No laptops, no phones, no problems

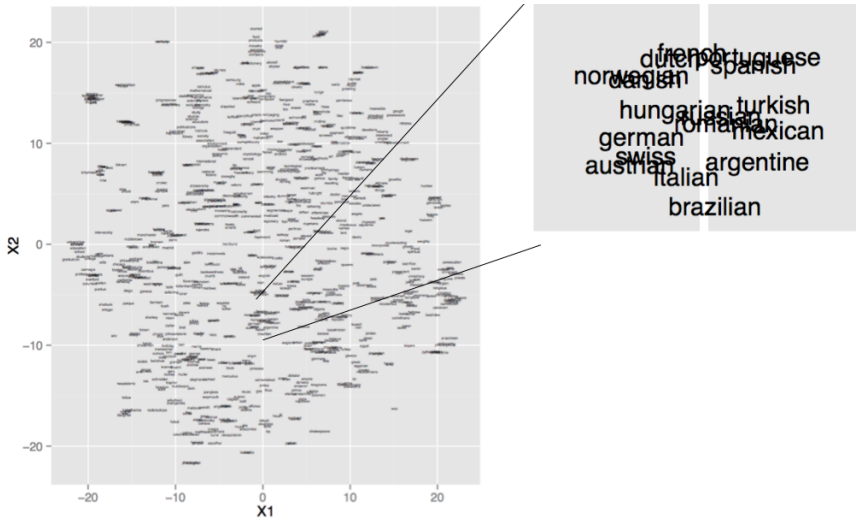
Multitasking senkt Lerneffizienz:

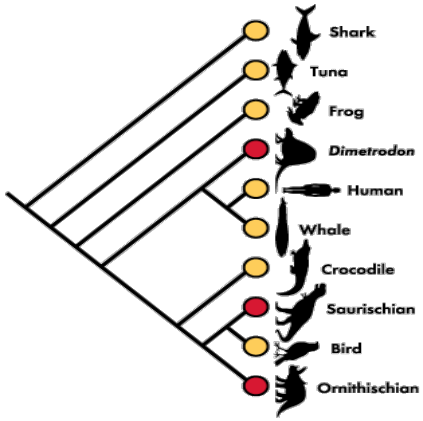
- **Keine Laptops im Theorie-Unterricht Deckel zu oder fast zu (Sleep modus)**

Overview of the semester

Part I (Unsupervised Learning)

- Dimension Reduction
  - PCA
- Similarities, Distance between objects
  - Euclidian, L-Norms, Gower,…
- Visualizing Similarities (in 2D)
  - MDS, t-SNE
- Clustering
  - K-Means
  - Hierarchical Clustering



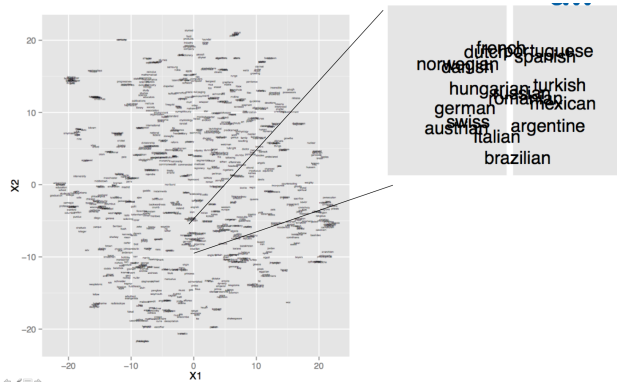


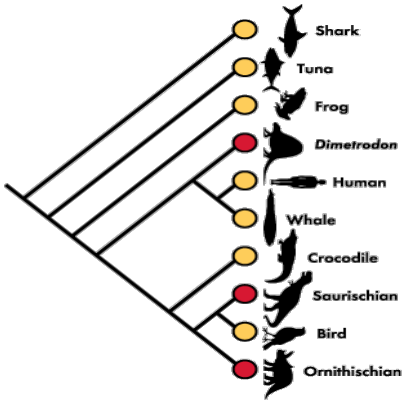
Part II (Supervised Learning)

- …

Overview: Unsupervised learning

- Methods to visualize Data (dimension reduction in metric spaces)
  - PCA
- Distances
  - **Definition of distances**
  - **Euclidean and Minkowski Distance**
  - Binary Data
  - Categorical Data
  - Mixed data types
- Methods to visualize distance (in 2D)
  - Multidimensional Scaling (MDS)
  - Linear Metric MDS
  - Non-Linear Metric MDS
  - isoMDS
  - t-SNE
- Clustering approaches
  - Grouping of data
- Skript Andreas Ruckstuhl





Dissimilarities for Categorical and Mixed Data

Similarity measures between binary vectors

$$o_1 = (o_{11}, o_{12}, ..., o_{1p}) \text{ and } o_2 = (o_{21}, o_{22}, ..., o_{2p})$$

Common situation is that objects, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$, have only binary attributes, like for example gender (f/M), driving license (yes/no), Nobel price holder (yes/no). We code them with 0 and 1.

We distinguish between symmetric and asymmetric binary variables.

In symmetric binary variable both levels have roughly comparable frequencies
example: gender

In asymmetric binary variable both levels have very different frequencies
many 0s few 1s.

Example: Nobel price holder = 1. It's nothing discriminative to be not a noble price winner. Therefore 0 don't count.

Matching Coefficient
Similarity measures for "symmetric" binary vectors

$$o_1 = (o_{11}, o_{12}, ..., o_{1p}) \text{ and } o_2 = (o_{21}, o_{22}, ..., o_{2p})$$

The objects, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$, have only binary attributes

Compute for the symmetric binary variable (could be only a subset of the p binary variables) the **S**imple **M**atching **C**oefficients:

SMC = # matches / # attributes

Corresponding to the proportion of matching features over **all** features

$$\mathbf{SMC = (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00})}$$

M_{01} = the number of attributes where o_{1i} was 0 and o_{2i} was 1
M_{10} = the number of attributes where o_{1i} was 1 and o_{2i} was 0
M_{00} = the number of attributes where o_{1i} was 0 and o_{2i} was 0
M_{11} = the number of attributes where o_{1i} was 1 and o_{2i} was 1

1 – SMC is a distance

Matching Coefficient
Similarity measures for "asymmetric" binary vectors

$$o_1 = (o_{11}, o_{12}, ..., o_{1p}) \text{ and } o_2 = (o_{21}, o_{22}, ..., o_{2p})$$

The objects, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$, have only binary attributes

Compute for the asymmetric binary variable (could be only a subset of the p binary variables) the Jaccard Coefficient:

J = # both-1-matches / # of not-both-zero attributes values

Corresponding to the proportion of matching features over **those** features which are 1 in at least one of both observations. "0's don't count'

$$J = (M_{11}) / (M_{01} + M_{10} + M_{11})$$

M_{01} = the number of attributes where o_{1i} was 0 and o_{2i} was 1
M_{10} = the number of attributes where o_{1i} was 1 and o_{2i} was 0
M_{11} = the number of attributes where o_{1i} was 1 and o_{2i} was 1

1 – J is a distance (Jaccard Distance)

Example: How similar are two given binary vectors?

p = 1 0 0 0 0 0 0 0 0 0

q = 0 0 0 0 0 0 1 0 0 1

M_{01} = 2 (the number of attributes where p was 0 and q was 1)
M_{10} = 1 (the number of attributes where p was 1 and q was 0)
M_{00} = 7 (the number of attributes where p was 0 and q was 0)
M_{11} = 0 (the number of attributes where p was 1 and q was 1)

$$SMC = (M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00})$$

$$SMC = (M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00}) = (0+7) / (2+1+0+7) = 0.7$$

$$J = (M_{11}) / (M_{01} + M_{10} + M_{11})$$

$$J = (M_{11}) / (M_{01} + M_{10} + M_{11}) = 0 / (2 + 1 + 0) = 0$$

More than 2 levels (Nominal Data)

- Simple matching coefficient
- mm: Number of variables in which object i and j mismatch
- p number of mismatch

$$d(i,j) = \frac{mm}{p}$$

Proportion of variables, in which people disagree

- Character strings can be understood as nominal data.
- Also called Hamming-Distance if with strings of same length (sometimes w/ o dividing by p)
- What is the Hamming-Distance between:
  - `HOUSE`
  - `MOUSE`

Gower's dissimilarity for mixed data types

Idea: Use distance measure d_{ij} between 0 and 1 for each variable or feature:

- k_{th} variable is binary, nominal: Use discussed methods, e.g.

