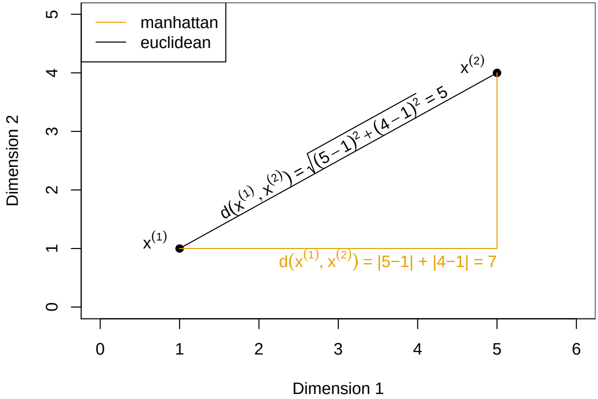
$$d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = ||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}||_1 = \sum_{k=1}^{p} |x_k^{(i)} - x_k^{(j)}|$$

  - euclidean distance:

$$d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = ||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}||_2 = \sqrt{\sum_{k=1}^{p} (x_k^{(i)} - x_k^{(j)})^2}$$

- distances between two clusters (called linkage).

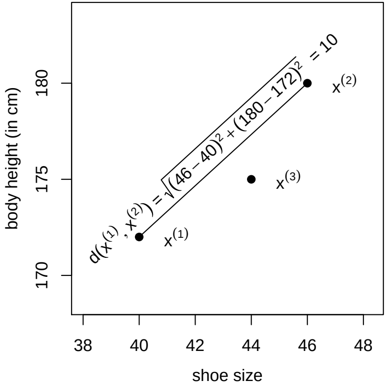
DISTANCES BETWEEN OBSERVATIONS

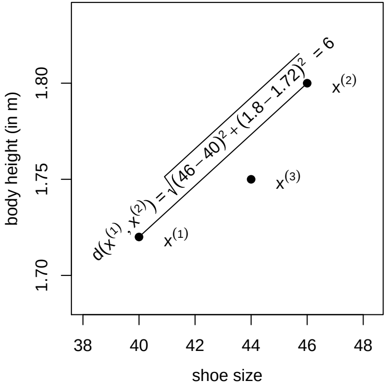


- manhattan: sum up the absolute distances in each dimension.
- euclidean: remember Pythagoras theorem from school?
- gower: can be used for mixed variables (categorical and numeric).

DISTANCES BETWEEN OBSERVATIONS

It is often a good idea to *normalize* the data before computing distances, especially when the scale of features is different, e.g.:





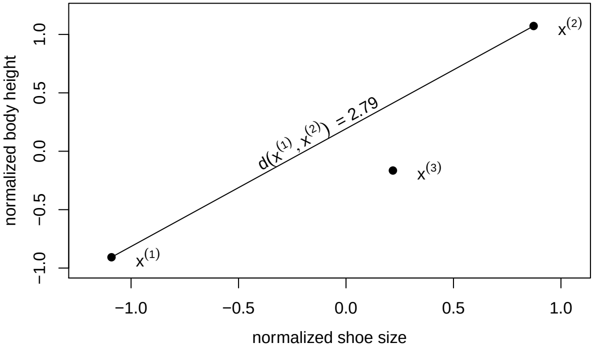
On the right plot, the distance is dominated by `shoe size`.

DISTANCES BETWEEN OBSERVATIONS

One possibility to normalize feature $\mathbf{x}_{\texttt{height}}$ is to compute

$$\tilde{\mathbf{x}}_{\texttt{height}} = \frac{\mathbf{x}_{\texttt{height}} - \text{mean}(\mathbf{x}_{\texttt{height}})}{\text{sd}(\mathbf{x}_{\texttt{height}})}.$$

Distances based on normalized data are better comparable and robust in terms of linear transformations (e.g. unit conversion).



DISTANCES BETWEEN CLUSTERS (LINKAGE)

- Assume that all observations $\left\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right\}$ belong to $k < n$ different clusters.
- For an arbitrary cluster j define its *index space* by

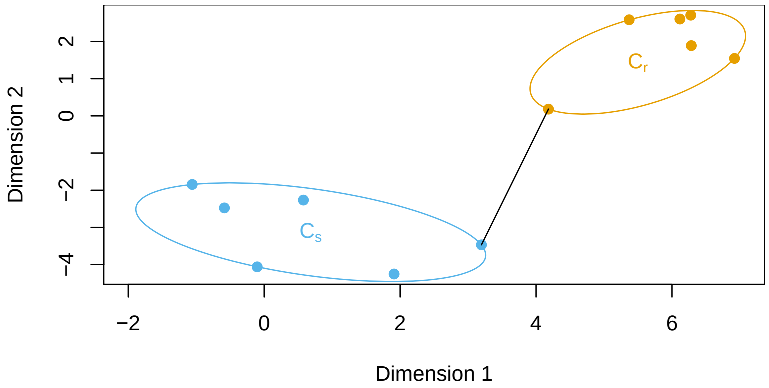
$$C_j := \{i \subset \{1, \dots, k\} | \mathbf{x}^{(i)} \text{cbelongs to cluster } j\}$$

- The linkage of two clusters C_r and C_s is a “score” describing their distance.

