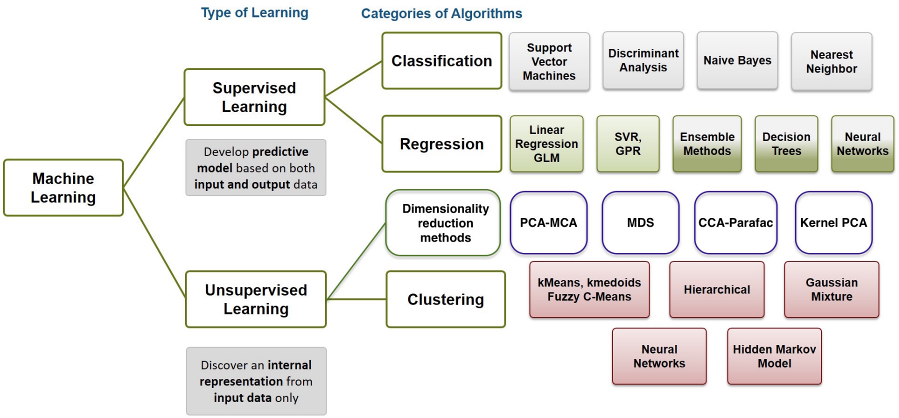
Unsupervised Learning
Introduction to clustering

MAP 573, 2019 – Julien Chiquet

École Polytechnique, Autumn semester, 2019

https://github.com/jchiquet/CourseUnsupervisedLearningX

Machine Learning



Supervised vs Unsupervised Learning

Supervised Learning

- Training data $\mathcal{D}_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}, X_i \sim^{\text{i.i.d}} \mathbb{P}$
- Construct a predictor $\hat{f} : \mathcal{X} \to \mathcal{Y}$ using $\mathcal{D}_n$
- Loss $\ell(y, f(x))$ measures how well $f(x)$ predicts y
- Aim: minimize the generalization error
- Task: Regression, Classification

$\rightsquigarrow$ The goal is clear: predict y based on x (regression, classification)

Unsupervised Learning

- Training data $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$
- Loss? , Aim?
- Task: Dimension reduction, Clustering

$\rightsquigarrow$ The goal is less well defined, and *validation* is questionable

Outline

Outline

Packages required for reproducing the slides

```r
library(tidyverse)  # opinionated collection of packages for data manipulation
library(corrplot)   # fancy plots of matrices as images
library(GGally)     # extension to ggplot vizualization system
library(ggfortify) # extension to ggplot vizualization system
library(mclust)     # Gaussian mixture models
library(aricode)    # fast computation of clustering measures
library(animation)  # kmeans animation slides
# color and plots themes
library(RColorBrewer)
pal <- brewer.pal(10, "Set3")
theme_set(theme_bw())
```

Outline

Companion data set

Morphological Measurements on Leptograpsus Crabs

Description

The crabs data frame has 200 rows and 8 columns, describing 5 morphological measurements on 50 crabs each of two colour forms and both sexes, of the species *Leptograpsus variegatus* collected at Fremantle, W. Australia.

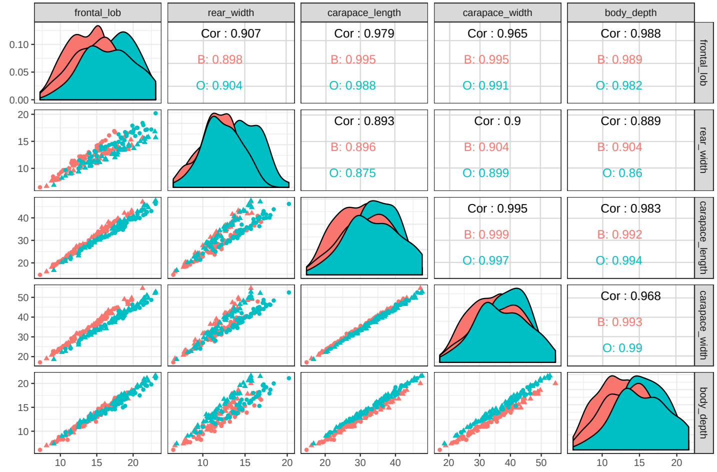
```r
crabs <- MASS::crabs %>% select(-index) %>%
  rename(sex = sex,
         species        = sp,
         frontal_lob    = FL,
         rear_width     = RW,
         carapace_length = CL,
         carapace_width  = CW,
         body_depth     = BD)
crabs %>% select(sex, species) %>% summary() %>% knitr::kable("latex")
```

	sex	species
	F:100	B:100
	M:100	O:100

Companion data set II

Pairs plot of attributes

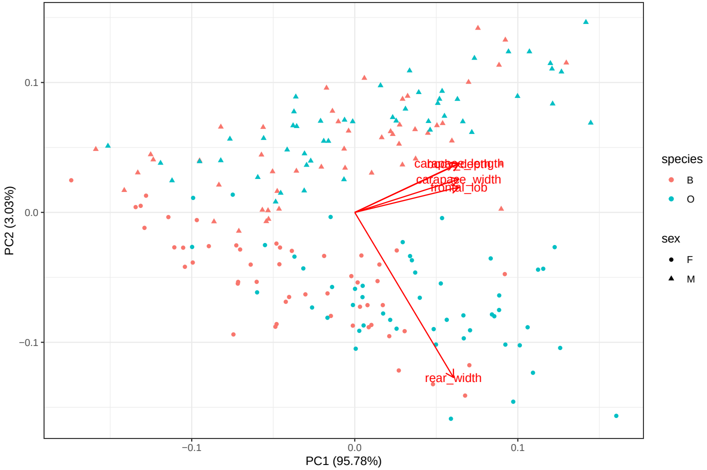
```
ggpairs(crabs, columns = 3:7, aes(colour = species, shape = sex))
```



