Hierarchical Clustering

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Introduction to the HC paradigm

... forget about partitional methods ;)

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What HC is

- In brief, HC algorithms build a whole hierarchy of clustering solutions
  - Solution at level k is a *refinement* of solution at level k-1
- Two main classes of HC approaches:
  - Agglomerative: solution at level k is obtained from solution at level k-1 by merging two clusters
  - Divisive: solution at level k is obtained from solution at level k-1 by splitting a cluster into two parts
    - Less used because of computational load

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Agglomerative HC

1. At start, each input pattern is assigned to a singleton cluster
2. At each step, the two *closest* clusters are merged into one
   - So the number of clusters is decreased by one at each step
3. At the last step, only one cluster is obtained

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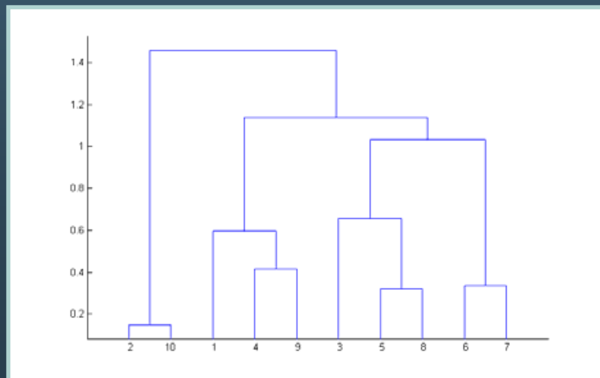
Dendrograms

- The clustering process is represented by a *dendrogram:*



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Dendrograms

- The resulting dendrogram has to be cut at some level to get the final clustering:
  - Cut criterion: number of desired clusters, or threshold on some features of resulting clusters

Computing dissimilarities

Dissimilarity between pairs of single points ➡

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Dissimilarity between pairs of clusters ➡

- Different distances/indices of dissimilarity…
  - E.g. euclidean, city-block, correlation…
- … and agglomeration criteria: Merge clusters C_i and C_j such that *diss(i, j)* is minimum
  - Single linkage:
    - diss(i,j) = min d(x, y), where x is in C_i , y in cluster C_j
  - Complete linkage:
    - diss(i,j) = max d(x, y), where x is in cluster i, y in cluster j
  - Group Average and Weighted Average Linkage:
    - diss(i j) = $\sum_{x\in C_i}\sum_{y\in C_j} w_i w_j d(x,y) \Big/ \sum_{x\in C_i}\sum_{y\in C_j} w_i w_j$

GA: $w_i = w_j = 1$
WA: $w_i = n_i$, $w_j = n_j$

Computing dissimilarities (cont.)

Dissimilarity between pairs of clusters ➡

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- Other agglomeration criteria: Merge clusters C_i and C_j such that *diss(i, j)* is minimum
  - Centroid Linkage:
    - diss(i, j) = d(μ_i, μ_j)
  - Median Linkage:
    - diss(i,j) = d(center$_i$ center$_j$), where each center$_i$ is the average of the centers of the clusters composing C_i
  - Ward's: Method:
    - diss(i, j) = increase in the total error sum of squares (ESS) due to the merging of C_i and C_j

Squared Euclidean distances should be used

- Single, complete, and average linkage: *graph methods*
  - *All points in clusters are considered*
- Centroid, median, and Ward's linkage: *geometric methods*
  - Clusters are summed up by their centers

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Ward's criterion

- Also known as minimum variance method
- Each merging step minimizes the increase in the total ESS:

$$ESS_i = \sum_{x \in C_i} (x - \mu_i)^2 \qquad ESS = \sum_i ESS_i$$

  - When merging clusters C_i and C_j, the increase in the total ESS is

$$\Delta ESS = ESS_{i,j} - ESS_i - ESS_j$$

- Spherical, compact clusters are obtained
- The solution at each level k is an <u>approximation</u> to the optimal solution for that level (the one minimizing ESS)

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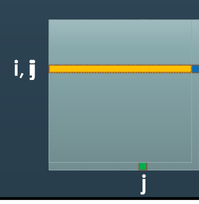
The dissimilarity matrix

- HC algorithms operate on a dissimilarity matrix:
  - For each pair of existant clusters, their dissimilarity value is stored
- When clusters C_i and C_j are merged, only dissimilarities for the new resulting cluster have to be computed
  - The rest of the matrix is left untouched



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The Lance-Williams formula

- Used for iterative implementation
- The dissimilarity value between newly formed cluster $\{C_i, C_j\}$ and every other cluster C_k is computed as

$$diss(k,(i,j)) = \alpha_i\, diss(k,i) + \alpha_j\, diss(k,j) + \beta\, diss(i,j) + \\ + \gamma \left| diss(k,i) - diss(k,j) \right|$$

- Only values already stored in the dissimilarity matrix are used
- Different sets of coefficients correspond to different criteria

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The Lance-Williams formula - coefficients

$$diss(k,(i,j)) = \alpha_i\, diss(k,i) + \alpha_j\, diss(k,j) + \beta\, diss(i,j) + \\ + \gamma \left| diss(k,i) - diss(k,j) \right|$$

Criterion	α_i	α_j	β	γ
Single Link.	½	½	0	-½
Complete Link.	½	½	0	½
Group Avg.	$n_i/(n_i+n_j)$	$n_j/(n_i+n_j)$	0	0
Weighted Avg.	½	½	0	0
Centroid	$n_i/(n_i+n_j)$	$n_j/(n_i+n_j)$	$-n_in_j/(n_i+n_j)^2$	0
Median	½	½	- ¼	0
Ward	$(n_i+n_k)/(n_i+n_j+n_k)$	$(n_j+n_k)/(n_i+n_j+n_k)$	$-n_k/(n_i+n_j+n_k)$	0

e.g. for single linkage…
diss(k, (i,j) = min(diss(k, i), diss(k,j))

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Pros and cons of HC algorithms

- Pros:
  - Indipendence from initialization
  - No need to specify a desired number of clusters from the beginning
- Cons:
  - Computational complexity at least $O(N^2)$
  - Sensitivity to outliers
  - No reconsideration of possibly misclassified points
  - Possibility of inversion phenomena and multiple solutions

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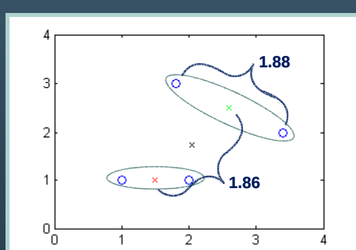
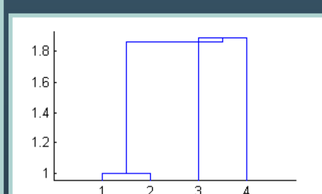
Inversions

- We have an inversion when the sequence of dissimilarity values selected by the HC algorithm is nonmonotonic





- Inversions may be produced when using the centroid or the median criterion