The most popular and simplest linkages are

- *Single Linkage*
- *Complete Linkage*
- *Average Linkage*
- *Centroid Linkage*

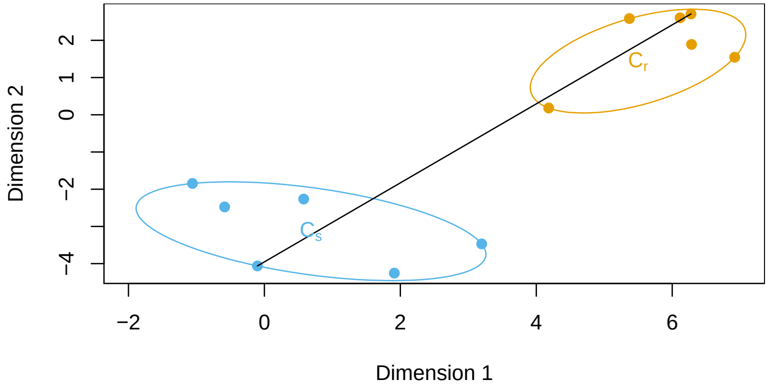
SINGLE LINKAGE



Single linkage defines the distance of the *closest point pairs* from different clusters as the distance between two clusters:

$$d_{\text{single}}(C_r, C_s) = \min_{i \in C_r, j \in C_s} d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

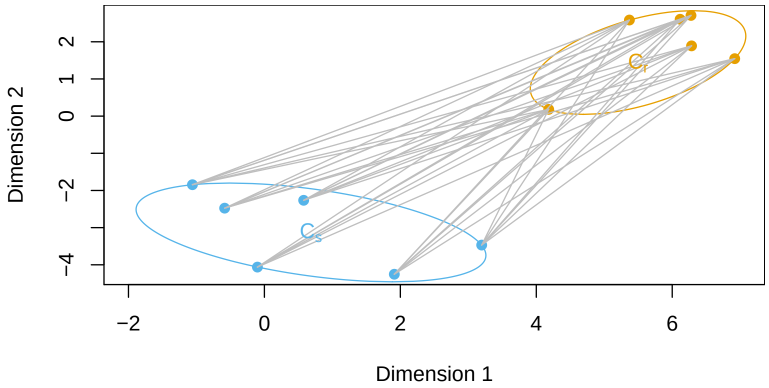
COMPLETE LINKAGE



Complete linkage defines the distance of the *furthest point pairs* of different clusters as the distance between two clusters:

$$d_{\text{complete}}(C_r, C_s) = \max_{i \in C_r, j \in C_s} d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

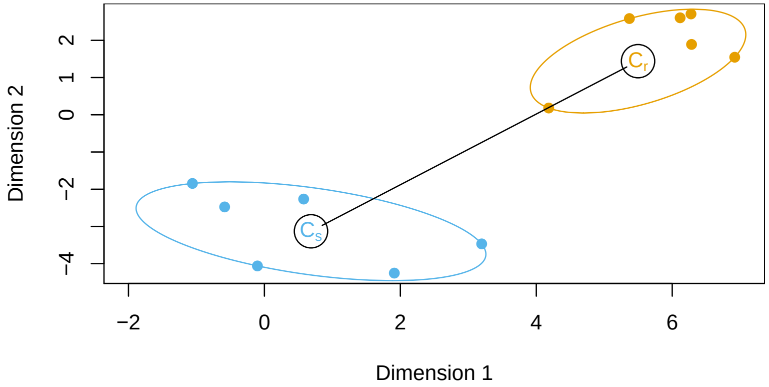
AVERAGE LINKAGE



In average linkage, the distance between two clusters is defined as the average distance across *all* pairs of two different clusters:

$$d_{\text{average}}(C_r, C_s) = \frac{1}{n_r n_s} \sum_{i \in C_r} \sum_{i \in C_s} d(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

CENTROID LINKAGE



Centroid linkage defines the distance between two clusters as the distance between the two cluster centroids. The centroid of a cluster C_s with n_s points is the mean value of each dimension:

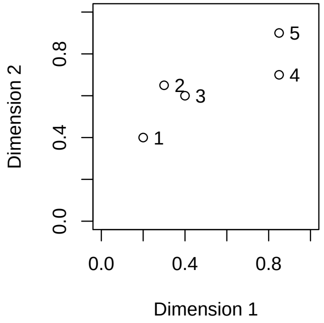
$$\bar{\mathbf{x}}_s = \frac{1}{n_s} \sum_{i \in C_s} \mathbf{x}^{(i)}$$

EXAMPLE: HIERARCHICAL CLUSTERING

Agglomerative hierarchical clustering starts with all points forming their own cluster and iteratively merges them until all points form a single cluster containing all points.

Example:

Step 1: $\{1\}, \{2\}, \{3\}, \{4\}, \{5\}$

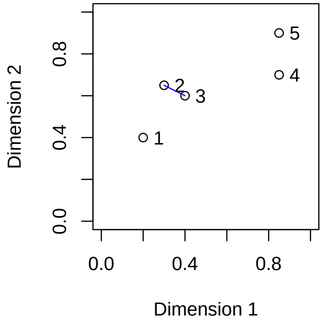


EXAMPLE: HIERARCHICAL CLUSTERING

Agglomerative hierarchical clustering starts with all points forming their own cluster and iteratively merges them until all points form a single cluster containing all points.

Example:

Step 1: $\{1\}, \{2\}, \{3\}, \{4\}, \{5\}$
Step 2: $\{1\}, \{2, 3\}, \{4\}, \{5\}$



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Example:

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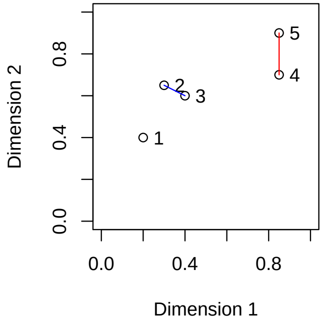
Step 2: $\{1\}, \{2, 3\}, \{4\}, \{5\}$
Step 3: $\{1\}, \{2, 3\}, \{4, 5\}$



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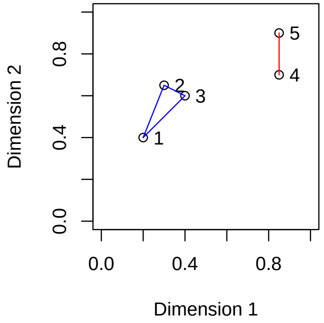
Step 3: $\{1\}, \{2, 3\}, \{4, 5\}$
Step 4: $\{1, 2, 3\}, \{4, 5\}$



EXAMPLE: HIERARCHICAL CLUSTERING

Agglomerative hierarchical clustering starts with all points forming their own cluster and iteratively merges them until all points form a single cluster containing all points.