Companion data set III

PCA on the attributes

```
prcomp(select(crabs, -species, -sex), scale. = TRUE) %>%
  autoplot(loadings = TRUE, loadings.label = TRUE,
           data = crabs, colour = 'species', shape = 'sex')
```



Remove size effect I

Carried by the 1st principal component

PCA is solved by SVD

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top.$$

We remove the best rank-1 approximation of $\mathbf{X}$ to remove the *size effect*, carried by the first axis, that is,

$$\tilde{\mathbf{X}}^{(1)} = \mathbf{U}_{\bullet 1} d_{11} \mathbf{v}_{\bullet 1}^\top.$$

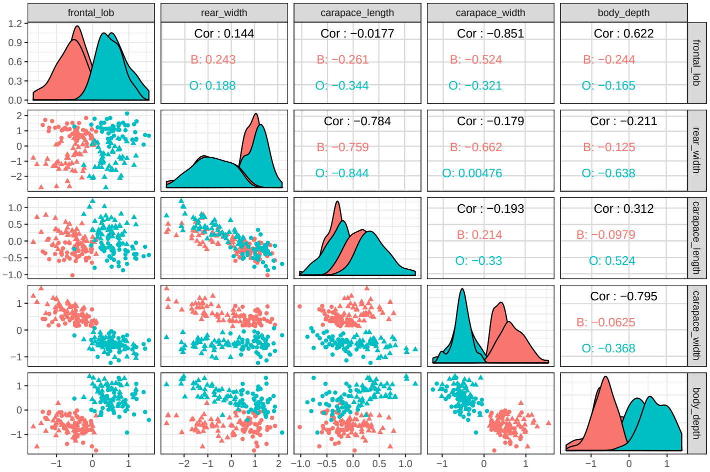
```r
attributes <- select(crabs, -sex, -species)
SVD <- svd(attributes)
attributes_rank1 <- tcrossprod(SVD$u[, 1] * SVD$d[1], SVD$v[, 1])
crabs_corrected <- crabs
crabs_corrected[, 3:7] <- attributes - attributes_rank1
```

$\rightsquigarrow$ Axis 1 explains a latent effect, here the size in the case at hand, common to all attributes.

Remove size effect II

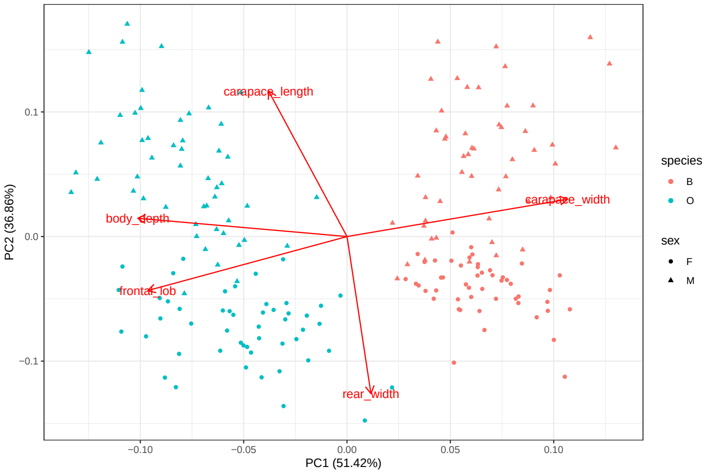
Carried by the 1st principal component

```
ggpairs(crabs_corrected, columns = 3:7, aes(colour = species, shape = sex))
```



PCA on corrected data

```r
prcomp(select(crabs_corrected, -species, -sex), scale. = TRUE) %>%
  autoplot(loadings = TRUE, loadings.label = TRUE,
           data = crabs_corrected, colour = 'species', shape = 'sex')
```



Questions

1. Could we automatically identify some grouping (clustering) between samples ?
2. Would this clustering correspond to some known labels (sex, species)?
3. Does it matter?

Outline

Clustering: general goals

Objective: construct a map f from $\mathcal{D}$ to $\{1, \ldots, K\}$ where K is a fixed number of clusters.

Careful! classification $\neq$ clustering

- Classification presupposes the existence of classes
- Clustering labels only elements of the dataset
  - $\rightsquigarrow$ no ground truth (no given labels)
  - $\rightsquigarrow$ discovers a structure "natural" to the data
  - $\rightsquigarrow$ not necessarily related to a known classification

Motivations

- describe large masses of data in a simplified way,
- structure a set of knowledge,
- reveal structures, hidden causes,
- use of the groups in further processing,
- ...