$$d_{ij}^{(k)} = \frac{M_{11} + M_{00}}{M_{01} + M_{10} + M_{11} + M_{00}}$$

- k_{th} variable is numeric:

  x_{ik}: Value for object i in variable k
  R_k: Range of variable k for all objects

$$d_{ij}^{(k)} = \frac{|x_{ik} - x_{jk}|}{R_k}$$

- Ordinal: Use ranks, then same like with numeric variables

Aggregate distance measures over all variables/feature/dimensions:

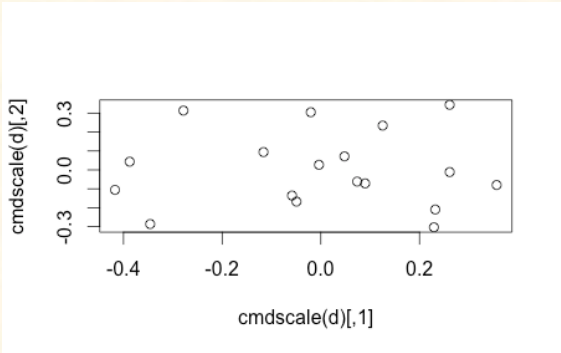
$$d_{ij} = \frac{1}{p} \sum_{k=1}^{p} d_{ij}^{(k)}$$

Dissimilarity for mixed data types with R-function "daisy" calculating Gower's dissimilarity

```
> str(flower)
'data.frame':  18 obs. of  8 variables:
 $ V1: Factor w/ 2 levels "0","1": 1 2 1 1 1 1 1 1 2 2 ...
 $ V2: Factor w/ 2 levels "0","1": 2 1 2 1 2 2 1 1 2 2 ...
 $ V3: Factor w/ 2 levels "0","1": 2 1 1 2 1 1 1 2 1 1 ...
 $ V4: Factor w/ 5 levels "1","2","3",..: 4 2 3 4 5 4 4 2 3 5 ...
 $ V5: Ord.factor w/ 3 levels "1"<"2"<"3": 3 1 3 2 2 3 3 2 1 2 ...
 $ V6: Ord.factor w/ 18 levels "1"<"2"<"3"<..: 15 3 1 16 2 12 ...
 $ V7: num  25 150 150 125 20 50 40 100 25 100 ...
 $ V8: num  15 50 50 50 15 40 20 15 15 60 ...

> dist=daisy(flower, type=list(asymm=c(1, 3), symm=2, ordratio=7))
> str(dist)
Classes 'dissimilarity', 'dist'  atomic [1:153] 0.901 0.618 ...
  ..- attr(*, "Size")= int 18
  ..- attr(*, "Metric")= chr "mixed"
  ..- attr(*, "Types")= chr [1:8] "A" "S" "A" "N" ...

> plot(cmdscale(d))
```



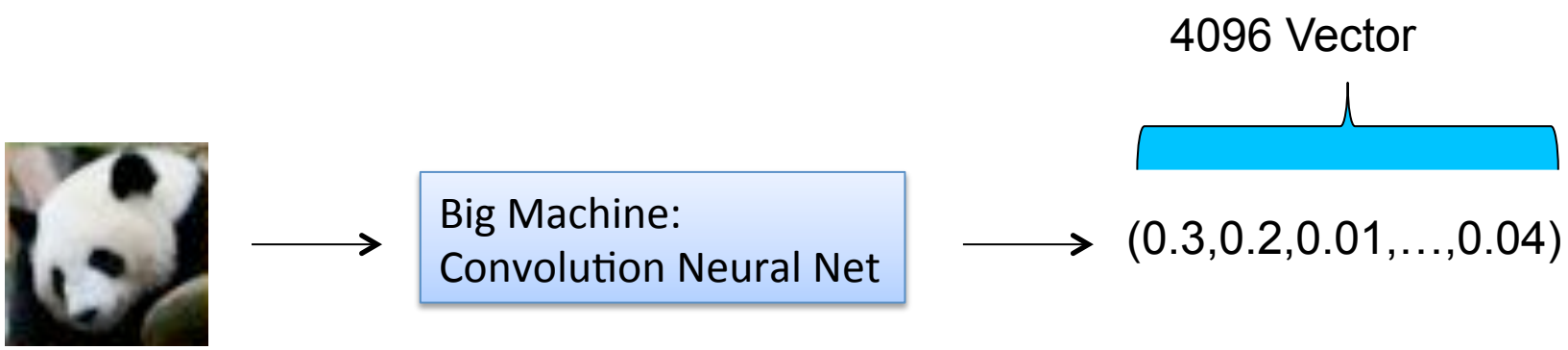
Special Distances

String Distances

- Package stringdist
  - Hamming Distance (see before)
    - Just count the number of mismatches
  - More distances
    - Longest common substring (Bioinformatic)
    - …
- Many distances used in bioinformatics comparing DNAs
- Or use embeddings like word2vec
  - String (complicated procedure) → 100 (or so) dimensional vector
  - Calculate Euclidean Distance

Distances between images [just for completeness]

- Dump approach use Euclidean distance between pixel values directly.
- Current state of the art, for image similarities: convolutional neural network