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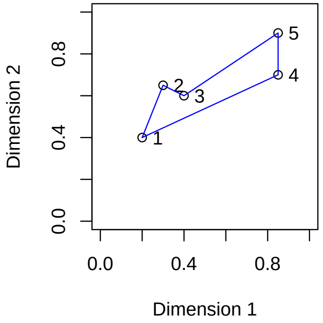
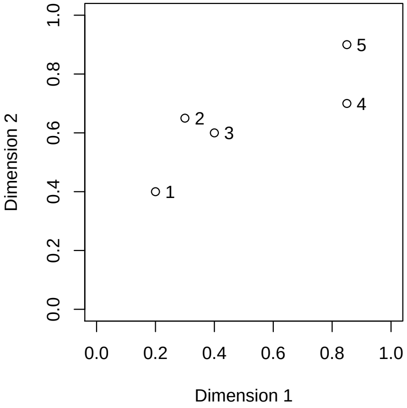
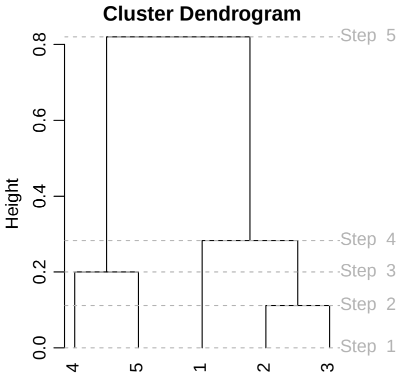
Step 2: $\{1\}, \{2, 3\}, \{4\}, \{5\}$
Step 3: $\{1\}, \{2, 3\}, \{4, 5\}$
Step 4: $\{1, 2, 3\}, \{4, 5\}$
Step 5: $\{1, 2, 3, 4, 5\}$



DENDROGRAM

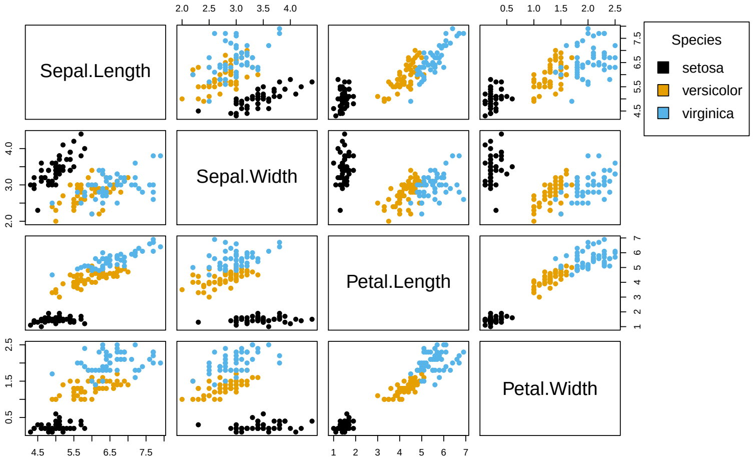
A Dendrogram is a tree showing which clusters / observations are merged after each step. The "height" is proportional to the distance between the two merged clusters:





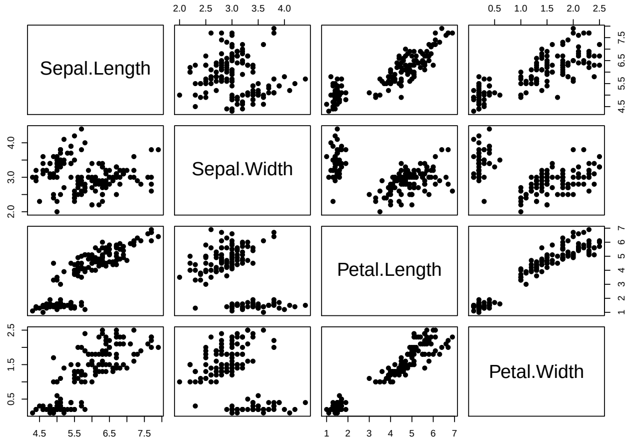
EXAMPLE: IRIS DATA

The data contains 150 leaf measurements for 3 flower species:

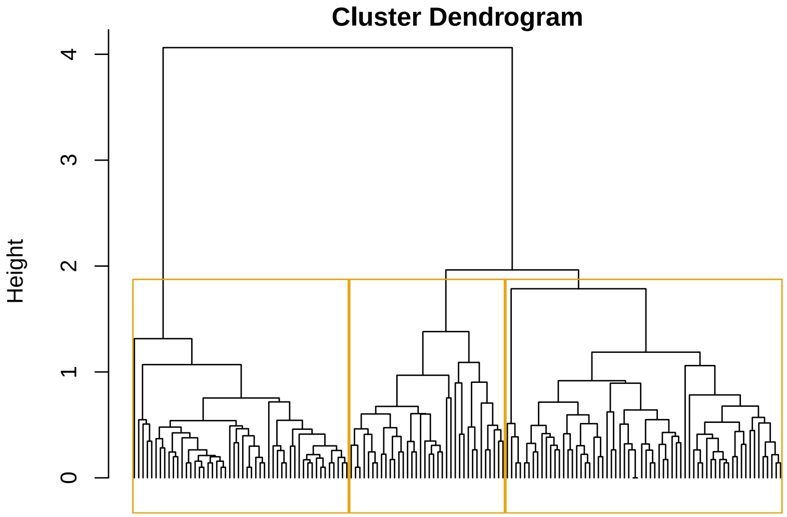


R EXAMPLE WITH IRIS DATA

We now “forget” the real groups specified by the `Species` variable and try to find clusters based on the leaf measurements.

