Hierarchical agglomerative
Cluster Analysis

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Classification

- Basic (unconscious & conscious) human strategy to reduce complexity
- *Always* biased
  - ➢ Cluster analysis
    - to find or confirm types in data
    - to uncover relations between objects
    - The more entities and the more attributes – the more difficulties classifying them manually
      - ➢ Computer-based cluster analysis

Cluster analysis – overview

- Selection of objects to be classified
- Selection of relevant attributes of these objects
- Calculation of distances between objects
- Cluster analysis
- Check of results
- (Modifications + rerun analyis)

Objects

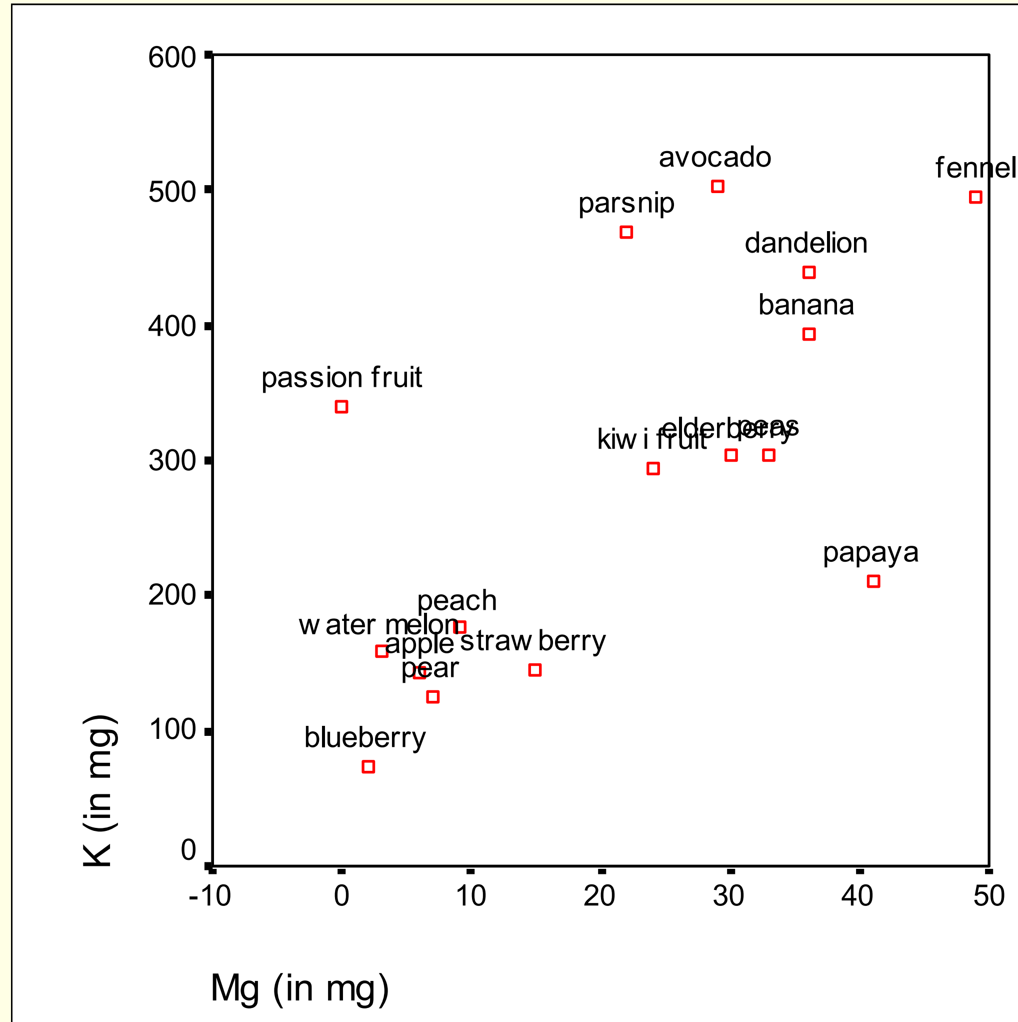
- Selection of objects depends on intention
- If clusters are expected:
  - Number of objects should be balanced
- Many objects = large distance matrix
  - $\frac{n \times (n-1)}{2}$ values (e.g. 200 objects = 19900 distance values)

Attributes

- Selection of attributes depends on intention
- *Not:* The more attributes the surer groups will appear
- Avoid correlations between attributes
- Values of attributes have to be comparable
- Treat missing values
- (Weight attributes to influence clustering)

Attributes – example

Position of selected fruits/vegetables in the 2 dimensions magnesium & potassium



Distance measures

- Based on the attribute values the distances between the objects have to be determined.
- Distance measures have to ensure:
  - Symmetry $d(x,y) = d(y,x) \geq 0$
  - Triangle inequality $d(x,y) \leq d(x,z) + d(y,z)$
  - Distinguishability of nonidenticals $if\ d(x,y) \neq 0,\ then\ x \neq y$
  - Indistinguishability of identicals $d(x,x') = 0$