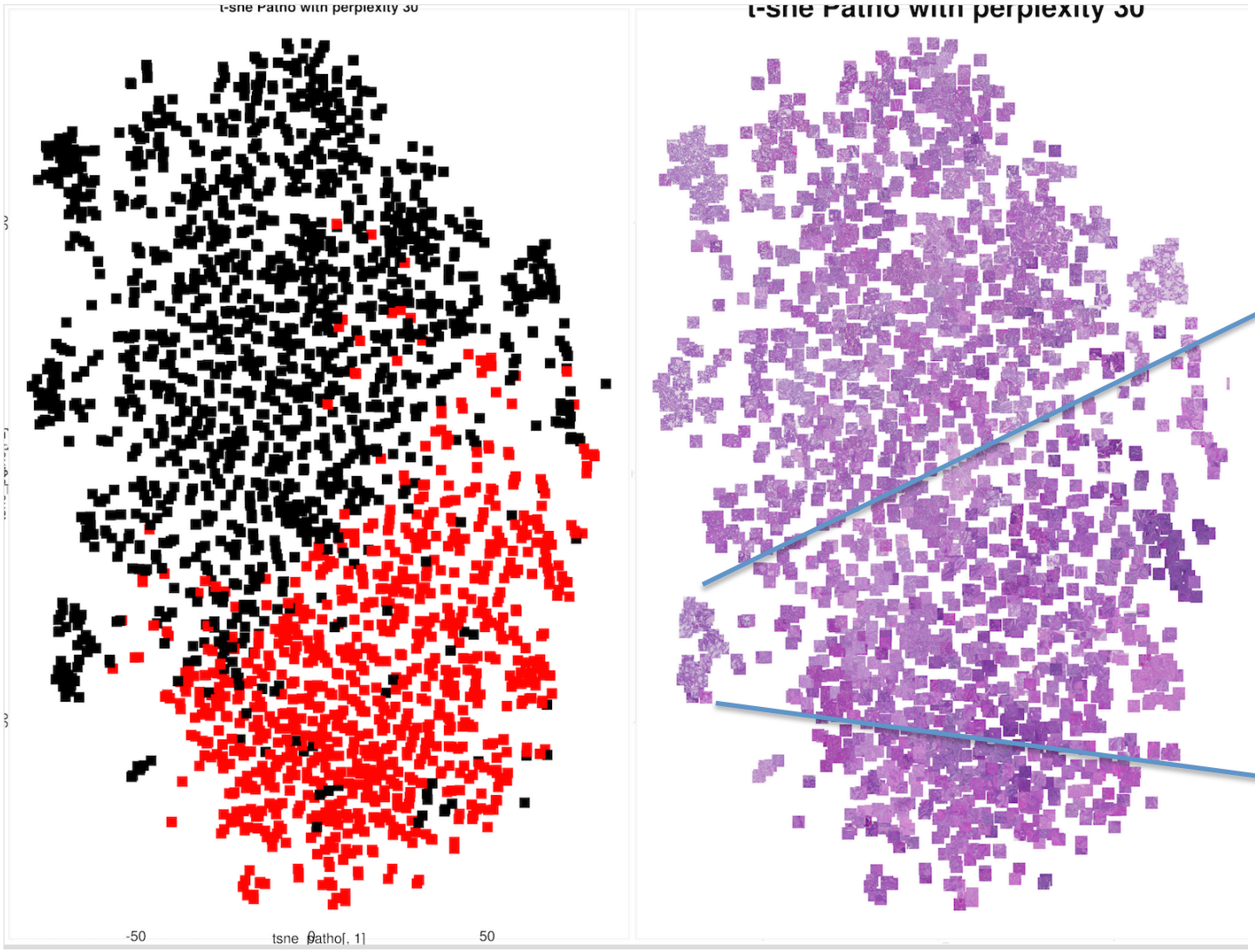


See: http://cs.stanford.edu/people/karpathy/cnnembed/

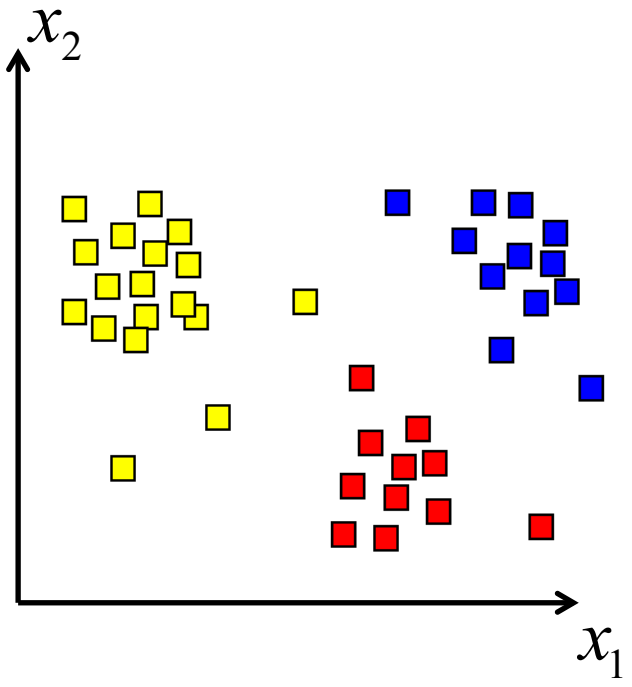
Semantic similarities not pixel wise!

See: http://cs.stanford.edu/people/karpathy/cnnembed/ for more images

Example Project with Uni-Spital ZH



Clustering



Now again in line with ILSR

- Inline again with ILSR
- See section 10.3 Clustering Methods in ILSR

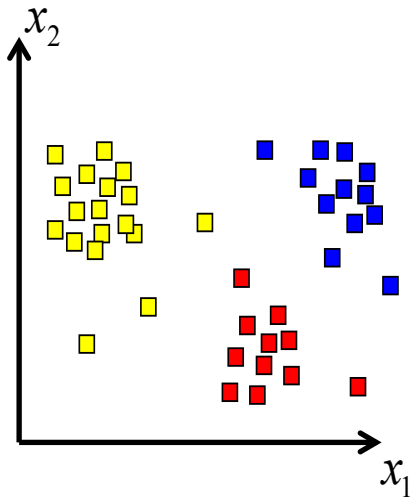
- Aims:
  - PCA (and other dimension reduction methods) look to find a low-dimensional representation of the observations
  - Clustering looks to find homogeneous subgroups among the observations.

- Examples of applications
  - Personalized medicine
    - Segment into subgroups needing different medication
  - Market segmentation
  - …

Descriptive and unsupervised: Cluster Analysis

Cluster analysis or clustering is the task of assigning a set of objects into groups.

Objects in the same cluster should be more similar to each other than to those in other clusters.



To perform clustering one must define a measure of similarity or distance based on the observed values describing different properties of the objects.

$$e.g.\ euclidean\ :\ dist(o_k, o_l) = \sum_{i=1}^{p} (x_{ki} - x_{li})^2$$

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

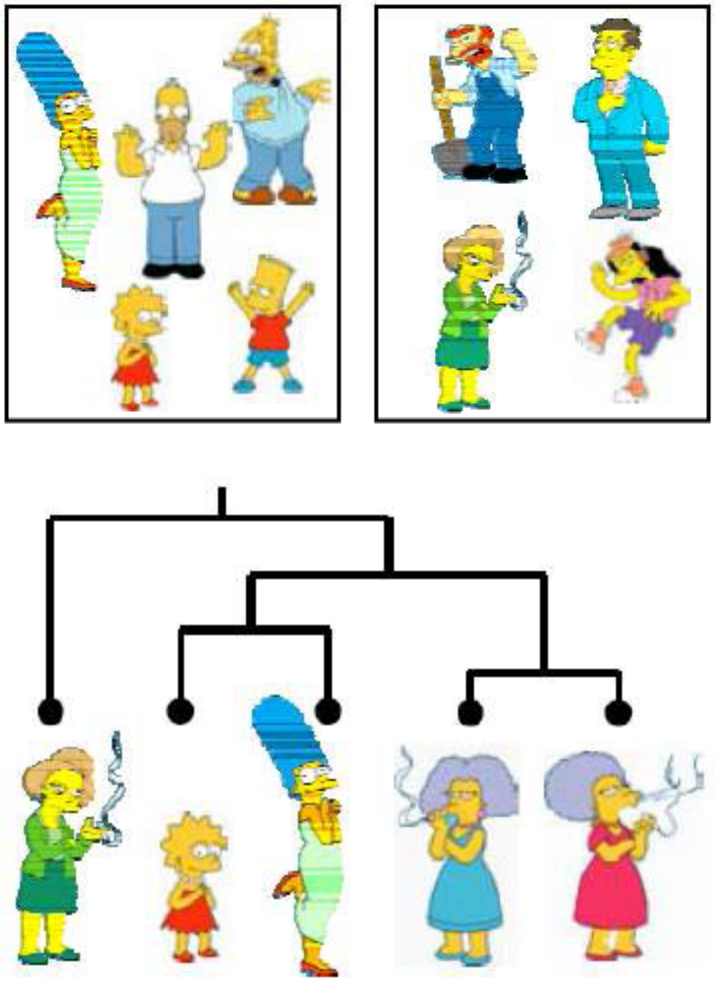
Four Clusters

Types of Clustering

- **Important distinction between hierarchical and partitional sets of clusters**
- **Partitional Clustering**

  A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- **Hierarchical clustering**

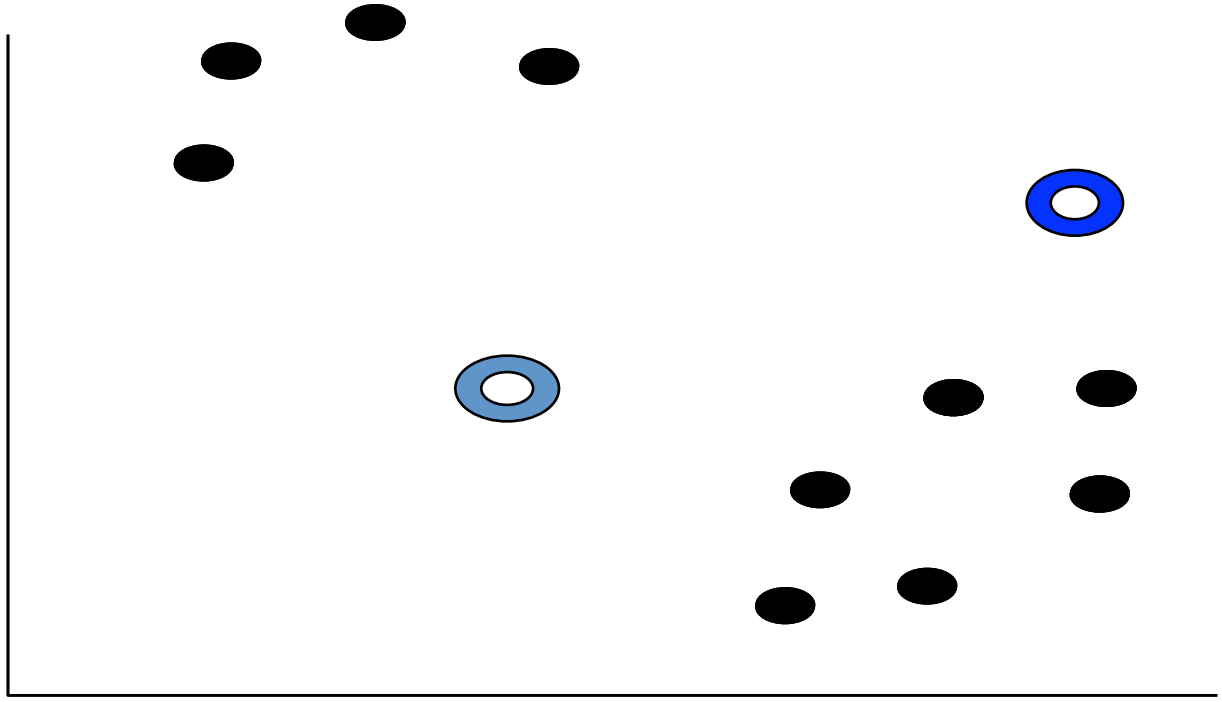
  A set of nested clusters organized as a hierarchical tree