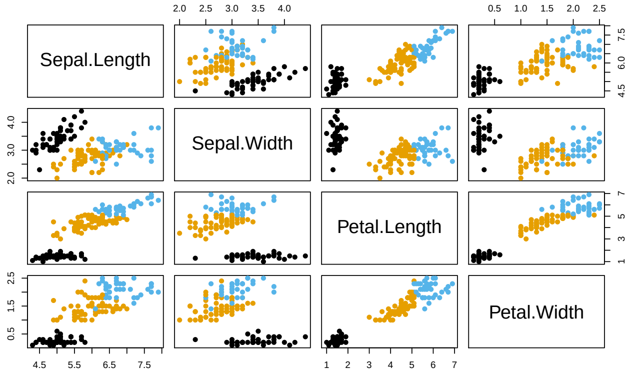


EXAMPLE: IRIS DATA



EXAMPLE: IRIS DATA

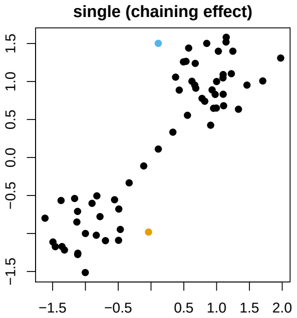
We can extract the clustering assignments by cutting the dendrogram, e.g. using $k = 3$ clusters:

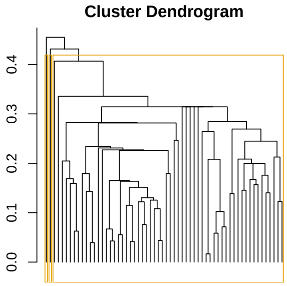


PROPERTIES: SINGLE LINKAGE

Single linkage introduces the *chaining problem*:

- Only one pair of points needs to be close to merge clusters.
- A chain of points can expand a cluster over long distances.
- Points within a cluster can be too widely spread and not dense enough.

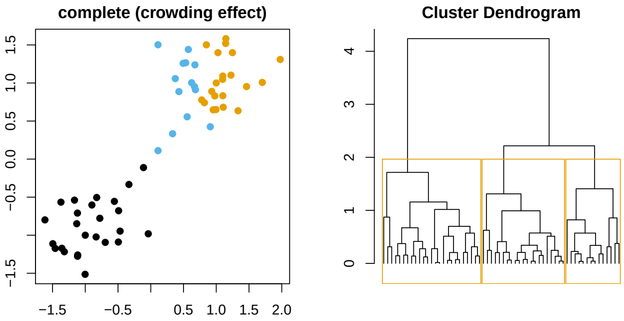




PROPERTIES: COMPLETE LINKAGE

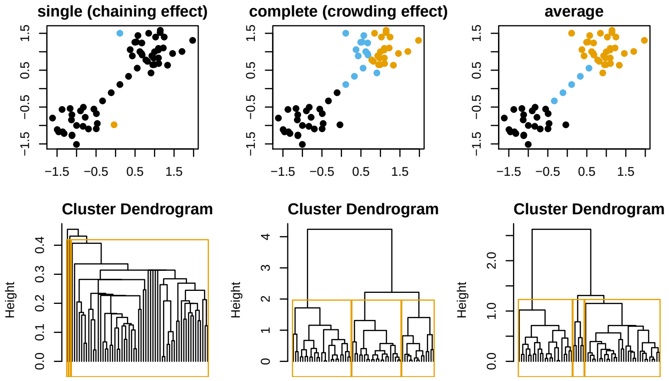
Complete linkage avoids chaining, but suffers from *crowding*:

- Merging is based on the furthest distance of point pairs from different clusters.
- Points of two different clusters can thus be closer than points within a cluster.
- Clusters are dense, but too close to each other.



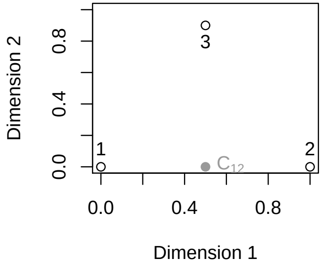
PROPERTIES: AVERAGE LINKAGE

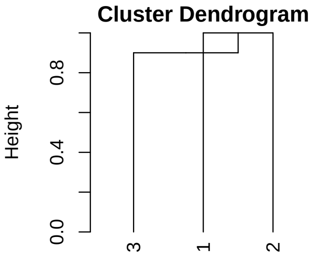
- Average linkage is based on the average distance between clusters and tries to avoid crowding and chaining.
- Produces clusters that are quite dense and rather far apart.



PROPERTIES: CENTROID LINKAGE

- Centroid linkage defines the distance based on **artificial data points** (the cluster centers), which produces dendrograms **with inversions**, i.e., the distance between the clusters to be merged can be smaller in the next step.
- In single, complete and average linkage, the distance between the clusters to be merged increases in each step. $\Rightarrow$ always produces dendrograms **without inversions**.





SUMMARY

- *Hierarchical agglomerative clustering methods* iteratively merge observations/clusters until all observations are in one single cluster.
- Results in a hierarchy of clustering assignments which can be visualized in a *dendrogram*. Each node of the dendrogram represents a cluster and its “height” is proportional to the distance of its child nodes.
- The most common linkage functions are *single, complete, average* and *centroid* linkage. There is no perfect linkage and each linkage has its own advantages and disadvantages.

Partitioning Clustering Methods

OPTIMAL PARTITIONING CLUSTERING

Hierarchical clustering:
Stepwise merging (agglomerative methods) or dividing (divisive methods) of clusters based on distances and linkages. The number of clusters are selected by splitting the dendrogram at a specific threshold for the "height" after visual inspection.

