Statistics and learning

Multivariate statistics 2 and clustering

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ISAE SupAero

Wednesday 2nd and 9th October 2013

Link to the previous session

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- introduce Correspondence analysis (CA): for 2 qualitative variables with several (many) levels.
- introduce clustering methods like hierarchical clustering or Kmeans-like algorithms.

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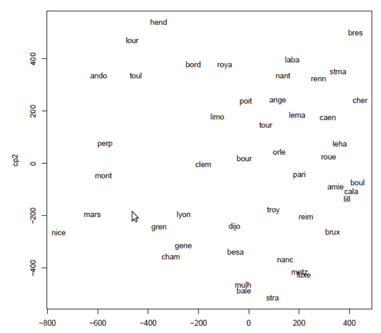
Easy example

Road distances between 47 French cities. Is it Euclidian ?



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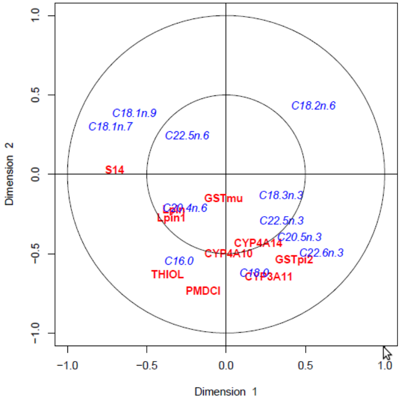
- Variables can be represented in either basis, it does not change the interpretation.

CCA (cont'd)

Need to have $p, q \leq n$. We kept 10 genes and 11 fatty acids.



More interpretation ? $\rightarrow$ Practical session

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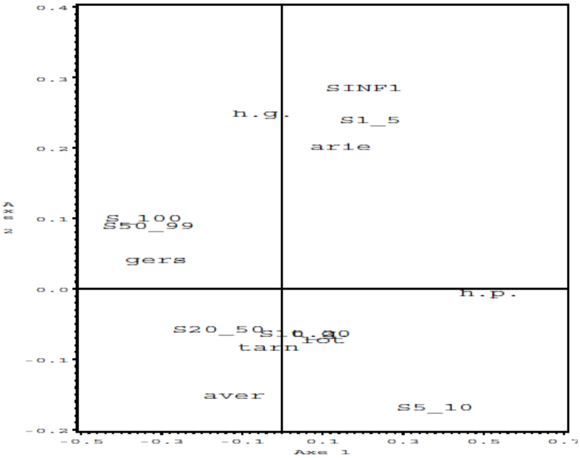
- Note that χ^2 writes $n \sum_i \sum_j \tilde{f_{i,j}} x_{i,j}^2$

CA: an example

Cultivated area in the Midi-Pyrénées region

Simultaneous representation of *département* and farm size (in 6 bins).



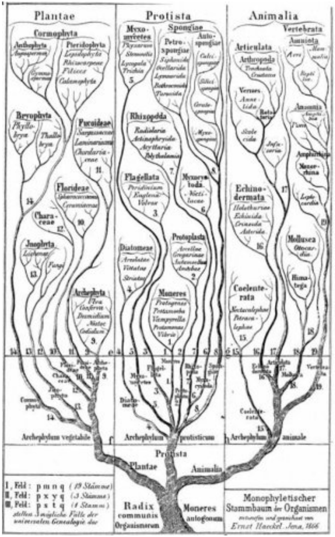
Today

- "Clustering: unsupervised classification". Distance, hierarchical clustering (divisive or agglomerative).
- Keep in mind that this is still exploratory statistics so the best clustering (including method, options, criterion, *etc.*) is the most useful ?!
- End of practical session on mice data set.
- And a new guided session on multivariate stats: CA on *presidential elections*, PCA and clustering (k-means and AHC) on *hotel data set* and multiple CA on 2 *multiple factor data sets*.

Clustering: grouping into classes

Ever heard of that in your background ??