Clustering: challenges

Clustering quality

No obvious measure to define the quality of the clusters. Ideas:

- Inner homogeneity: samples in the same group should be similar
- Outer inhomogeneity: samples in different groups should be different

Number of clusters

Choice of the number of clusters K often complex

- No ground truth in unsupervised learning!
- Several solutions might be equally good

Two general approaches

- distance-based: require a distance/dissimilarity between $\{\mathbf{x}_i\}$
- model-based: require assumptions on the distribution $\mathbb{P}$

Outline

Dissimilarity and Distance

Clustering requires a measure of ressemblance between object

Definition ((dis)similarity)

Similarity (*resp. Dissimilarity*) measures the ressemblance (*resp. discrepancy*) between objects based on several features.

For instance, two objects are similar if

- they share a certain feature
- their features are close according to a measure of proximity

Definition (distance/metric)

Dissimilairty can be measuresd by distances, *i.e.* a function d_{ij} between pairs in $\{\mathbf{x}_i\}$ s.t.

- $d_{ij} \geq 0,$
- $d_{ij} = 0 \Leftrightarrow \mathbf{x}_i = \mathbf{x}_j,$
- $d_{ij} = d_{ji},$
- $d_{ik} \leq d_{ij} + d_{jk}.$

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Classification structures: Partition

Clustering leads to a grouping (or classification) of individuals into homogeneous classes

We consider two structures to describe this classification:

- partitions and
- hierarchies.

Definition (Partition)

A partition $\mathcal{P}$ is a decomposition $\mathcal{P} = \{P_1, \dots, P_K\}$ of a finite ensemble Ω such that

- $P_k \cap P_{k'} = \emptyset$ for any $k \neq k'$
- $\bigcup_k P_k = \Omega$

In a set $\Omega = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ partitioned into K classes, each element of the set belongs to a class and only one.

Classification structures: Hierarchy

Definition (Hierarchy)

A hierarchy $\mathcal{H}$ is a non empty subset of a finite ensemble Ω such that

- $\Omega \in \mathcal{H}$,
- $\forall \mathbf{x} \in \Omega, \{\mathbf{x}\} \in \mathcal{H}$,
- $\forall H, H' \in \mathcal{H}$, then either $H \cap H' = \emptyset$, $H \subset H'$ or $H' \subset H$.

Definition (Index of a Hierarchy)

The index is a function $i : \mathcal{H} \to \mathbb{R}_+$ such that

- if $H \subset H'$ then $i(H) < i(H')$;
- if $\mathbf{x} \in \Omega$ then $i(\mathbf{x}) = 0$.

Properties (Partition and Hierarchy)

- *Each level of an indexed hierarchy is a partition;*
- $\{\Omega, P_1, \dots, P_K, \mathbf{x}_1, \dots, \mathbf{x}_n\}$ *is a hierachy.*

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Clusterings Comparison: Contingency table

Definition

Consider two clusterings U and V of elements in Ω, into respectively $|U|$ and $|V|$ classes. The $|U| \times |V|$ contingency matrix stores at position (i, j) the number of elements that are simultaneously in cluster i of U and j of V.

$\mathbf{U}\backslash\mathbf{V}$	V_1	V_2	$\ldots$	$V_{\|V\|}$	Sums
U_1	n_{11}	n_{12}	$\ldots$	$n_{1\|V\|}$	$n_{1.}$
U_2	n_{21}	n_{22}	$\ldots$	$n_{2\|V\|}$	$n_{2.}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$U_{\|U\|}$	$n_{\|U\|1}$	$n_{\|U\|2}$	$\ldots$	$n_{\|U\|\|V\|}$	$n_{\|U\|.}$
Sums	$n_{.1}$	$n_{.2}$	$\ldots$	$n_{.\|V\|}$	$n_{..} = n$

Clusterings Comparison: Measures (I)

Definition (Rand index)

Given a set Ω of n elements and two partitions U and V to compare, define the following:

- a, the number of pairs in the same subset in U and in in V
- b, the number of pairs in different subsets in U and in V

The Rand index, $RI \in [0, 1]$ is

$$RI = \frac{a + b}{\binom{n}{2}}$$

The Rand index can be viewed as a measure of the percentage of correct decisions:

$$RI = \frac{TP + TN}{\binom{n}{2}},$$

where TP, TN are true positive and true negative decisions.

Clusterings Comparison: Measures (II)

The ARI (most popular) is a version of the RI adjusted for chance grouping of element (i.e., the expected similarity of all pair-wise comparisons).

Definition (Adjusted Rand-index)

$$ARI(U,V) = \frac{\sum_{i,j}\binom{n_{ij}}{2} - \left[\sum_i \binom{n_{i.}}{2} \sum_j \binom{n_{.j}}{2}\right] / \binom{n}{2}}{\frac{1}{2}\left[\sum_i \binom{n_{i.}}{2} + \sum_j \binom{n_{.j}}{2}\right] - \left[\sum_i \binom{n_{i.}}{2} \sum_j \binom{n_{.j}}{2}\right] / \binom{n}{2}}$$

Other popular measures:

- NVI, the normalized variation information
- NID, the normalized information distance
- NMI, the normalized mutual information

Outline

References

The Elements of Statistical Learning,
T. Hastie, R. Tibshirani, J. Friedman
Chapter: 14 Unsupervised Learning, Section 3: Cluster Analysis
https://web.stanford.edu/~hastie/ElemStatLearn/

Classification non-supervisées,
É. Lebarbier, T. Mary-Huard
Chapitre 2 - méthode de partitionnement
https://www.agroparistech.fr/IMG/pdf/ClassificationNonSupervisee-AgroParisTech.pdf