Partitioning clustering:
Partitions the n observations into a predefined number of k clusters by optimizing a numerical criterion. The most common partitioning methods are:

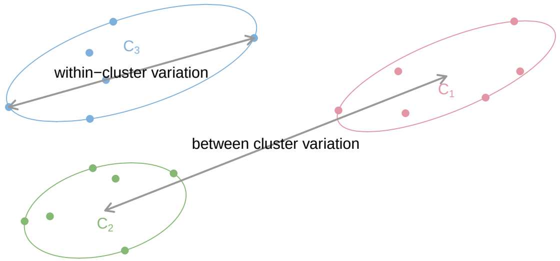
- k-means
- k-medians
- k-medoids (Partitioning Around Medoids (PAM))

K-MEANS

k-means partitions the *n* observations into *k* predefined clusters $C_1, C_2, \dots, C_k$ by minimizing the **compactness**, i.e. the **within-cluster variation** of all clusters using

$$\sum_{j=1}^{k} \sum_{i \in C_j} \|\mathbf{x}^{(i)} - \bar{\mathbf{x}}_j\|_2^2 \rightarrow \min,$$

where $\bar{\mathbf{x}}_j = \frac{1}{n_j} \sum_{i \in C_j} \mathbf{x}^{(i)}$ is the centroid of cluster *j* and n_j is the number of observations in cluster *j*.



K-**MEANS**

Idea: Consider every possible partition of n observations into k clusters and select the one with the lowest **within-cluster variation**.
Problem: Requires trying all possible assignments of n observations into k clusters, which in practice is nearly impossible (Hothorn et al., 2009, p.322):

n	k	Number of possible partitions
15	3	2.375.101
20	4	45.232.115.901
100	5	10^{68}

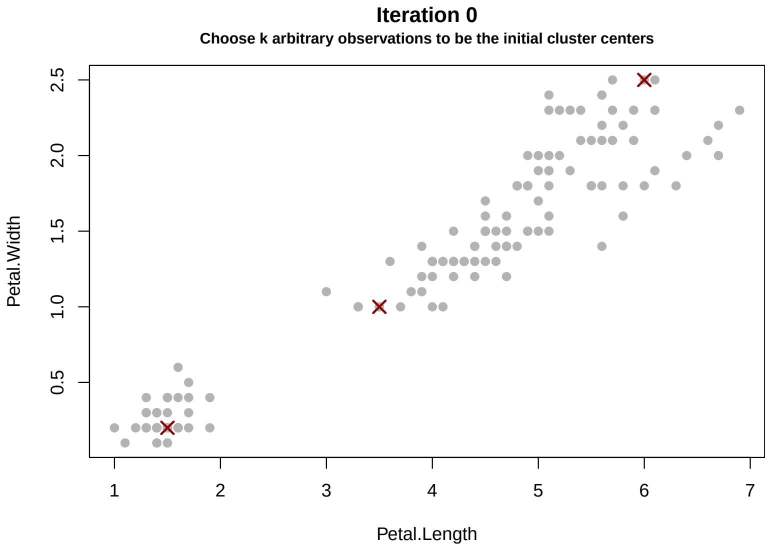
Hothorn, T., Everitt, B. S. (2009). A handbook of statistical analyses using R. Chapman and Hall/CRC.

K-MEANS

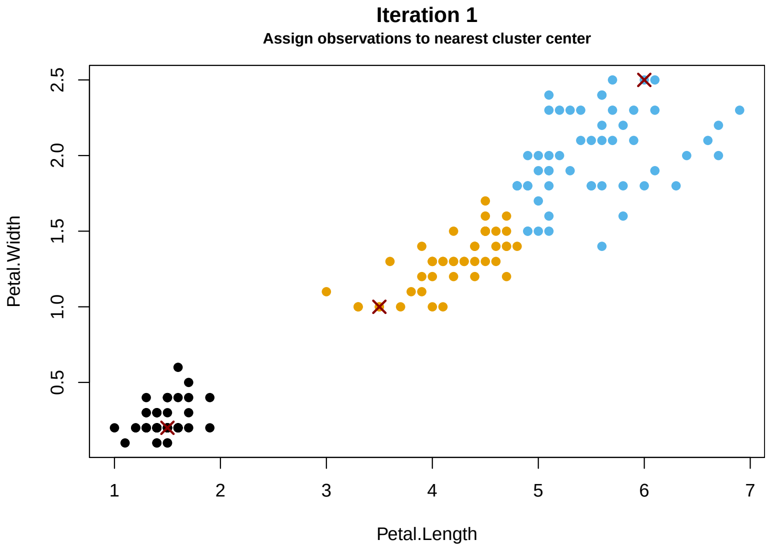
Use an approximation:

1. **Initialization:** Choose k arbitrary observations to be the initial cluster centers.
2. **Assignment:** Assign every observation to the cluster with the closest center.
3. **Update:** Compute the new center of each cluster as the mean of its members.
4. Repeat (2) and (3) until the centers do not move.