Clustering: grouping into classes



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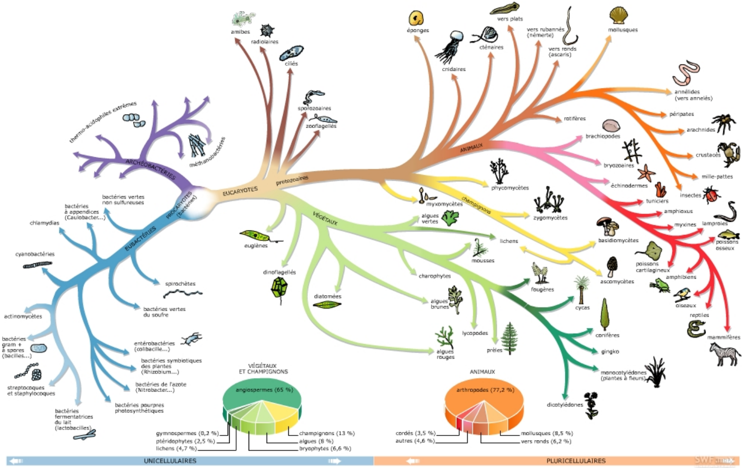

Cluster analysis or clustering

- Task of **grouping** objects so that objects belonging to the same group are 'more similar' to each other than to those in any other group $\rightarrow$ multiobjective optimisation task.

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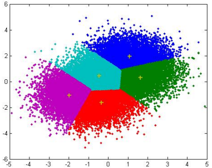

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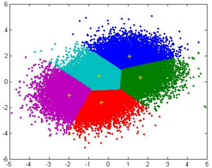

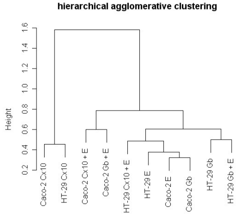

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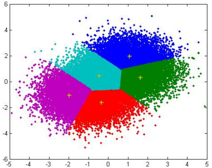

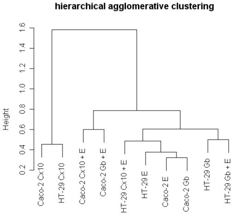

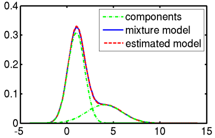

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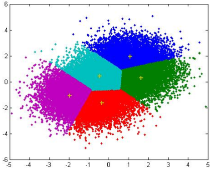

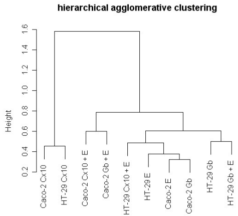

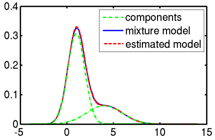

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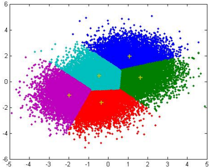

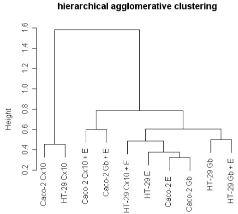

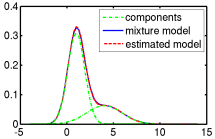

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- Possibly, different parameters (initialisation, distance used, ending criterion . . .) lead to different representations.

Clustering algorithms

Challenge: build your own clustering algorithm ?!

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Let's quote only few of widespread clustering algorithms:

- hierarchical clustering with dissimilarity `min` $\rightarrow$ single, *max* $\rightarrow$ complete or *mean* $\rightarrow$ average linkages)
- centroid models (*e.g.* K-means clustering)
- distribution models (statistical definition *e.g.* multivariate Gaussian distribution)
- graph or density models (*e.g.* clique)
- ...

Clustering: some formalism

- Define a similarity (symetry, self-similarity, bounded) $\rightarrow$ dissimilarity
- Distance need additional properties: $d(i,j) = 0 \Rightarrow i = j$ and triangular inequality (*Euclidian* dist. from scalar product)

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A goodness-of-fit of partitions can be defined: (i) external: TP, FP $\ldots \rightarrow$ precision, sensitivity or Rand/Jaccard index or (ii) internal: Dunn index $D = \min_i \min_{j \neq i} \frac{d(i,j)}{\max_k d^{'}(k)}$.

Homework

What do students choose after French baccalauréat ?

First describe and then represent this (simple) data set in some informative way.

Hint: CA...

origin	counselling			
	université	prep. clas.	other	Total
bac lit.	13	2	5	20
bac éco.	20	2	8	30
bac scient.	10	5	5	20
bac tech.	7	1	22	30
Total	50	10	40	100

Finished

Next time: tests

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But before that: practice with R ?!