Distance measures – examples

- Distance measures
  - (squared) Euclidian distance

$$\delta(X,Y) = \sqrt{\sum_{i=1}^{n}(X_i - Y_i)^2}$$

  - Manhattan distance

$$\delta(X,Y) = \sum_{i=1}^{n}|X_i - Y_i|$$

- Similarity measures
  - ➢ Pearson‘s correlation coefficient

$$r(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \overline{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \overline{Y})^2}}$$

Squared Euclidian distance – example

Distances of selected fruits/vegetables based on (standardized) content of Mg & K

Proximity Matrix

	Squared Euclidean Distance			
Case	1:banana	2:avocado	3:parsnip	4:dandelion
1:banana	,000	1,250	1,477	,183
2:avocado	1,250	,000	,346	,578
3:parsnip	1,477	,346	,000	1,070
4:dandelion	,183	,578	1,070	,000

This is a dissimilarity matrix

Cluster analysis

- Here discussed (because most common):
  - **S**equential **A**gglomerative **H**ierarchical **N**onoverlapping (SAHN)

- Other approaches for clustering:
  - Hierarchic divisive
  - Iterative partitioning
  - Factor analytic
  - Clumping
  - ...

Cluster analysis

- Iterative process
- n – 1 steps necessary to cluster all objects
- At every step the two most similar objects or clusters will be merged until all are aggregated in one cluster

Cluster analysis – example

	banana	avocado	parsnip	dandelion
banana		1.25	1.477	0.183
avocado			0.346	0.578
parsnip				1.07
dandelion				

$$d_{avocado[banana,dandelion]} = \frac{d_{avocado,banana}}{2} + \frac{d_{avocado,dandelion}}{2}$$

$$d_{avocado[banana,dandelion]} = \frac{1.25}{2} + \frac{0.578}{2} = 0.914$$

Cluster analysis – example

	banana-dandelion	avocado	parsnip
banana-dandelion		0.914	1.2735
avocado			0.346
parsnip			

	banana-dandelion	avocado-parsnip
banana-dandelion		1.09375
avocado-parsnip		

$$d_{[banana,dandelion][avocado,parsnip]} = \frac{d_{[banana,dandelion],avocado}}{2} + \frac{d_{[banana,dandelion],parsnip}}{2}$$

$$d_{[banana,dandelion][avocado,parsnip]} = \frac{0.914}{2} + \frac{1.2735}{2} = 1.09375$$

Matrix updating algorithms

- Several SAHN clustering algorithms
- They differ in how they calculate the distances of new formed clusters to the other elements.
- Not every algorithm equally suitable for every situation
  - ➢ **Results can be very different!!**

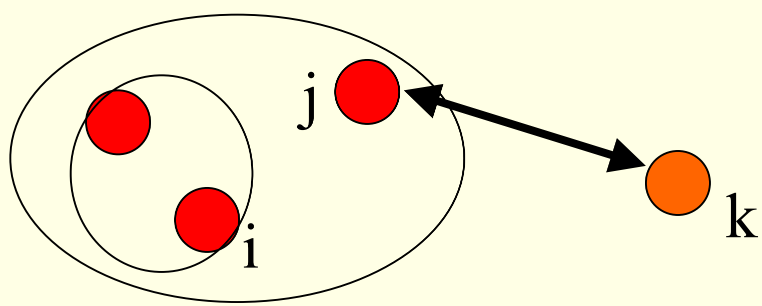
Matrix updating algorithms

- Single linkage
- Complete linkage
- Unweighted average linkage
- Weighted average linkage
- (Un)Weighted centroid linkage
- Ward‘s method

Single linkage

$$d_{k(ij)} = \min(d_{ki}, d_{kj})$$

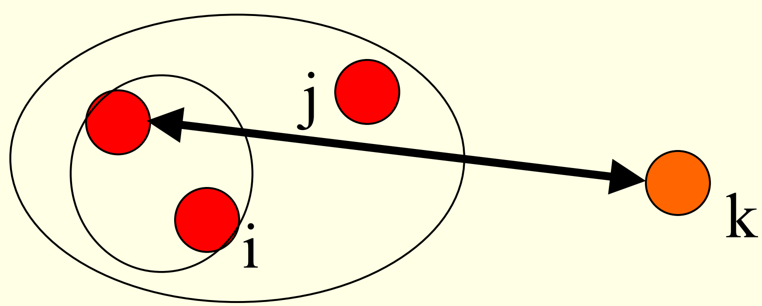
- Nearest neighbor
- Distance between new cluster and other elements equals the *smallest* in the cluster occurring distance to the other elements
- Tendency to very different sized clusters (outliers!)