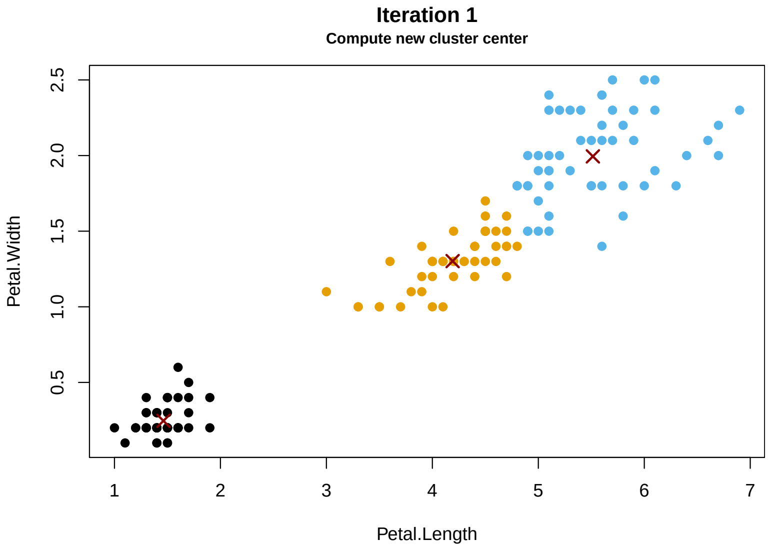
K-MEANS EXAMPLE



K-MEANS EXAMPLE



K-MEANS EXAMPLE



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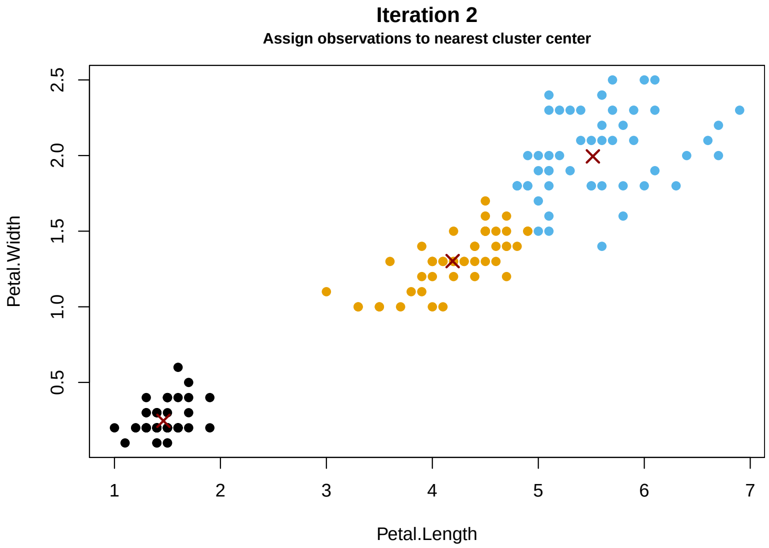
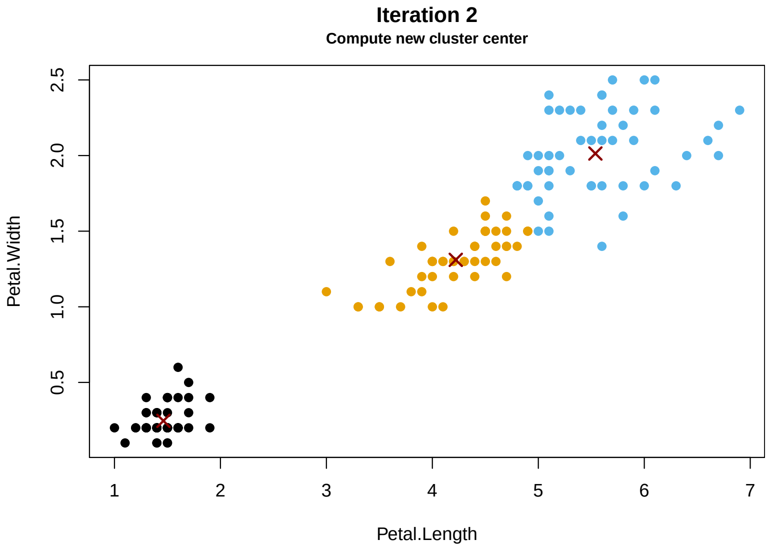


K-MEANS EXAMPLE



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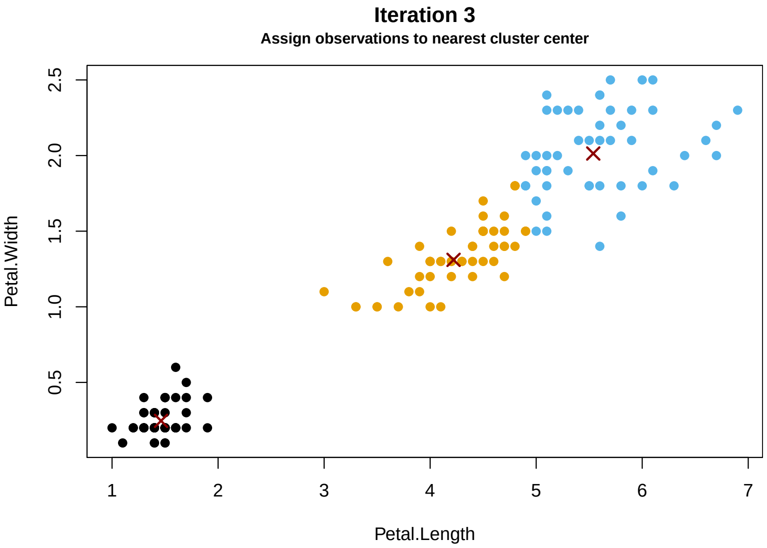
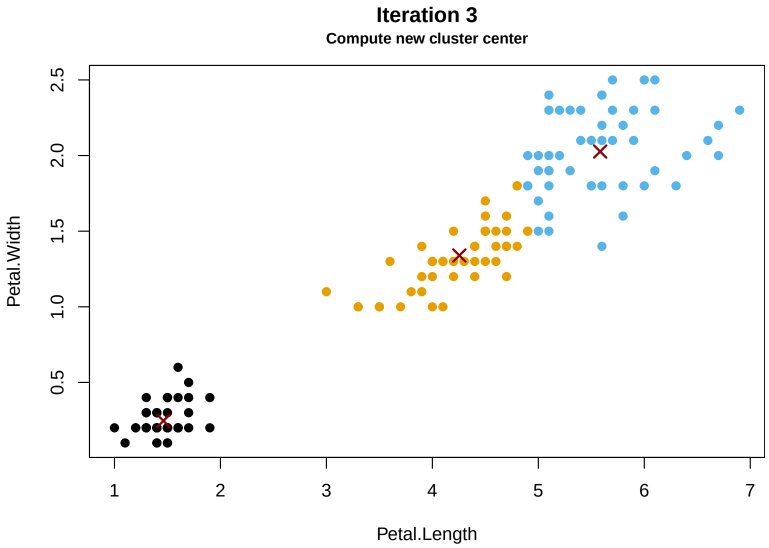