Outline

K-means heuristic

Idea

1. Clustering is defined by a partition in K classes
2. Minimize a criteria of clustering quality
3. Use Euclidean distances to measure dissimilarity

Criteria: intra-class variance/ Inertia "within"

Intra-class variance measures inner homogeneity

$$I_W = \sum_{k=1}^{K} \sum_{i=1}^{n} c_{ik} \left\| \mathbf{x}_i - \boldsymbol{\mu}_k \right\|_2^2 ,$$

where

- $\boldsymbol{\mu}_k$ are the centers (prototypes) of classes
- $c_{ik} = \mathbf{1}_{i \in \mathcal{P}_k}$ is a partition matrix

K-means algorithm

Ideally, one would solve

$$(\hat{\mathbf{c}}, \hat{\boldsymbol{\mu}}) = \arg\min_{(\mathbf{c},\boldsymbol{\mu})} I_w((\mathbf{c}, \boldsymbol{\mu})), \quad \text{s.t} \quad \mathbf{c} \text{ is a partion matrix.}$$

This problem is hard to solve but can be optimized locally as follows:

K-means algorithm (Loyds)

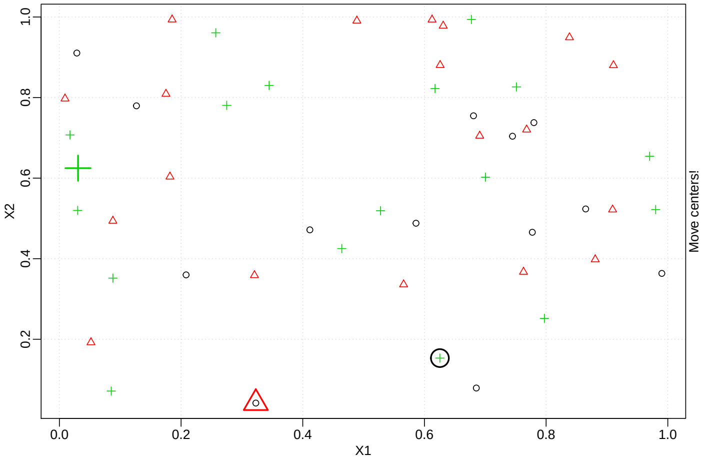
Initialization start by a (pseudo) random choice for the centers $\boldsymbol{\mu}_k$

Alternate until convergence

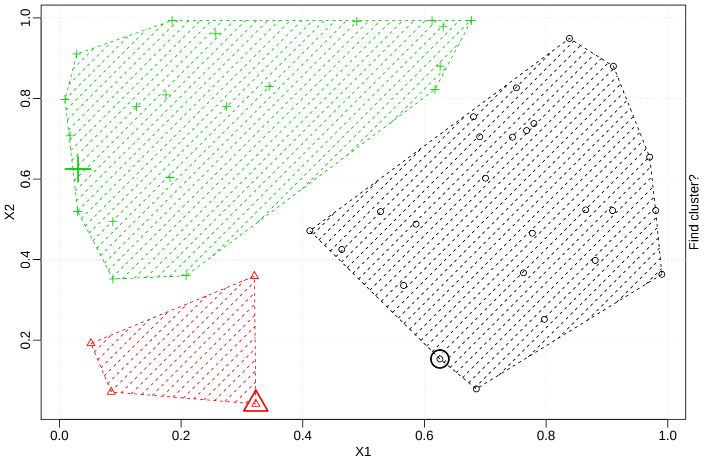
step 1 given $\boldsymbol{\mu}$, chose $\mathbf{c}$ minimizing $I_w \equiv$ assign $\mathbf{x}_i$ to the nearest prototype

step 2 given $\mathbf{c}$, chose $\boldsymbol{\mu}$ minimizing $I_w \equiv$ update $\boldsymbol{\mu}$ by the new means of classes