Complete linkage

$$d_{k(ij)} = \max(d_{ki}, d_{kj})$$

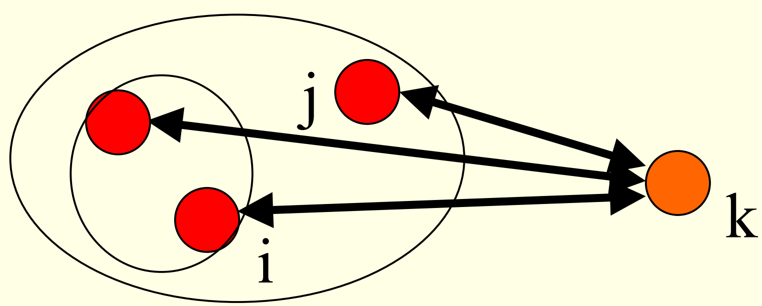
- Furthest neighbor
- Distance between new cluster and other elements equals the *largest* in the cluster occurring distance
- Clusters are only merged when dissimilarity is small.
  - Balanced and equally sized clusters



Unweighted average linkage

$$d_{k[ij]} = \frac{n_i}{n_i + n_j} \times d_{ki} + \frac{n_j}{n_i + n_j} \times d_{kj}$$

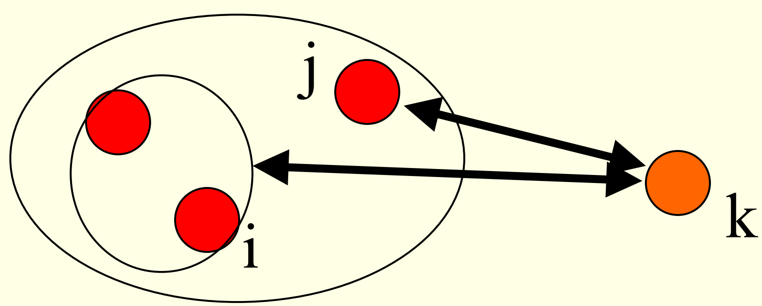
- UPGMA, Baverage, linkage *between* groups
- Uses averages instead of extreme values
- Number of elements in clusters is taken into account



Weighted average linkage

$$d_{k[ij]} = \frac{d_{ki}}{2} + \frac{d_{kj}}{2}$$

- WPGMA, Waverage, linkage *within* groups
- Equals UPGMA but the number of elements in clusters is *not* taken into account
- Can be necessary when the size of supposed clusters or the object density in them differs

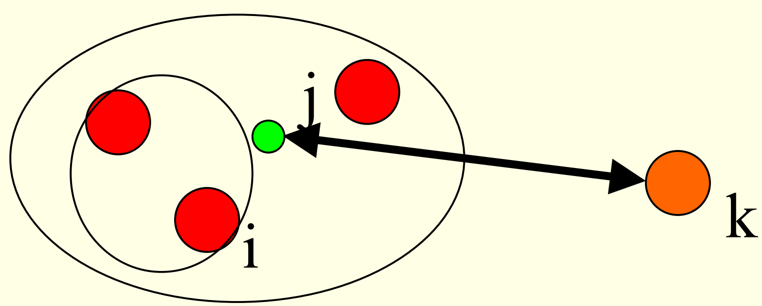


(Un)Weighted centroid linkage

$$d_{k[ij]} = \frac{n_i}{n_i + n_j} \times d_{ki} + \frac{n_j}{n_i + n_j} \times d_{kj} - \frac{n_i \times n_j}{(n_i + n_j)^2} \times d_{ij}$$

$$d_{k[ij]} = \frac{d_{ki}}{2} + \frac{d_{kj}}{2} - \frac{d_{ij}}{4}$$

- Centroid of cluster is calculated
- Distance to new cluster equals distance to centroid