K-MEANS EXAMPLE

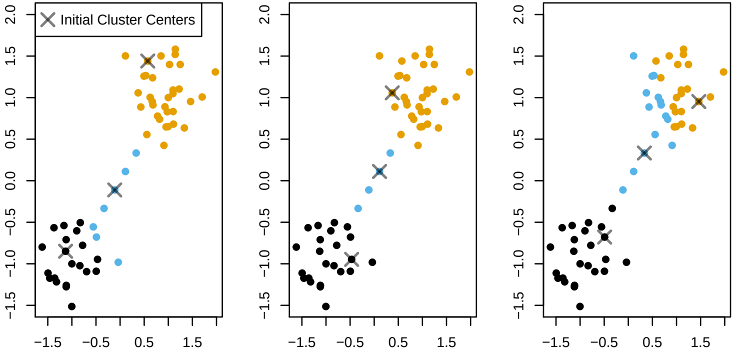


PROPERTIES OF *K*-MEANS

- *k*-means is based on computing the mean, which is sensitive to outliers and can only be computed for numerical data.
- The **within-cluster variation** is reduced in each iteration.
- The final result is typically not the best result that globally minimizes the **within-cluster variation**.
  $\rightarrow$ would only be possible after trying all possible partitions!
- *k*-means can be restarted multiple times. The clustering with the smallest within-cluster variation is then selected as the best solution.

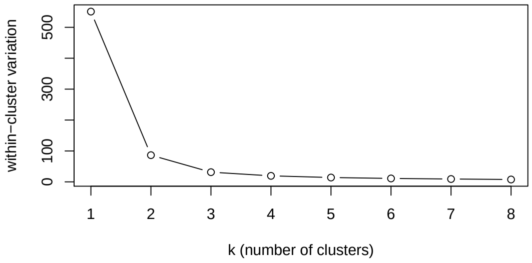
PROPERTIES OF K-MEANS

- k-means produces different clusters depending on the initial centers and always converges, e.g.:



CHOICE OF *K*

- Many methods exist for choosing the number of clusters *k* (there is no perfect solution).
- The easiest method is to apply *k*-means for different *k* and plot the **within-cluster variation** for each number of *k*.
- The **within-cluster variation** always decreases with increasing number of clusters.
- An **"elbow"** in the plot might indicate a useful solution.



K-MEDOIDS

- is strongly related to *k*-means and is realized by the **Partitioning Around Medoids (PAM)** algorithm.
- uses cluster medoids as representative clusters, i.e. **real data points** instead of **artificial data points** (such as the cluster centers as in *k*-means) are used.
- is less sensitive to outliers and more robust than *k*-means.
- can handle categorical features (*k*-means doesn't because it is based on calculating the cluster centers by taking the mean in each dimension).

THE PAM ALGORITHM

1. **Initialization:** Randomly select k data points as the medoids.
2. **Assignment:** Assign each data point $\mathbf{x}^{(i)}$ to its closest medoid m and calculate the within-cluster variation for each medoid (by summing up the distances of the current medoid m to all other data points associated to m) .
3. **Update:** Swap m and $\mathbf{x}^{(i)}$ and recompute the within-cluster variation to see if another medoid is more appropriate. Select the medoid m with the lowest within-cluster variation.
4. Repeat steps (2) and (3) until medoids do not change.

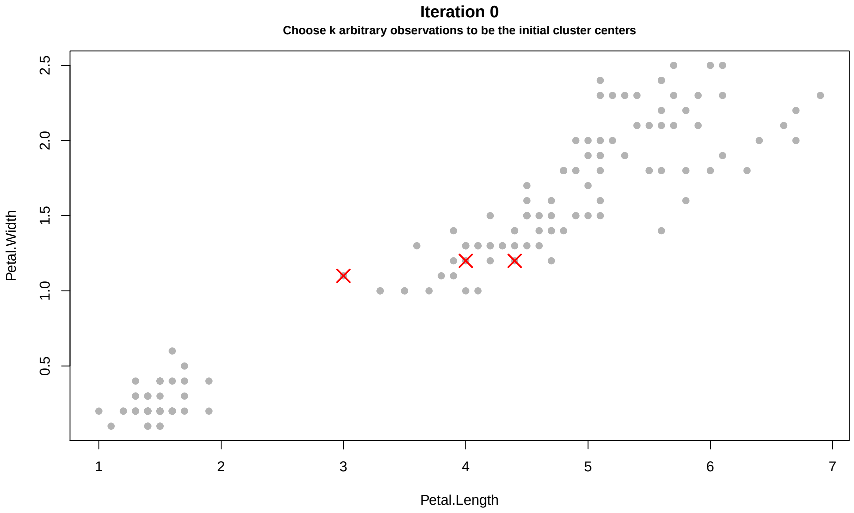
THE PAM ALGORITHM

The PAM algorithm typically uses the following two metrics to compute distances:

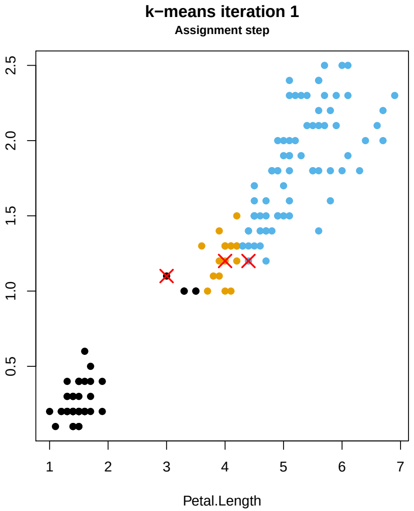
- The euclidean distance (root sum-of-squares of differences).
- The Manhattan distance (the sum of absolute distances).