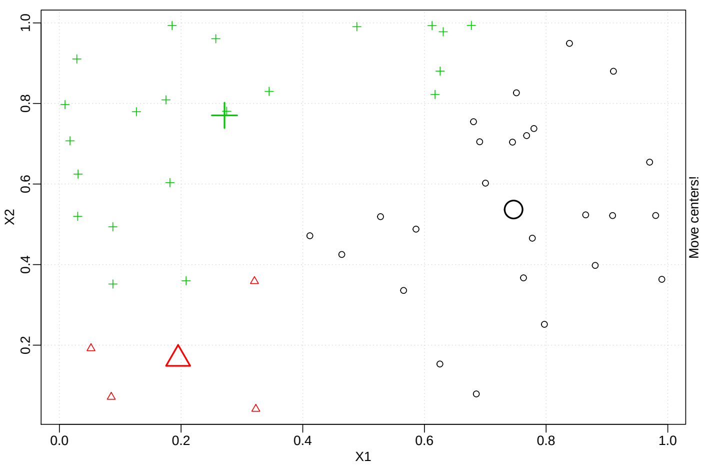
K-means in action I



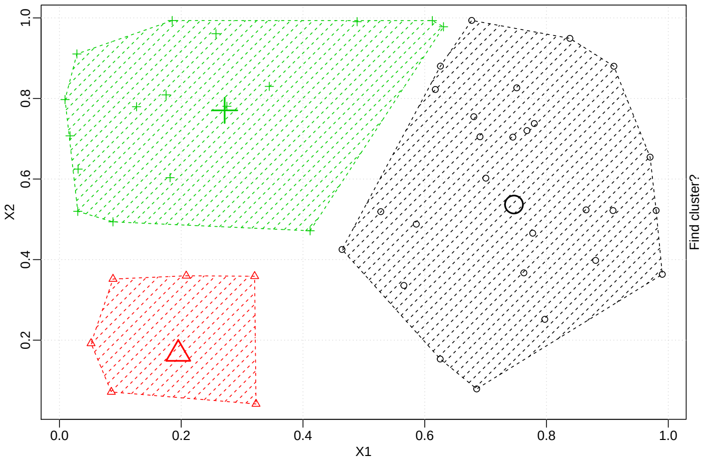
K-means in action II



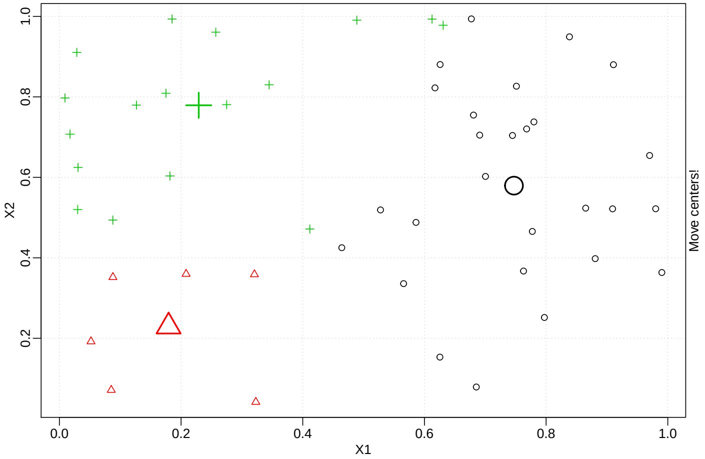
K-means in action III



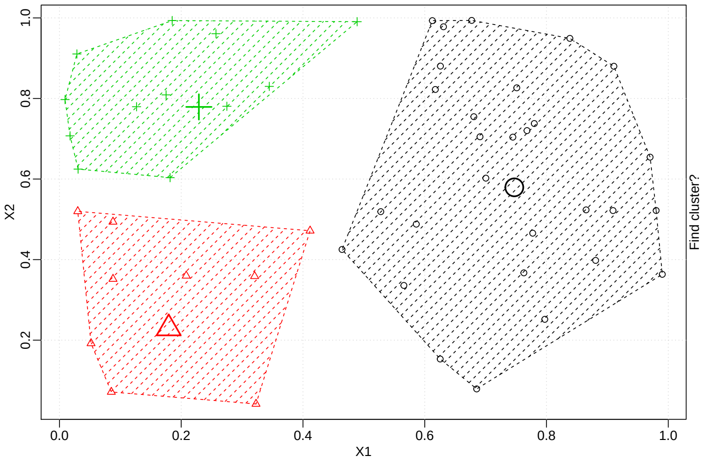
K-means in action IV



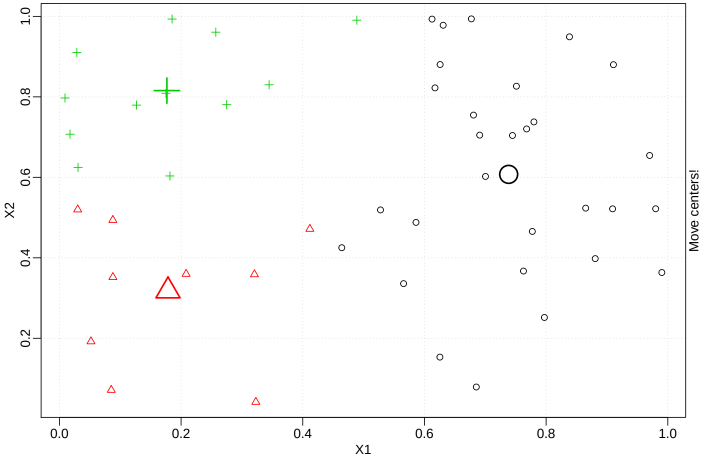
K-means in action V



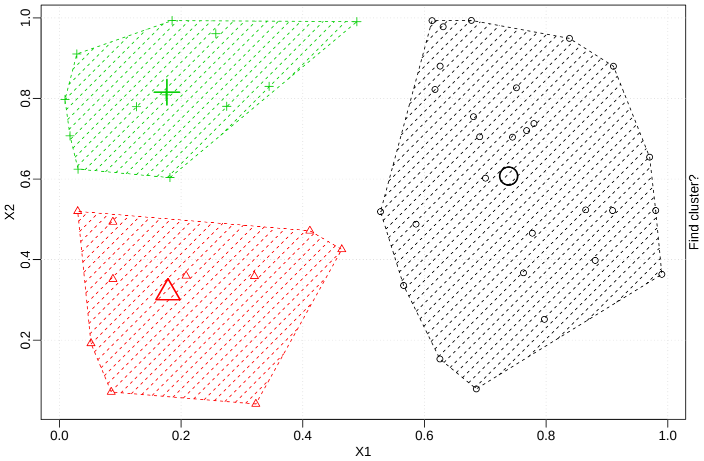
K-means in action VI



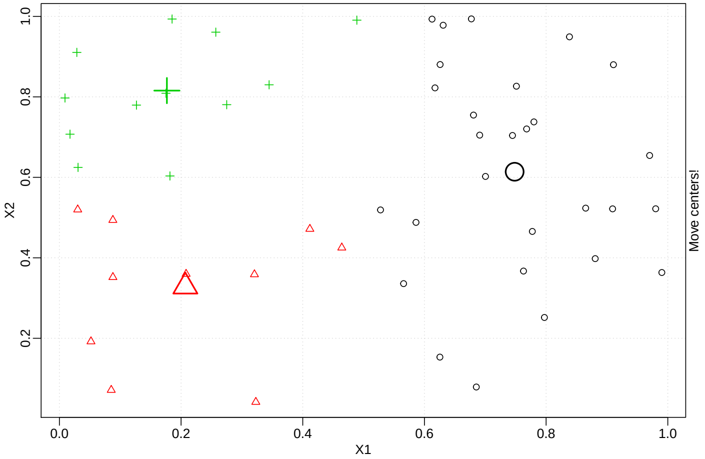
K-means in action VII



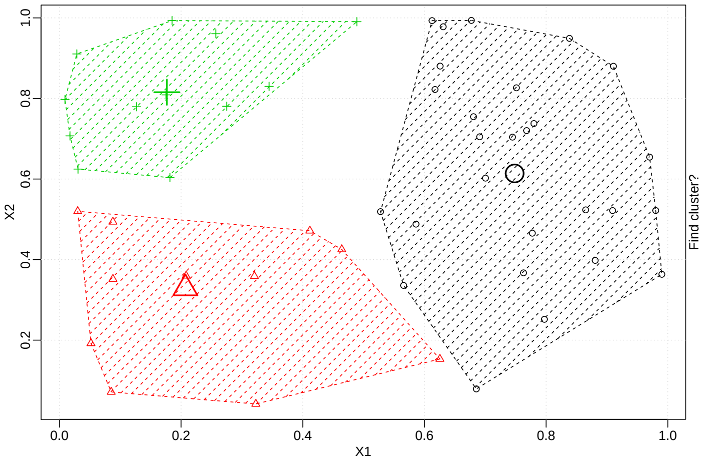
K-means in action VIII



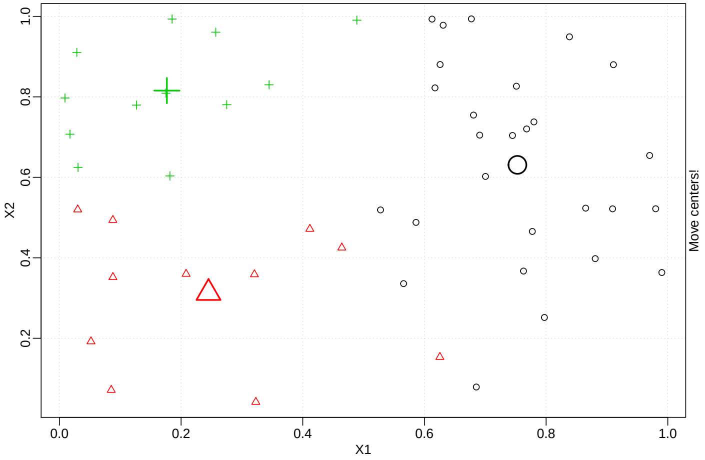
K-means in action IX



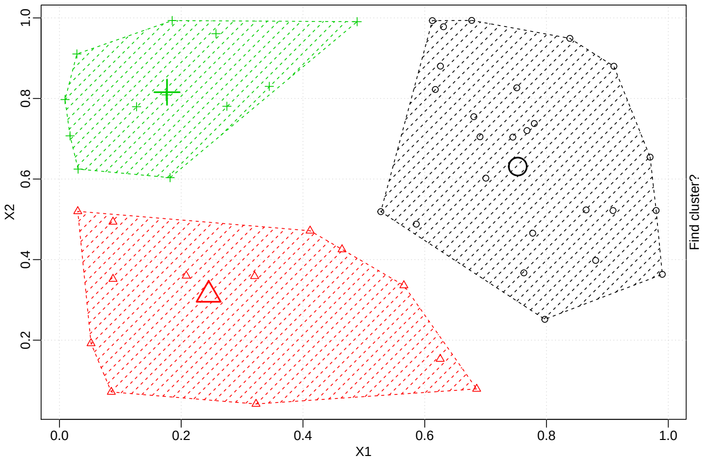
K-means in action X



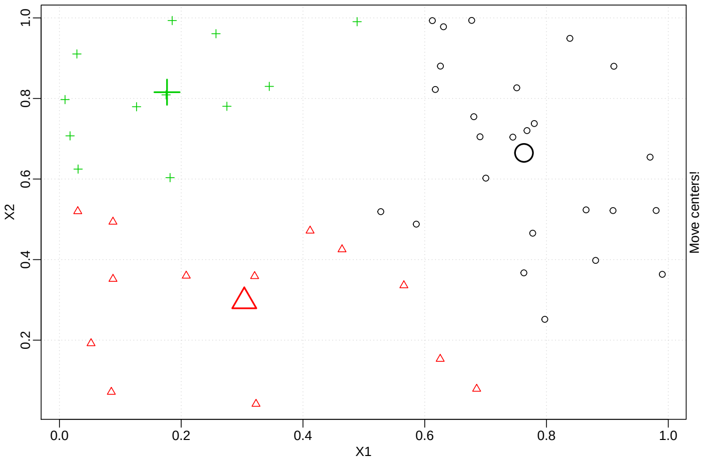
K-means in action XI



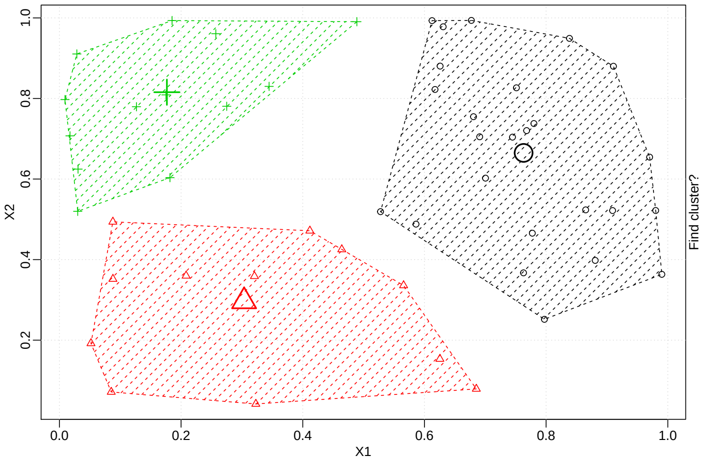
K-means in action XII



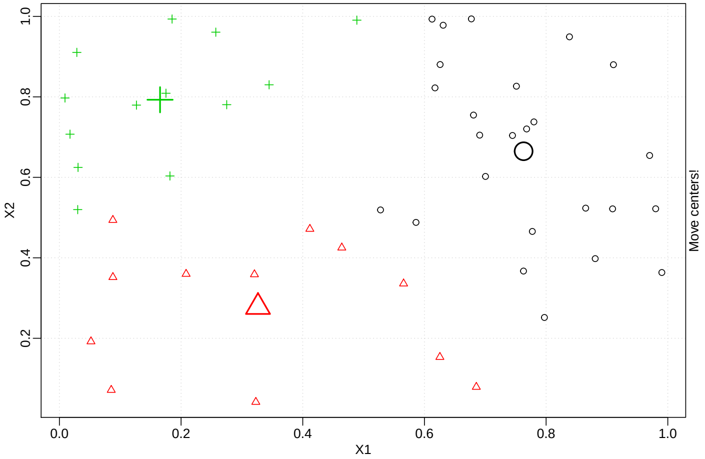