Partitional Clustering

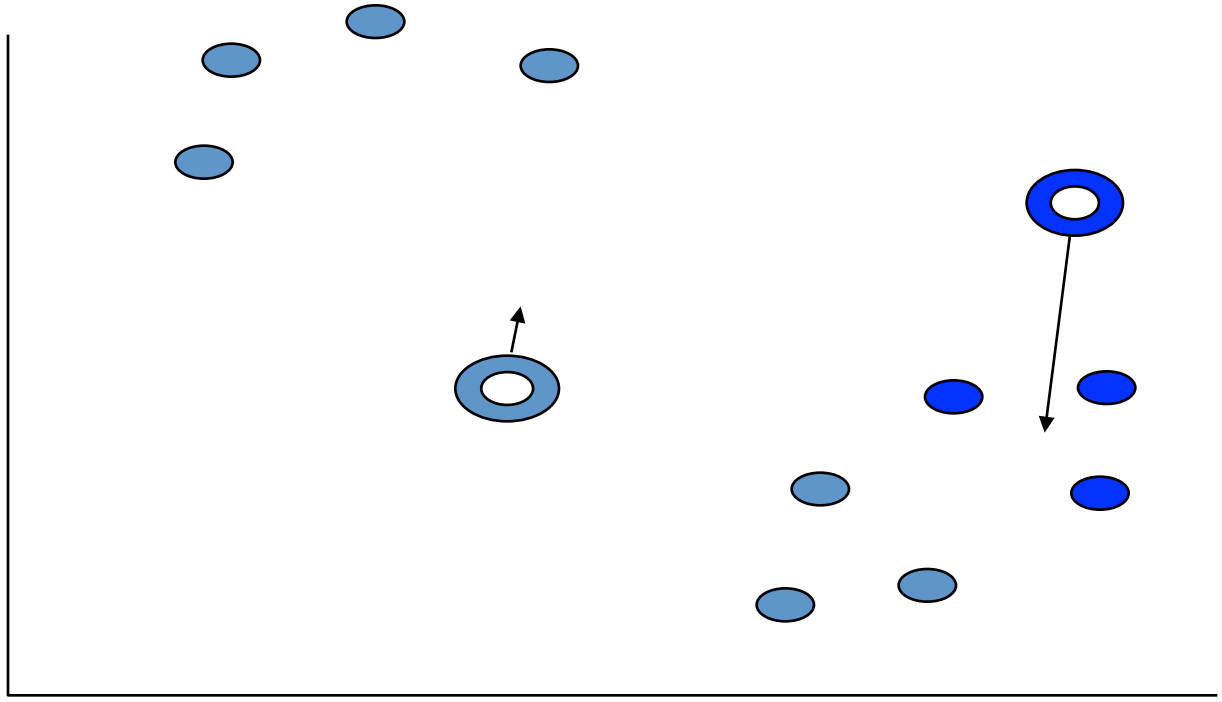
Partitioning Clustering: K-means

+ Given a number of objects and an initial (randomly choosen) set of cluster centers, assign each object to the closest cluster center



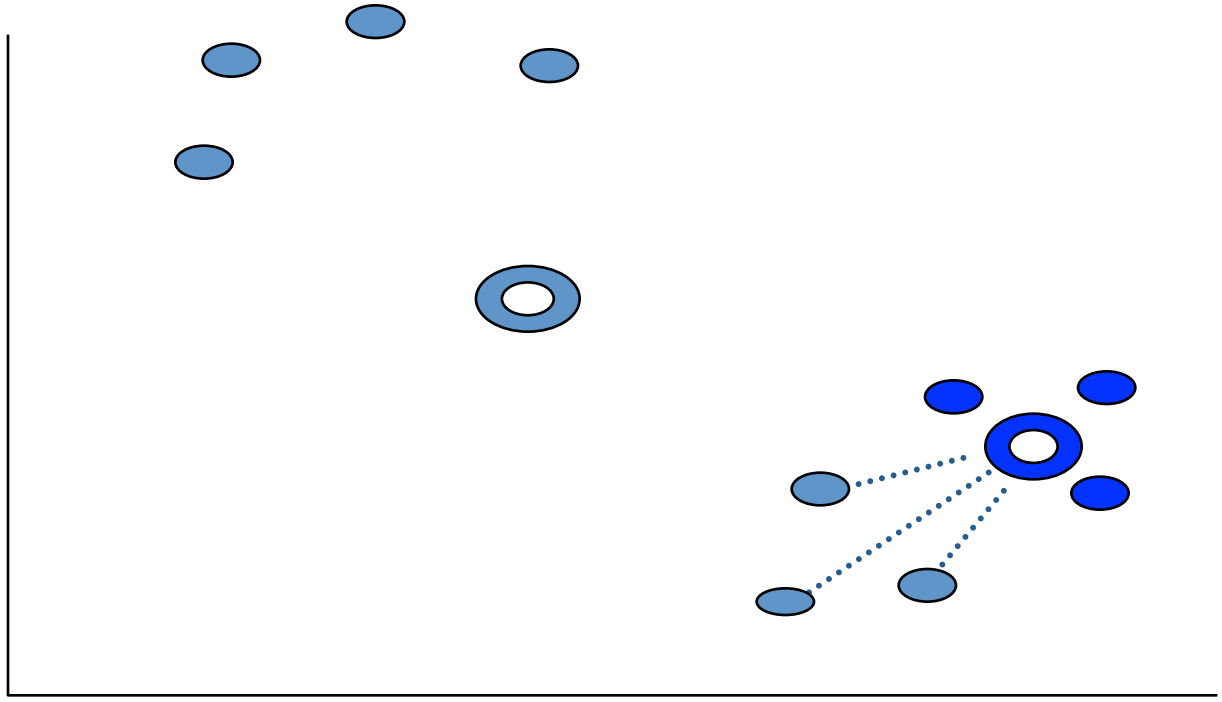
Partitioning Clustering: K-means

+ Update the coordinates of each cluster center to the average coordinate of the objects associated with it



