Statistics and learning

Multivariate statistics 2 and clustering

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Goal of multivariate (exploratory) statistics: understanding high-dimensional data sets, reducing their 'useful' dimensions, representing them, seeking hidden or latent factors . . . Today we will:

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- ▶ introduce Canonical correlation analysis (CCA): for p quantitative variables and q quantitative variables)
- ▶ 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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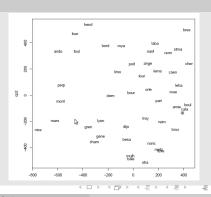
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Easy example

Road distances between 47 French cities. Is it Fuclidian?



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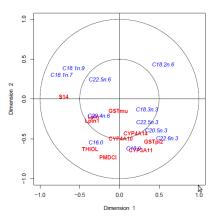
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- ► Consists in looking for a couple of vectors, one related to *X* (gene expressions) and one to *Y* (metabolite levels) which are maximally conected. And iteratively (without correlation between iterations).
- ► Variables can be represented in either 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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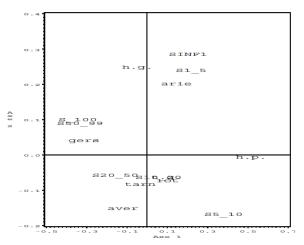
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- ▶ Note that χ^2 writes $n \sum_i \sum_j \tilde{f_{i,j}} x_{i,j}^2$

CA: an example

Cultivated area in the Midi-Pyrénées region

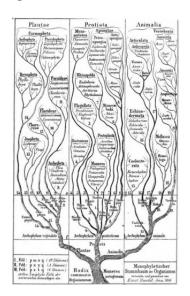
Simultaneous representation of département and farm size (in 6 bins).



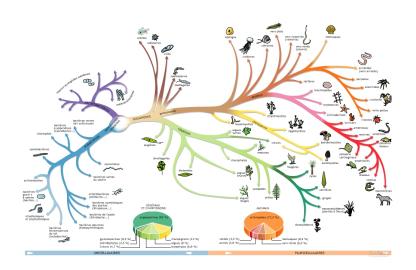
Clustering: grouping into classes

Ever heard of that in your background ??

Clustering: grouping into classes



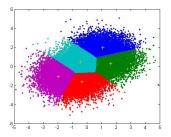
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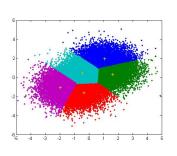
► Task of **grouping** objects so that objects belonging to the same group are 'more similar' to each other than to those in any other group → multiobjective optimisation task.

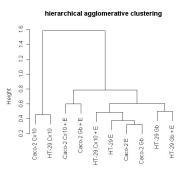
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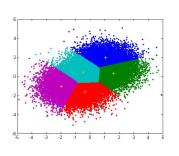


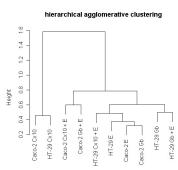
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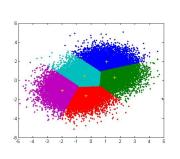
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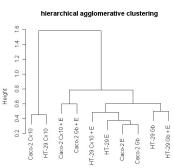




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- ► Several algorithms can do the job, their differences mainly being about used distance.
- ► Possibly, different parameters (initialisation, distance used, ending criterion . . .) lead to different representations.

Clustering algorithms

Challenge: build your own clustering algorithm ?!

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Let's quote only few of widespread clustering algorithms:

- ► hierarchical clustering (single, complete, average linkages)
- ► centroid models (e.g. Kmeans clustering)
- ▶ distribution models (statistical definition *e.g.* multivariate Gaussian distribution)
- ▶ graph or density models (e.g. clique)
- ▶ ...

Clustering: some formalism

- lacktriangle Define a similarity (symetry, self-similarity, bound) ightarrow dissimilarity
- ▶ Distance need additional property: $d(i, j) = 0 \Rightarrow i = j$ (Euclidian dist. from scalar product)

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A goodness-of-fit of partitions can be defined: (i) external: TP, FP ... \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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