Ward‘s method

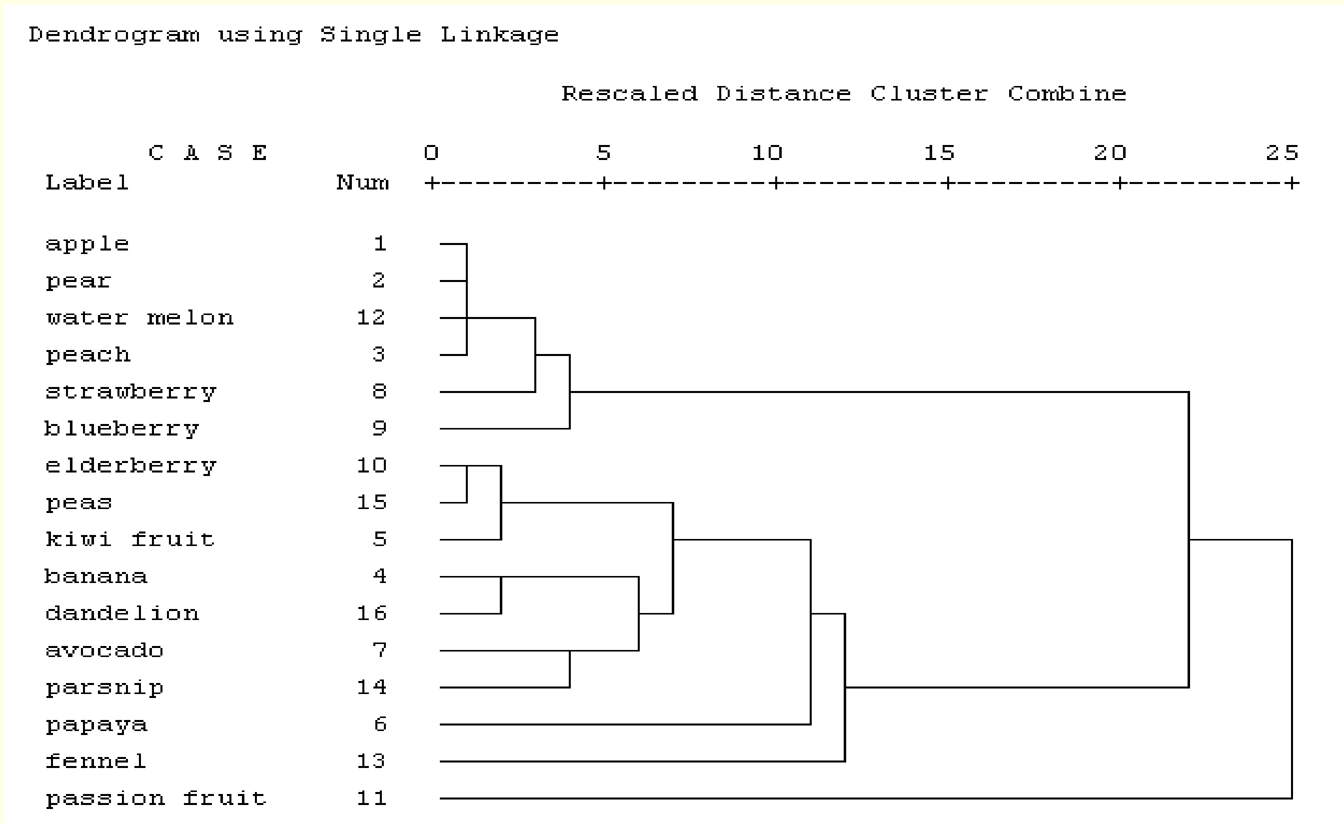
$$d_{k[ij]} = \frac{n_k + n_i}{n_k + n_i + n_j} \times d_{ki} + \frac{n_k + n_j}{n_k + n_i + n_j} \times d_{kj} - \frac{n_k}{n_k + n_i + n_j} \times d_{ij}$$

- Minimum variance
- Idea: Heterogenity is not a reasonable feature of clusters
  - Minimize variance
- To be used only with quantitative attributes and squared Euclidian distance!

Matrix updating algorithms

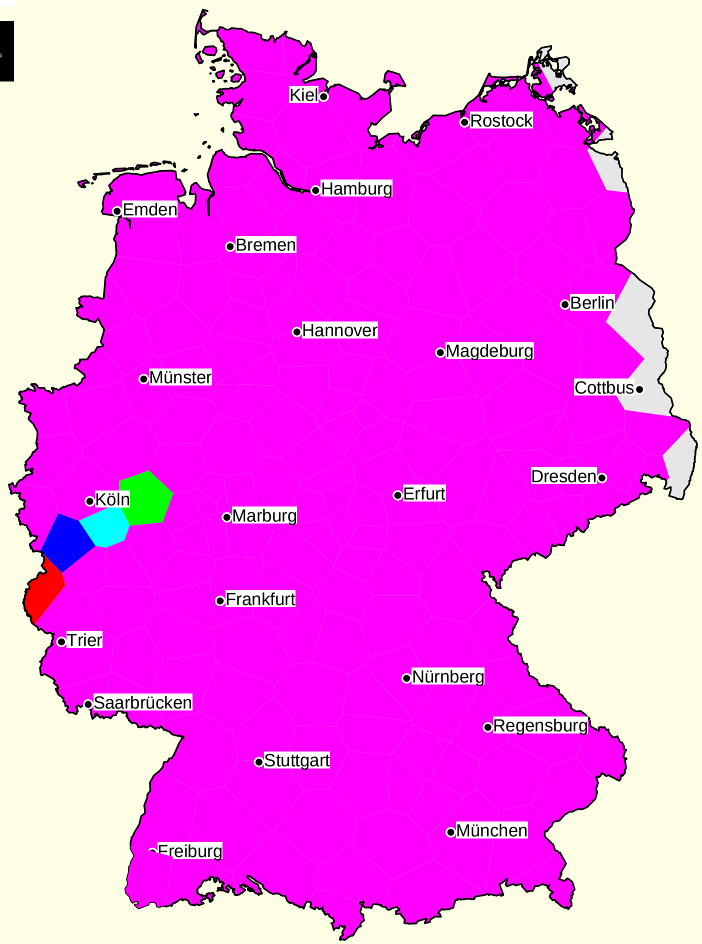
- Types of algorithms:
  - Space-contracting (Single & Centroid (?) Linkage)
    - Unequally sized clusters
    - Outliers visible
  - Space-dilating (Complete linkage & Ward’s method)
    - Balanced clustering
    - Clusters are often not easy to interpret
  - Space-conserving (Average linkage)
    - No unnaturally blown up clusters
    - Appearing clusters are often interpretable