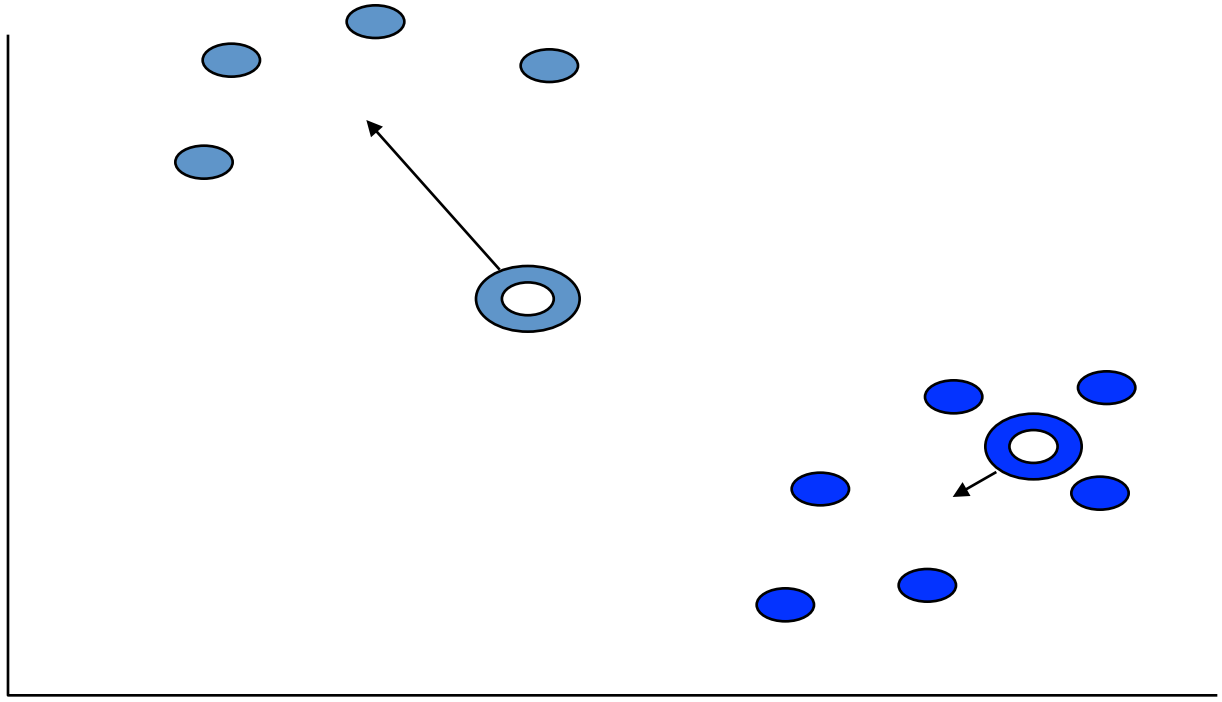
Partitioning Clustering: K-means

+ Re-assign each gene to the closest cluster centre



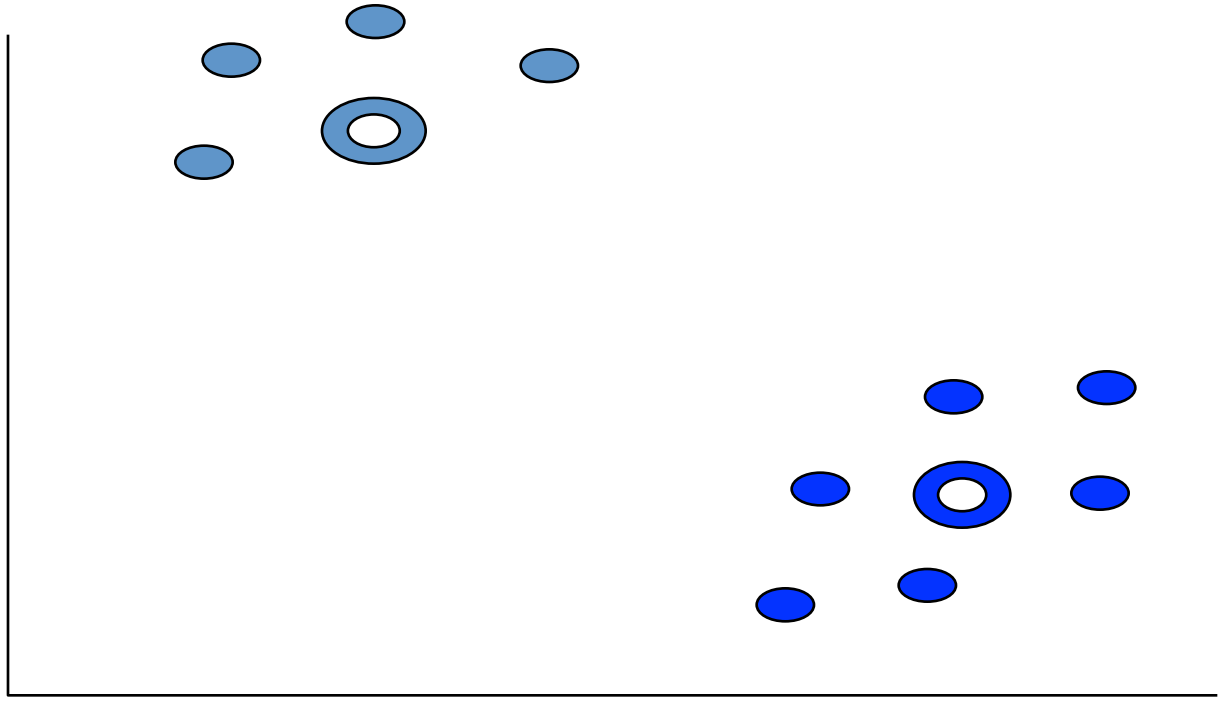
Partitioning Clustering: K-means

+ Recalculate the co-ordinates of each cluster centre according to the average co-ordinate of the genes associated with it



Partitioning Clustering: K-means

+ Repeat these steps until no reassignment is possible (or maximal number of iterations have been reached).



What is optimized in K-means Clustering ?

The goal in k-means is to partition the observations into K clusters such that the total within-cluster variation (WCV), summed over all K clusters C_k, is as small as possible.

$$\underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \text{WCV}(C_k) \right\}$$

WCV is often based on Euclidian distances

Squared Euclidian distance between data points i and i'

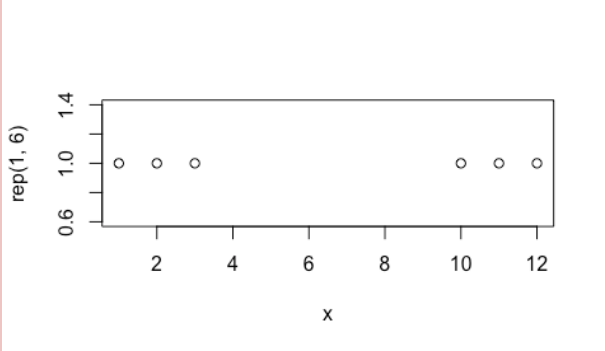
$$\text{WCV}(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

where $|C_k|$ denotes the number of observations in the kth cluster and p is the number of variables (dimensions).

Clustern von Hand

Find a senseful k=2 clustering for the data-points

x = c(1,2,3,10,11,12)

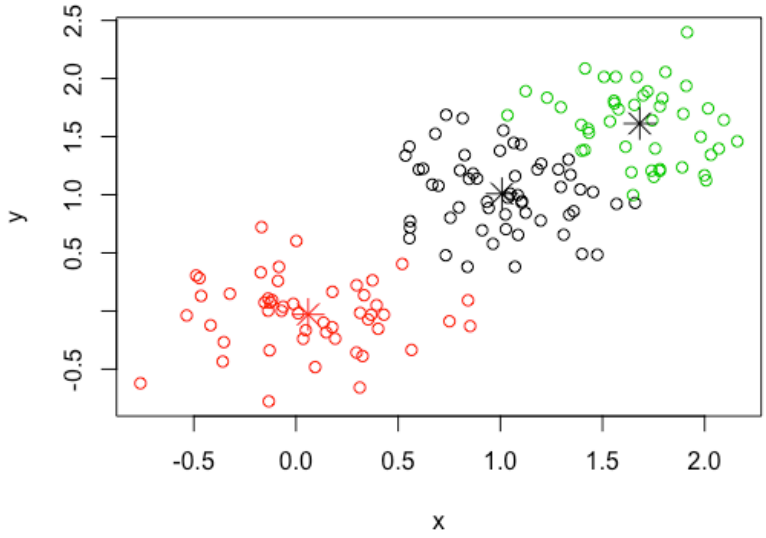


And calculate the within cluster variations

$$\mathrm{WCV}(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

K-means clustering in R

```
x <- rbind(matrix(rnorm(100, sd = 0.3), ncol = 2),
           matrix(rnorm(100, mean = 1, sd = 0.3), ncol = 2),
           matrix(rnorm(100, mean = 1.6, sd = 0.3), ncol = 2)
           )
colnames(x) <- c("x", "y")
(cl <- kmeans(x, 3))
plot(x, col = cl$cluster)
points(cl$centers, col = 1:2, pch = 8, cex = 2)
```



K-Means

- The k-means algorithm (see also animation) is a optimization of the total within cluster variation.

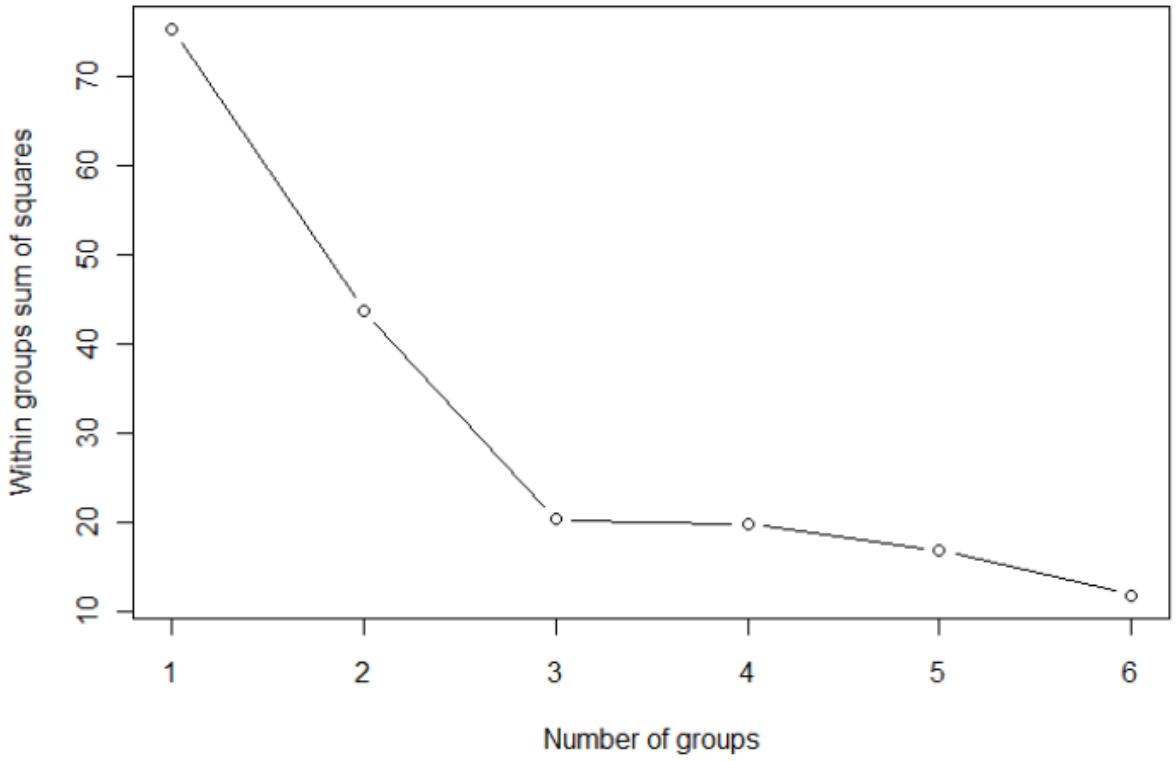
Algorithm 10.1 *K-Means Clustering*

1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
2. Iterate until the cluster assignments stop changing:
   (a) For each of the K clusters, compute the cluster *centroid*. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
   (b) Assign each observation to the cluster whose centroid is closest (where *closest* is defined using Euclidean distance).