K-means in action XIII



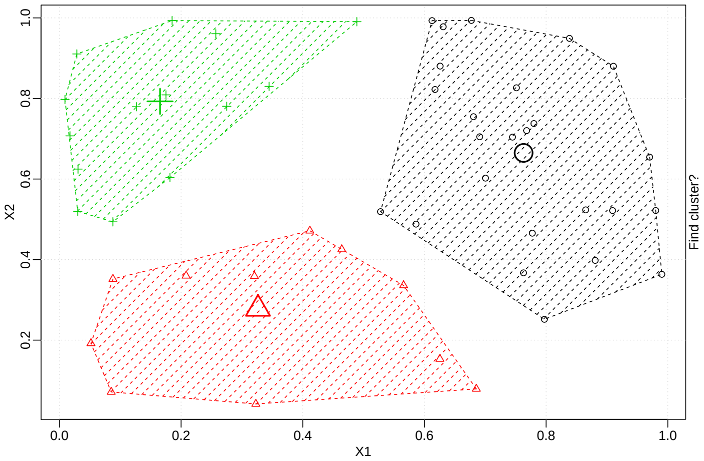
K-means in action XIV



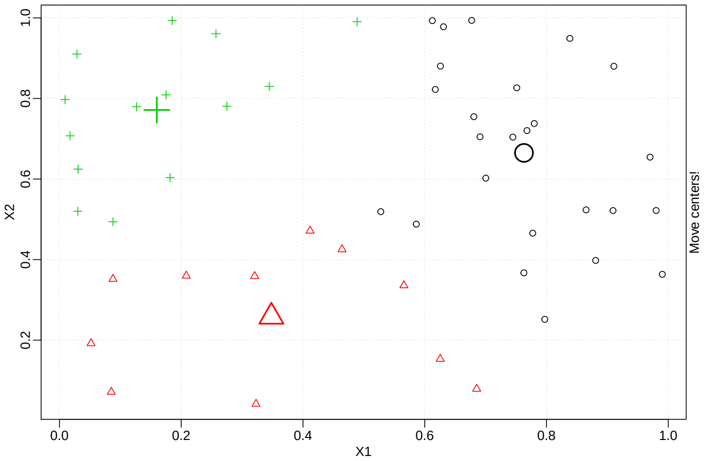
K-means in action XV



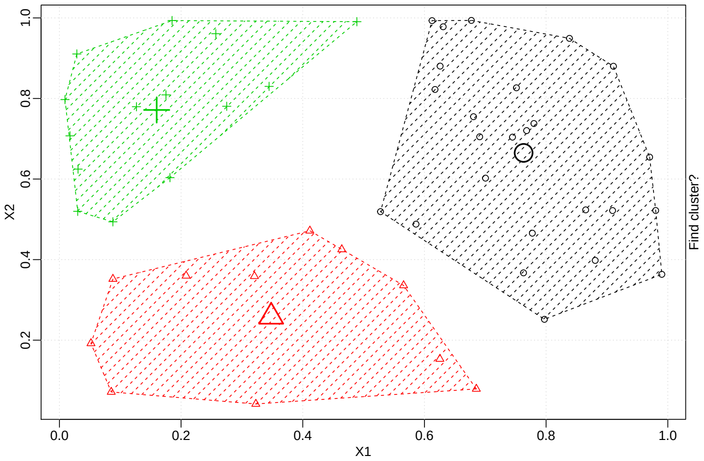
K-means in action XVI



K-means in action XVII



K-means in action XVIII



K-means: properties

Other schemes

- McQueen: modify the mean each time a sample is assigned to a new cluster.
- Hartigan: modify the mean by removing the considered sample, assign it to the nearby center and recompute the new mean after assignment.

Initialization

No guarantee to converge to a global optimum

- Repeat and keep the best result
- k-Mean$++$: try to take them as separated as possible.

Complexity

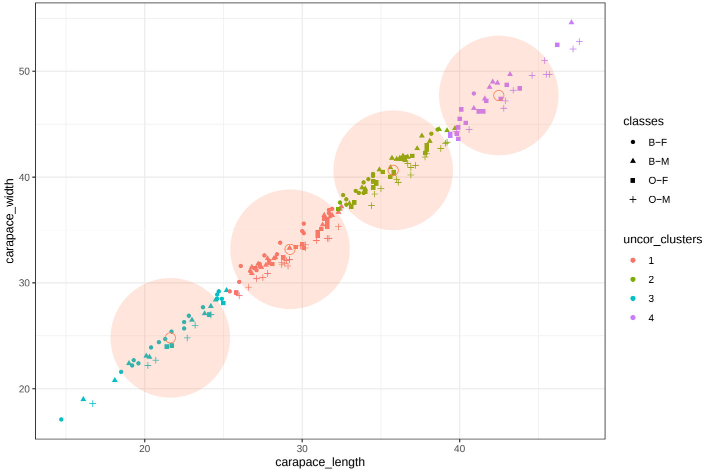
$O(nKT)$ where T is the number of step in the algorithm.