Space-contracting – example 1

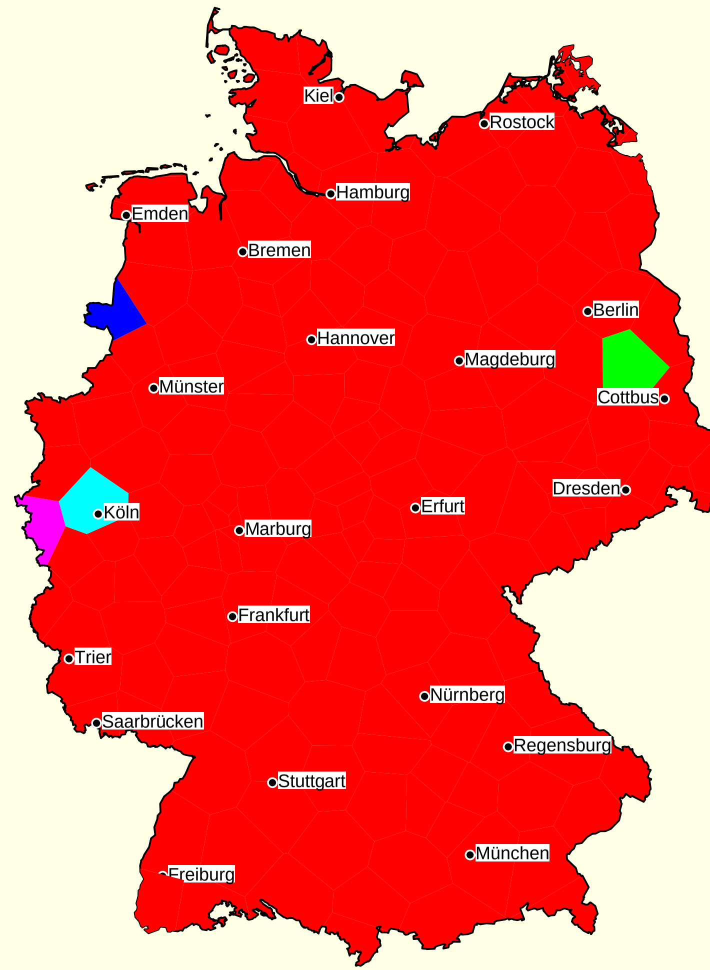


Dendrodram generated by Single-linkage

Space-contracting – example 2

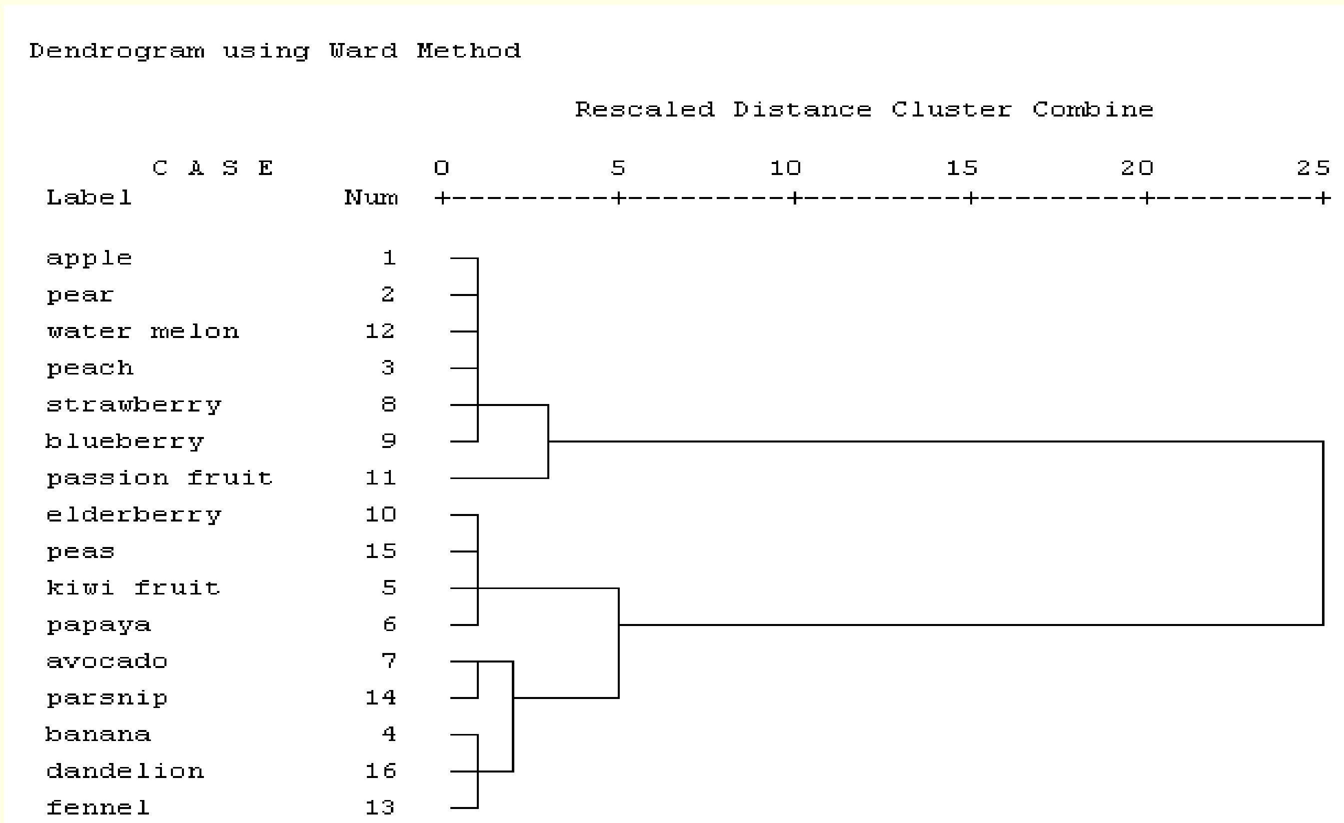


Single linkage



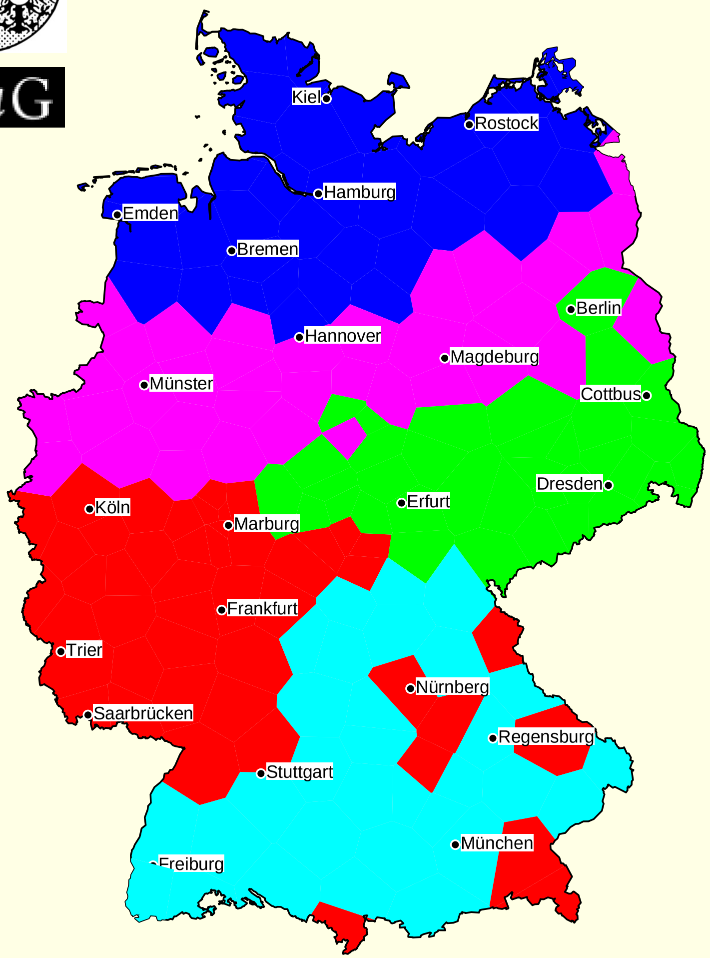
WPGMC

Space-dilating – example 1

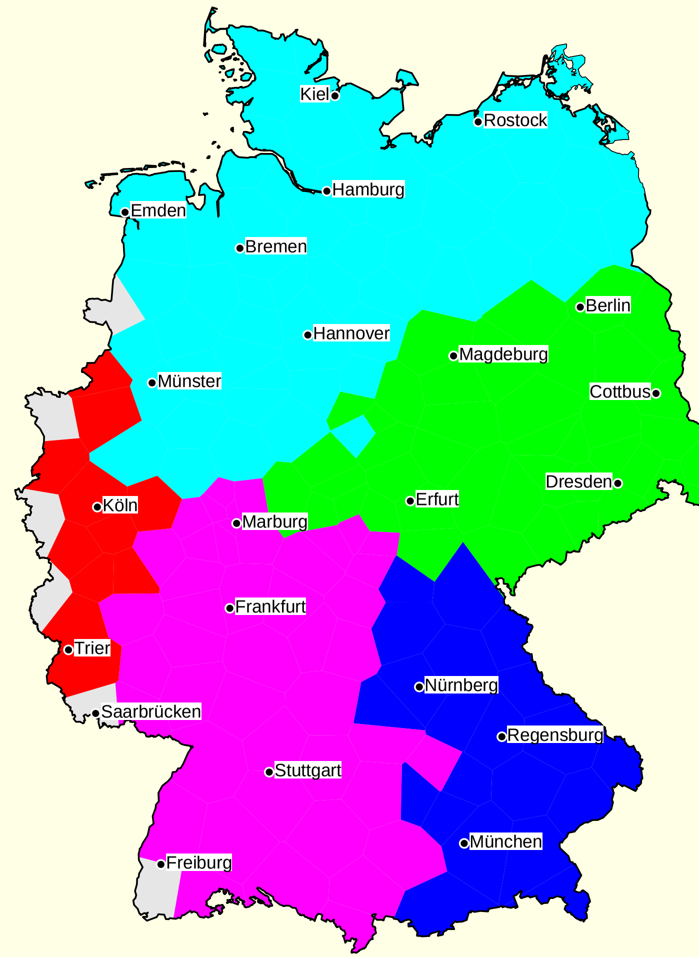


Dendrodram generated by Ward‘s method

Space-dilating – example 2

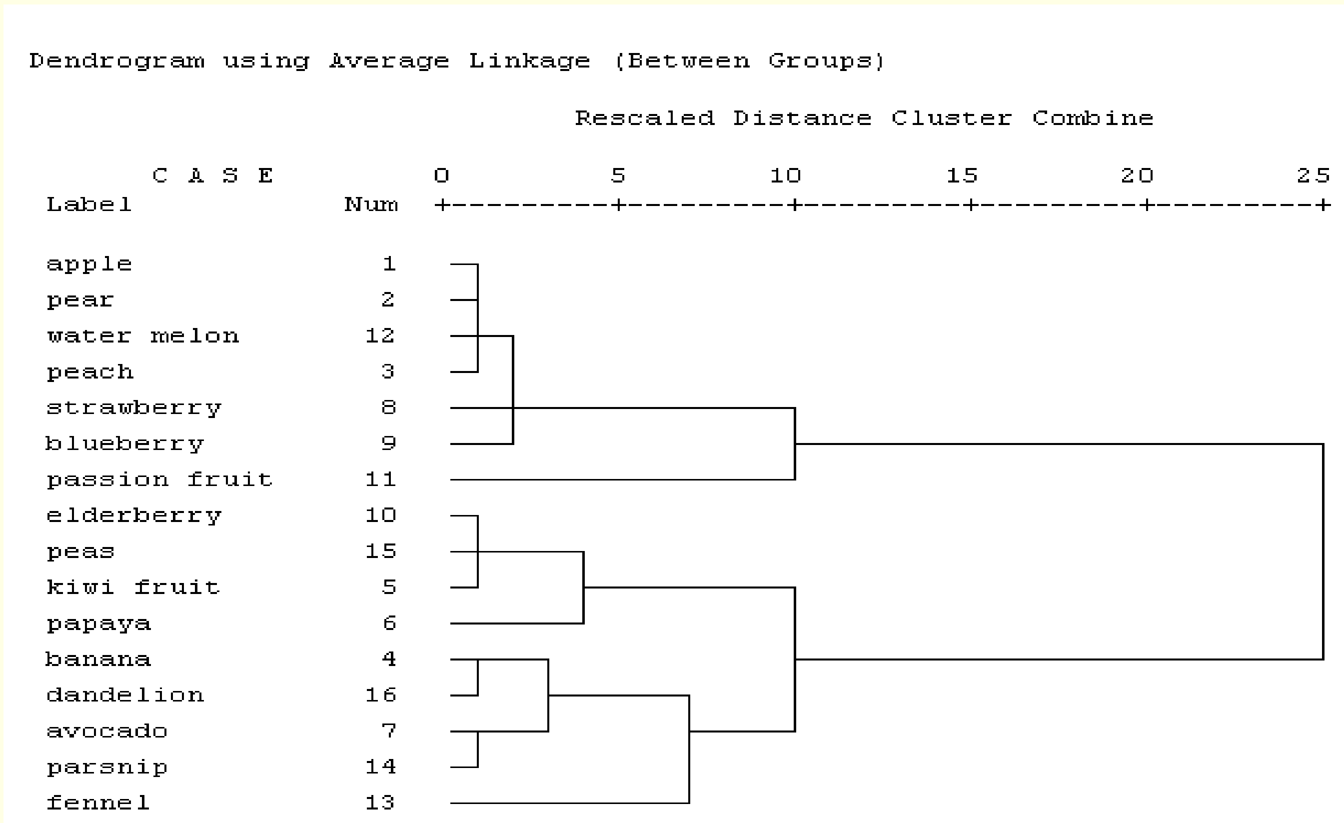


Ward’s method



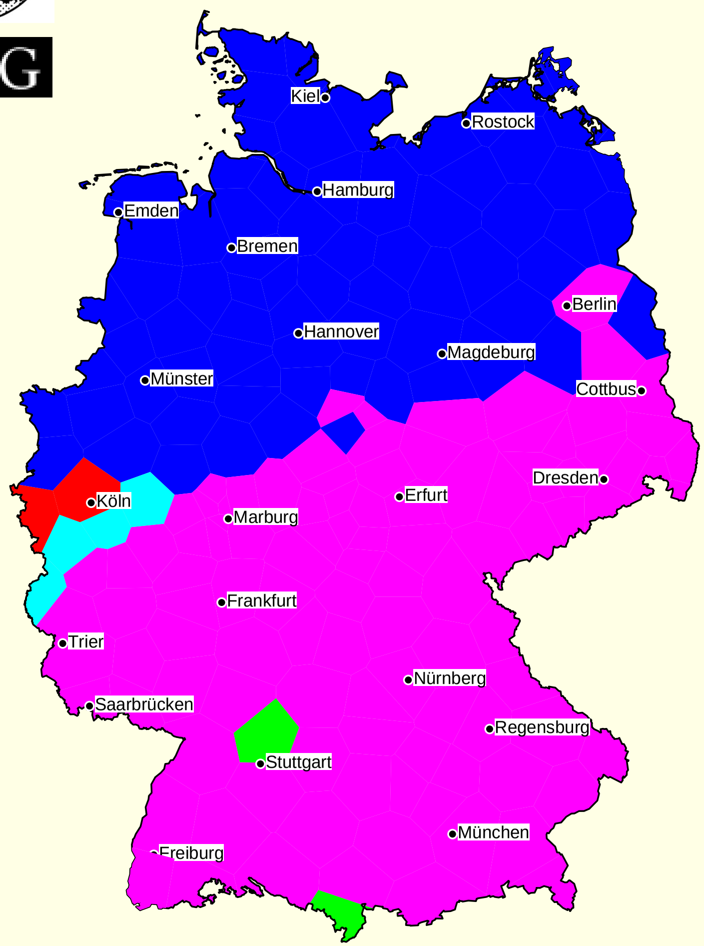
Complete linkage

Space-conserving – example 1

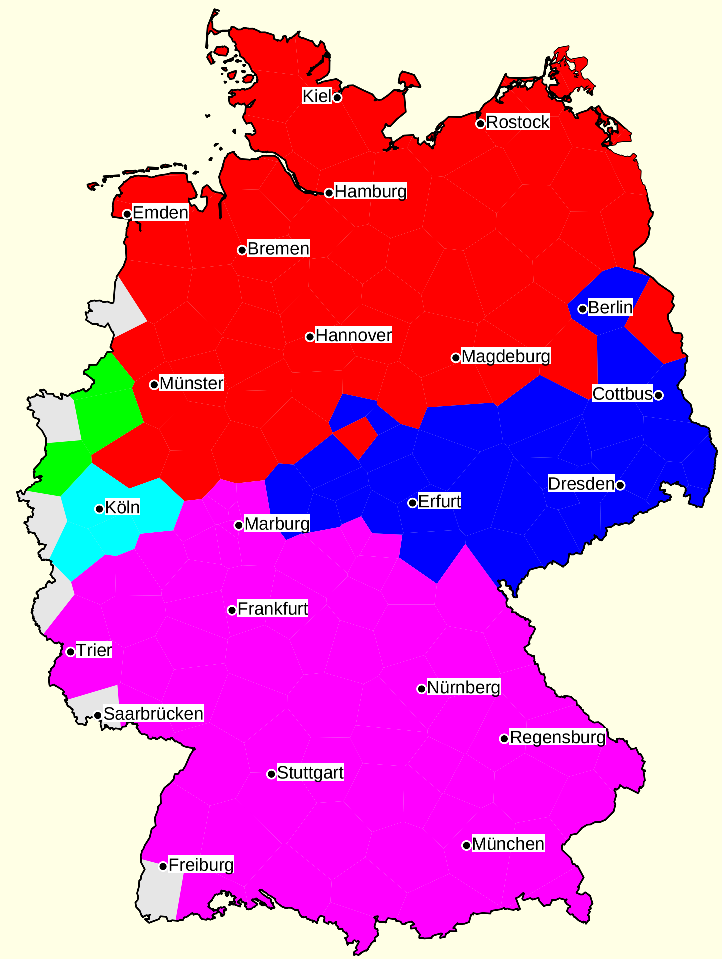


Dendrodram generated by UPGMA