- **Can be trapped in a local minima**, not a global optimization of WCV

How to choose the "best" number of clusters in K-means ?

- Run k-Means for several k - number of groups
- Determine minimized sum of WCV `sum(kmeans(dat, centers=k)$withinss)`
- Plot minimized sum of WCV vs. number of groups (k)
- Choose number of groups after the last big drop of



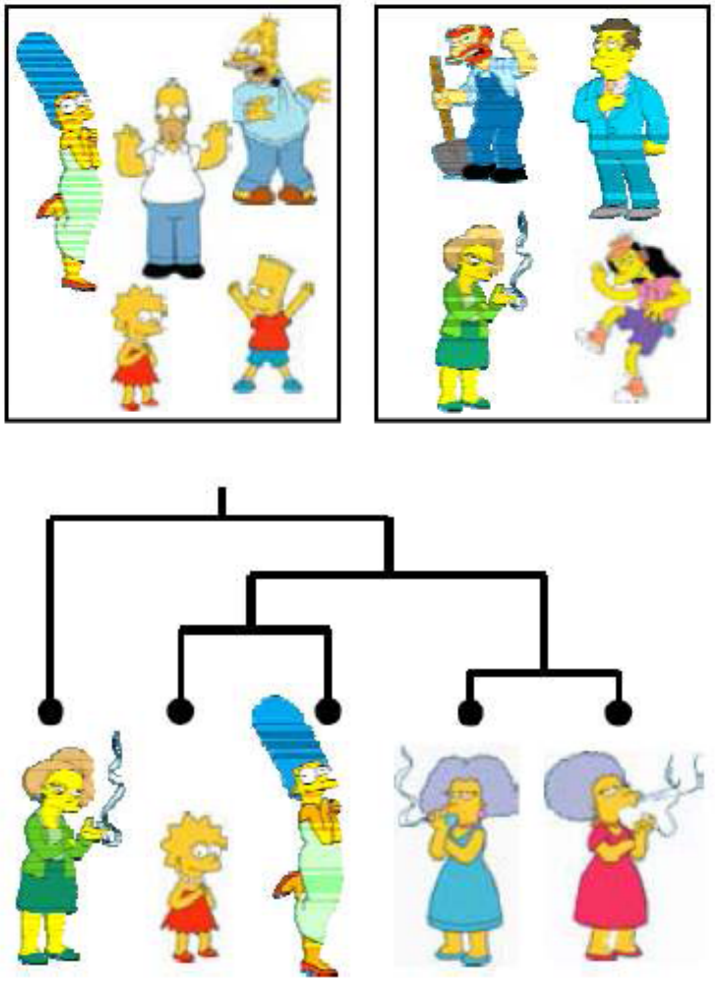
Hierarchical Clustering

Types of Clustering

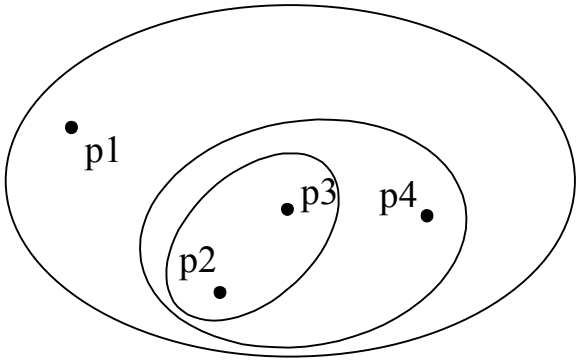
- **Important distinction between hierarchical and partitional sets of clusters**
- **Partitional Clustering**

  A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- **Hierarchical clustering**

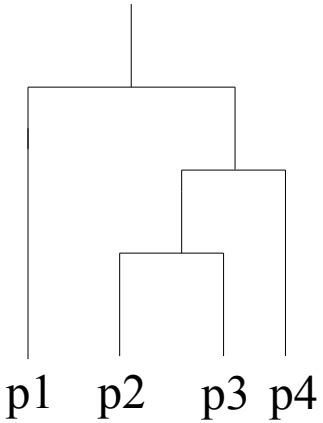
  A set of nested clusters organized as a hierarchical tree



Hierarchical Clustering



Hierarchical Clustering



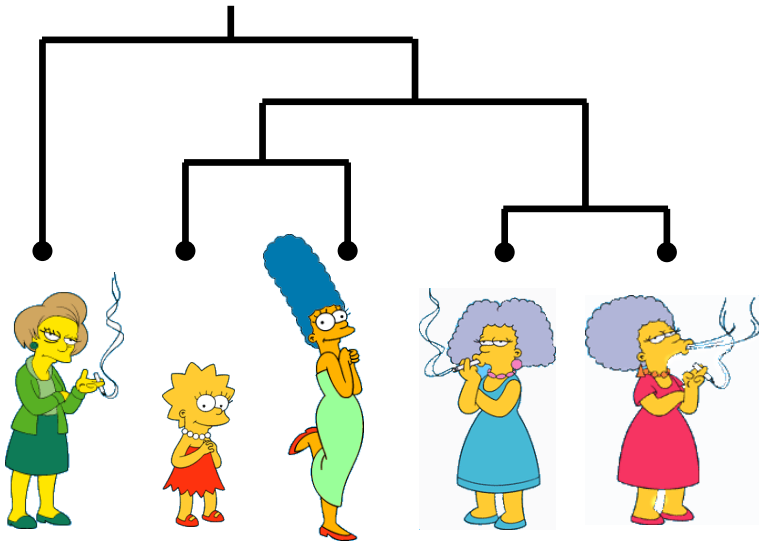
Dendrogram

- Wird der Baum von “unten nach oben” aufgebaut: agglomerativ.
- Von oben nach unten “divisive”

How to do hierarchical Clustering?

Without proof: The number of dendrograms with n leafs:
$= (2n-3)!/[(2^{(n-2)})\,(n-2)!]$

Number of Leafs	Number of Possible Dendrograms
2	1
3	3
4	15
5	105
...	…
10	34,459,425



Since we cannot test all possible dendrograms we will have to heuristic search of all possible dendrograms. We could do this..

Bottom-Up (agglomerative):
Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

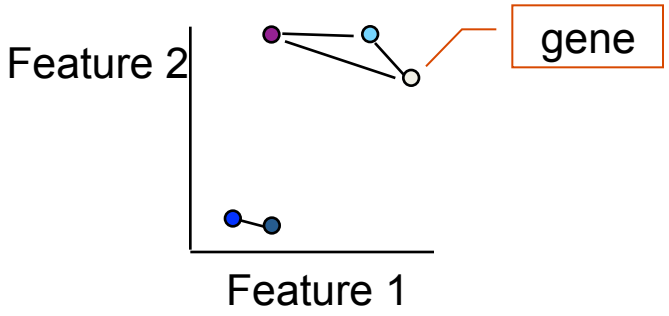
Top-Down (divisive):
Starting with all the data in a single cluster, consider every possible way to divide the cluster into two. Choose the best division and recursively operate on both sides.

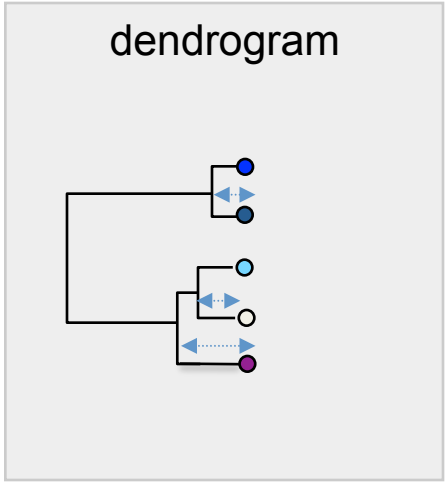
Dissimilarity between samples or observations

Any dissimilarity we have seen before can be used

- euclidean
- manhattan
- simple matching coefficent
- Jaccard dissimilarity
- Gower's dissimilarity
- etc.