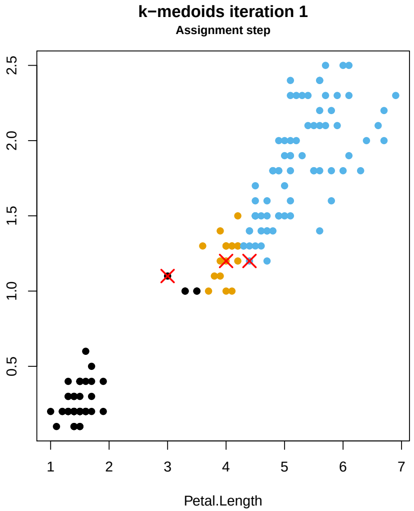
Note: The Manhattan distance should give more robust results if your data contains outliers. In all other cases, the results will be similar for both metrics.

K-MEANS VS. *K*-MEDOIDS

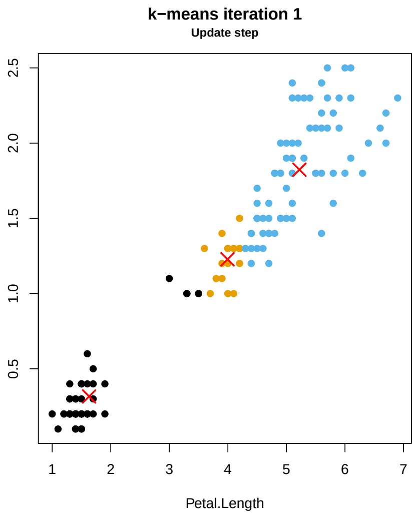


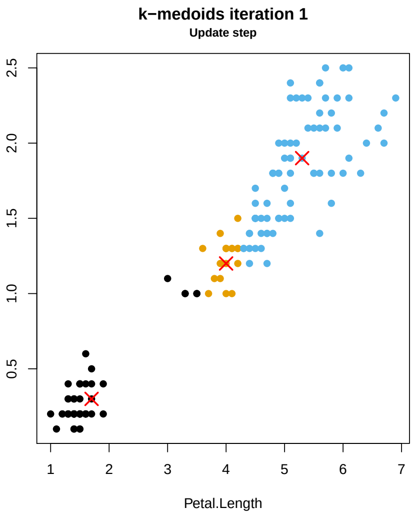
K-MEANS VS. *K*-MEDOIDS



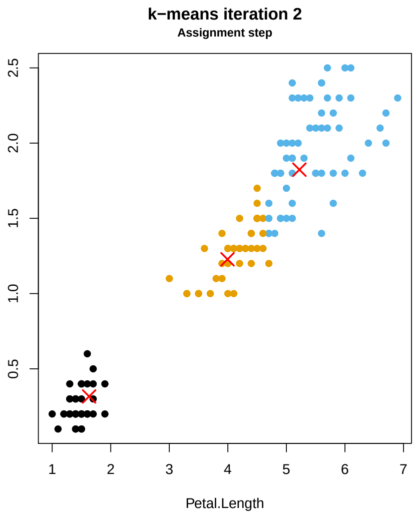


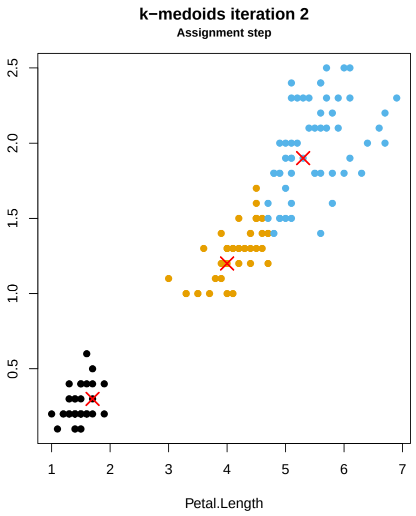
K-MEANS VS. *K*-MEDOIDS



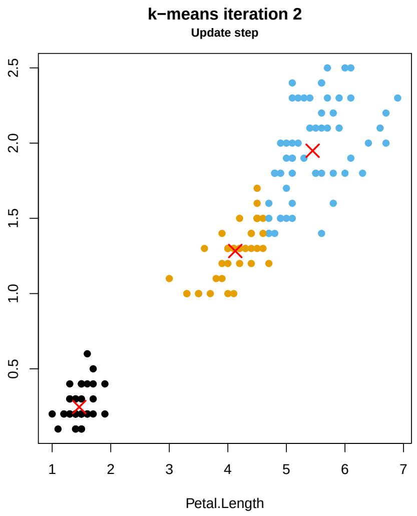


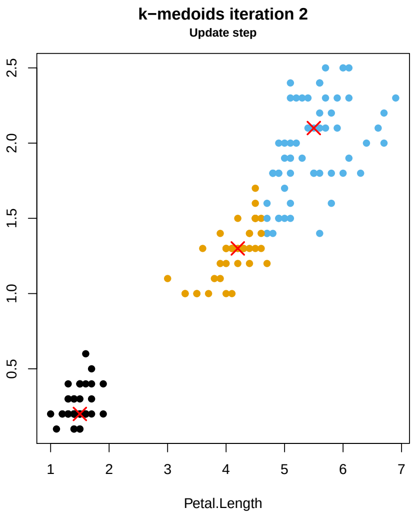
K-MEANS VS. *K*-MEDOIDS





K-MEANS VS. *K*-MEDOIDS





SUMMARY

- Minimizing the *within-cluster variation* exactly is not feasible and can be approximated by the k-means algorithm.
- k-means always converges, however, the cluster assignments strongly depend on the initial centers.
  $\rightarrow$ repeat it several times with different initial centers.
- A simple solution for choosing the number of clusters k is to plot the *within-cluster variation* for several k and look for an *"elbow"* which is a good guess for k.