Space-conserving – example 2



UPGMA



WPGMA

Matrix updating algorithms

- Which should be used?
  - Outliers shall be visible
    - Single linkage
  - Unequally sized clusters expected
    - *Not* space-dilating methods
  - Differing object density in expected clusters
    - WPGMA
- No-idea-just-try-order:
  - Space-conserving > space-dilating > space-contracting

Number of clusters

- How many ‚natural‘ classes has cluster analysis generated?
  - ➢ Subjective decision of researcher
  - ➢ Analysis of merging values
    - Large step = rather dissimilar clusters = stop
  - ➢ Plot number of clusters against merging values
    - Graph flattens = no new information = stop
  - ➢ Ward’s method: Significance test possible

Validation of results

- Results should be stable
- Plausible interpretation possible
- Repeat cluster analysis with different samples of the same population
  - Different results = both invalid, but
  - Same results = not necessarily valid and
  - not always possible due to lack of data
- Cophenetic correlation, but
  - Normal distribution (wrongly?) assumed
  - In dendrogram fewer (different) values

Validation of results

- Significance tests
  - Used attributes: Useless because always significant
  - Not used (but relevant) attributes: Useful but only possible when knowledge about classes already exists…
- Monte Carlo procedures
  - Data set is created which has the same global properties as original data but contains no classes
  - Both sets are clustered & results compared
  - Significant differences => results valid

Attention!

- A lot of factors determine the results of cluster analysis
  - *Very* careful selection of objects, attributes, (dis)similarity measure, cluster method and matrix updating algorithm

- **Cluster analysis will *always* output clusters – if there are natural classes or not!**