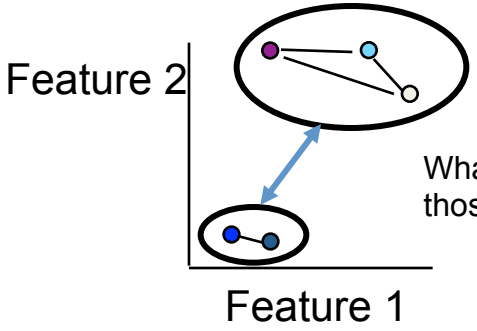
Aglomatrative Hierarchical Clustering





Problem:

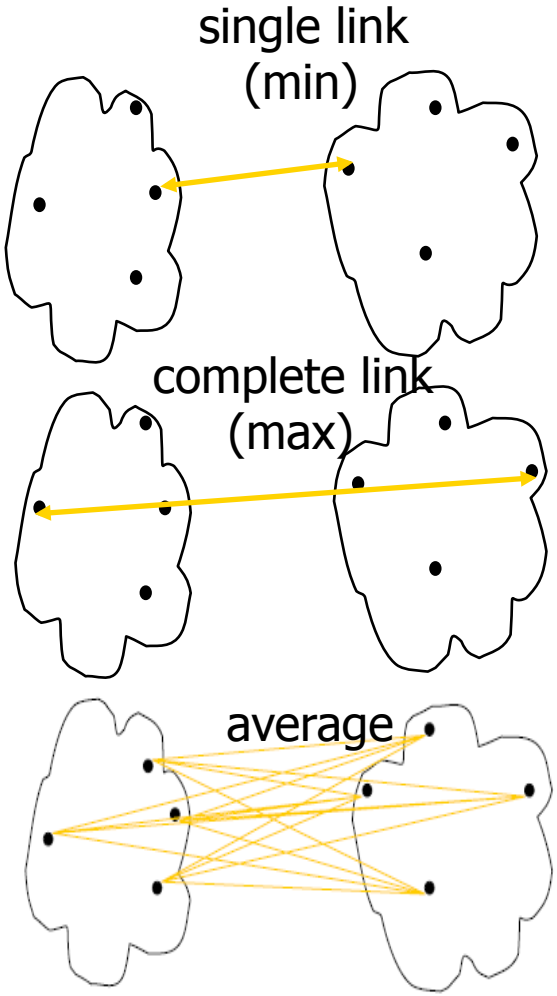
Need a generalization of the distance between the objects to compound of objects.

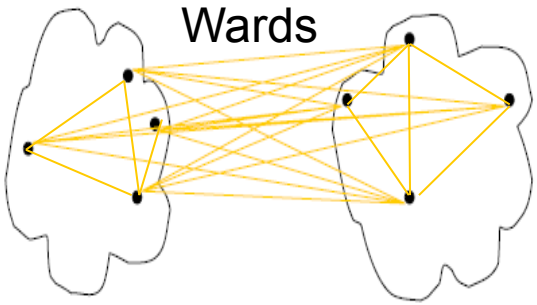


What is the distance between those objects. -> **Linkage**

Dissimilarity between clusters: Linkages

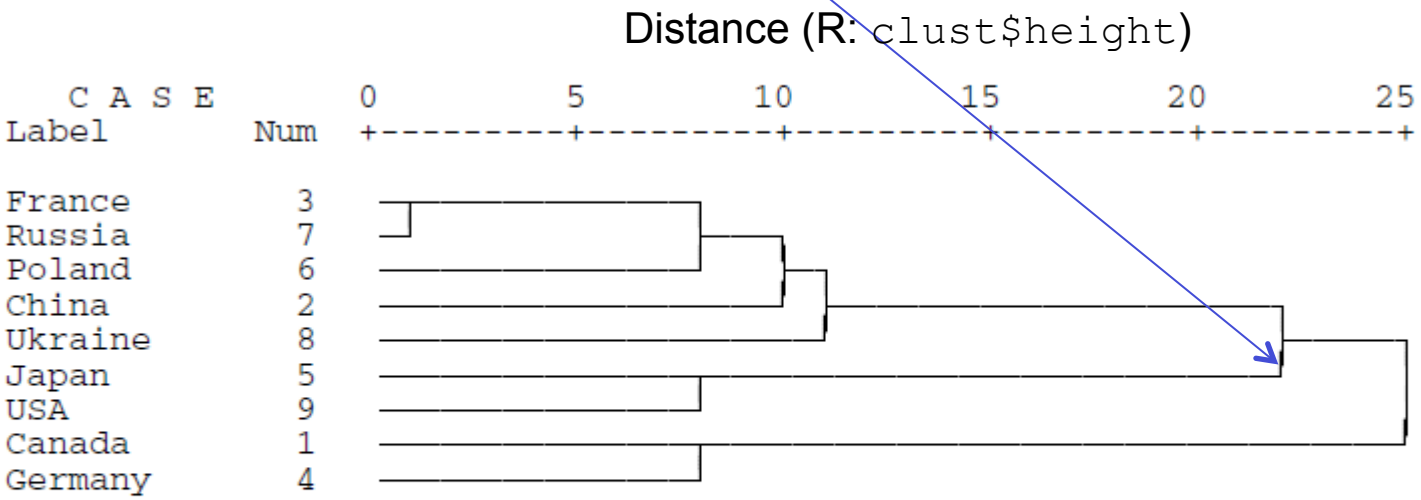
- Single link: smallest distance between point-pairs linking both clusters
- Complete link: largest distance
- Average: avg distance between
- Wards: In this method, we try to minimize the variance of the merged clusters





How to read a dendrogram

The position of the join node on the distance-scale indicates the distance between clusters (this distance depends on the linkage method). For example, if you see two clusters merged at a height 22, it means that the distance between those clusters was 22 .



When you read a dendrogram, you want to determine at what stage the distance between clusters that are combined is large.
You look for large distances between sequential join nodes (here vertical lines).

Simple example

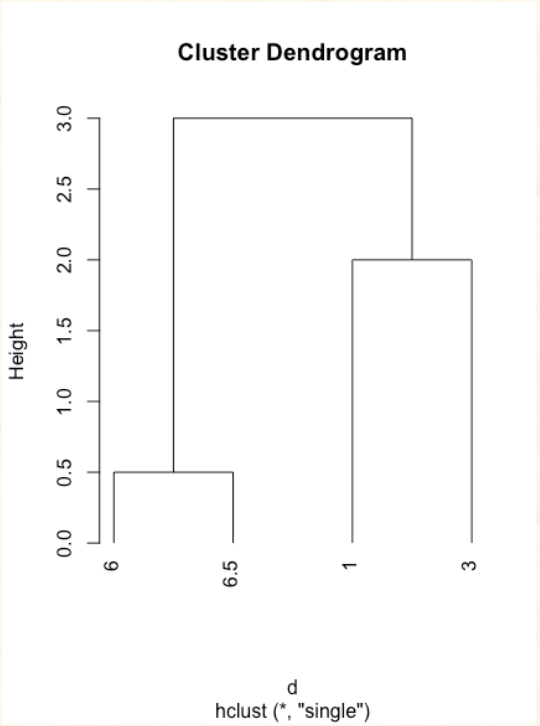
Zeichnen sie das Dendrogram für die eindimensionale Datenmatrix

feature
1
3
6
6.5

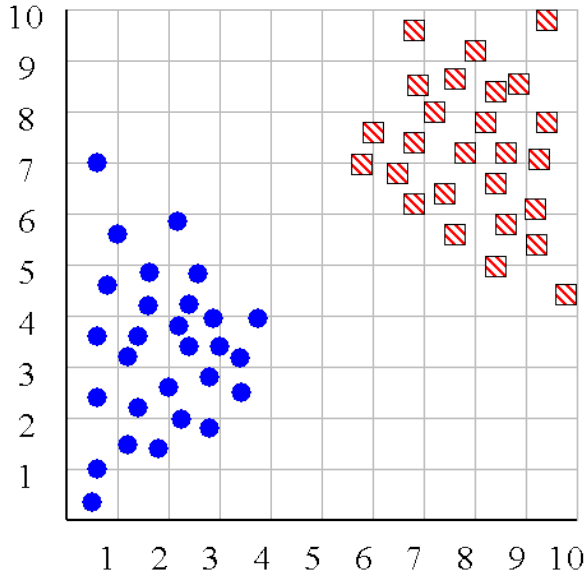
Verwenden Sie dazu die Euklidische Distanzen und die single-linkage

Simple example

```
x = c(1,3,6,6.5)
names(x) = c('1','3','6', '6.5')
d = dist(x)
cluster = hclust(d, method = 'single')
plot(cluster, hang=-10, axes = FALSE)
axis(2)
```

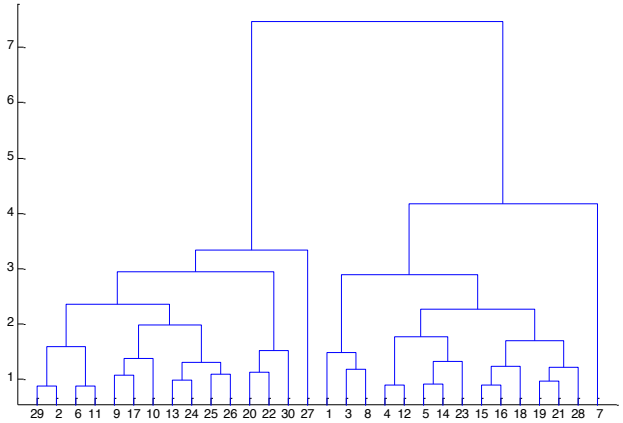


Compare linkage methods

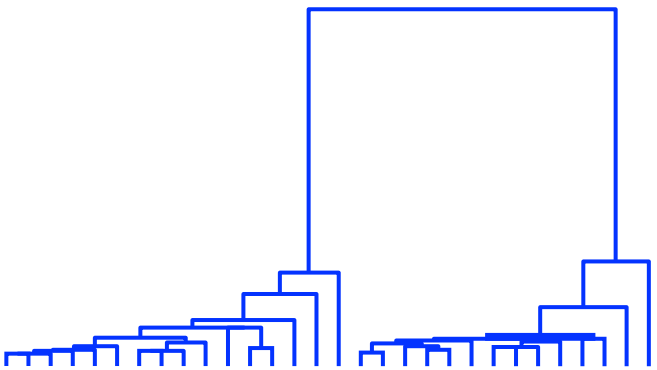


- Single-Linkage produce long and skinny clusters.
- Wards produce of ten very separated clusters
- Average linkage yield more round clusters

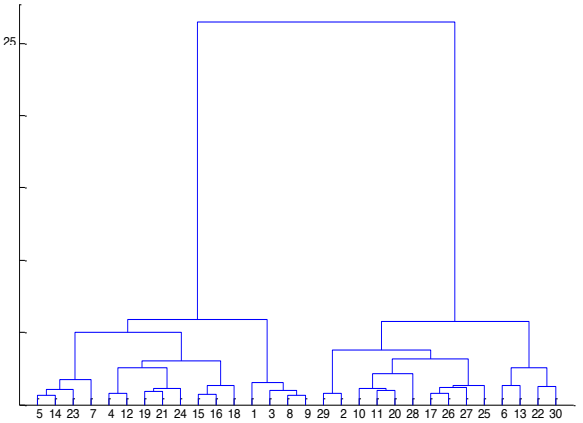
•Generally clustering is an exploratory tool.
Use the linkage which produces the “best” results.



Average linkage



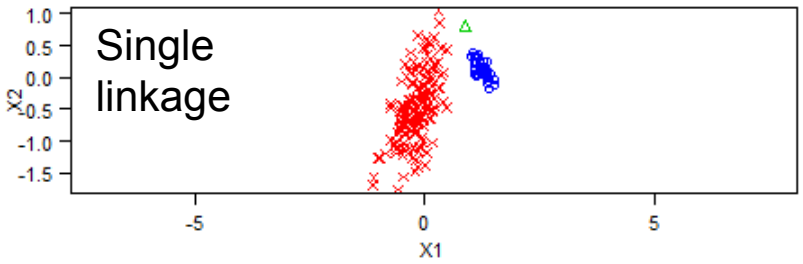
Single linkage

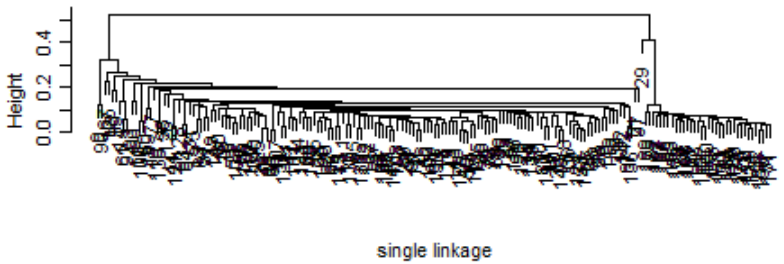


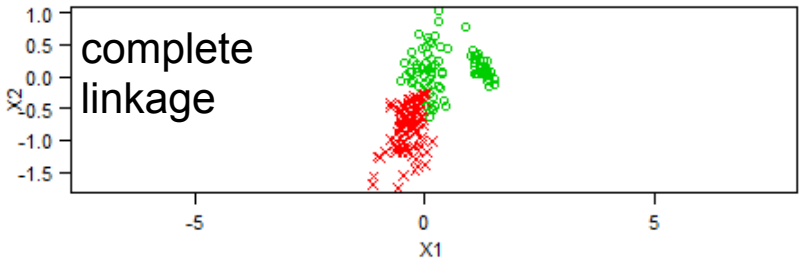
Wards linkage

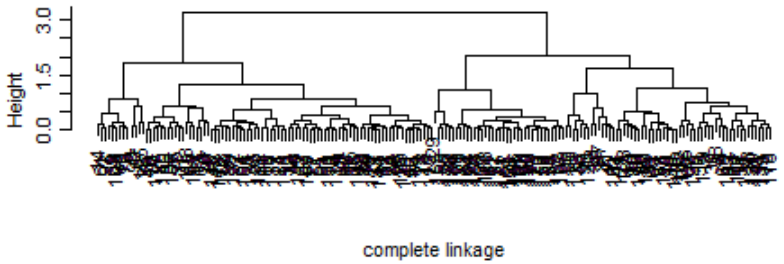
Cluster result depend on data structure, distances and linkage methods

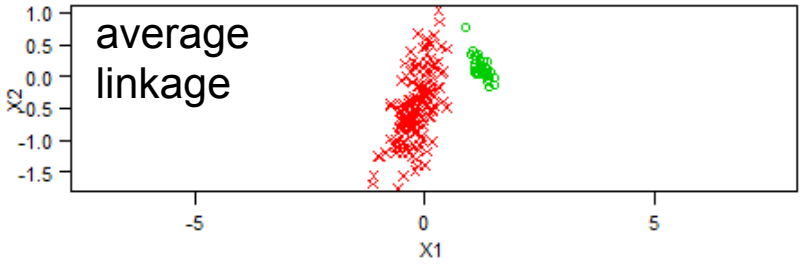
Data: we simulated 2 2D-Gaussian Clusters with very different sizes

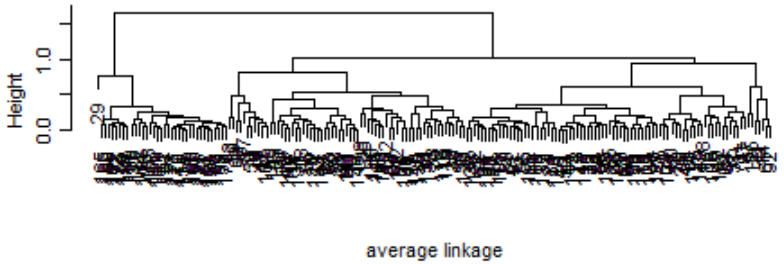


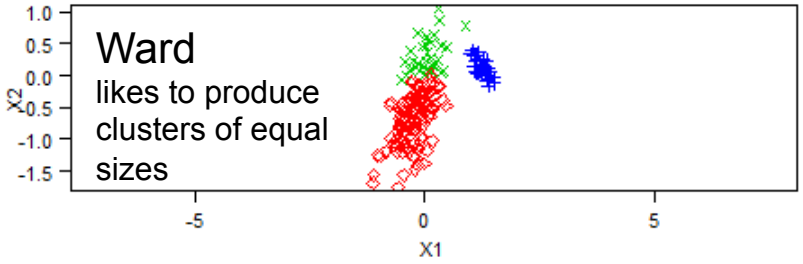


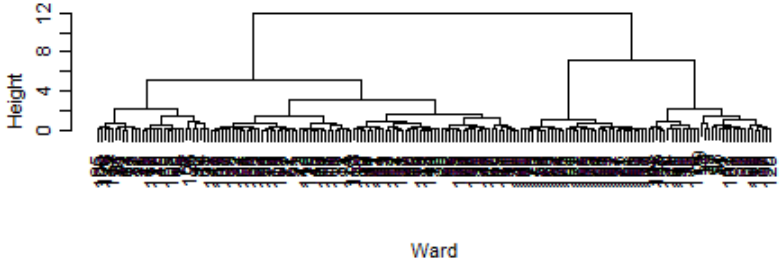












Heatmaps