K-means in R on uncorrected data set I

```r
uncor_kmeans_res <- crabs %>%
  select(-species, -sex) %>%
  kmeans(4, nstart = 10)
uncor_clusters <- as.factor(uncor_kmeans_res$cluster)
uncor_centers  <- as_tibble(uncor_kmeans_res$centers)
classes <- paste(crabs_corrected$species, crabs_corrected$sex, sep = "-")

crabs %>%
  ggplot(aes(x = carapace_length, y = carapace_width, color = uncor_clusters)) +
  geom_point(aes(shape = classes)) +
  geom_point(data = uncor_centers, color = 'coral', size = 4 , pch = 21) +
  geom_point(data = uncor_centers, color = 'coral', size = 50, alpha = 0.2)
```

K-means in R on uncorrected data set II



K-means in R on corrected crabs data set I

```r
kmeans_res <- crabs_corrected %>%
  select(-species, -sex) %>%
  kmeans(4, nstart = 10)
clusters <- as.factor(kmeans_res$cluster)
centers  <- as.tibble(kmeans_res$centers)
classes <- paste(crabs_corrected$species, crabs_corrected$sex, sep = "-")

crabs_corrected %>%
  ggplot(aes(x = carapace_length, y = carapace_width, color = clusters)) +
  geom_point(aes(shape = classes)) +
  geom_point(data = centers, color = 'coral', size = 4 , pch = 21) +
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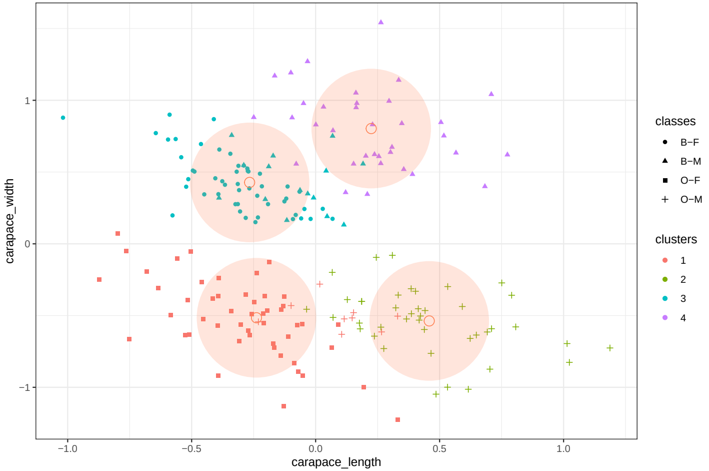
K-means in R on corrected crabs data set II



Clustering comparison

```
aricode::ARI(clusters, classes)

## [1] 0.7223637

aricode::ARI(uncor_clusters, classes)

## [1] 0.01573617
```

```
knitr::kable(table(clusters, classes),
caption = "Estimating structure with k-means")
```

Table: Estimating structure with k-means

B-F	B-M	O-F	O-M
0	0	50	9
0	0	0	41
50	15	0	0
0	35	0	0

Outline

Agglomerative Clustering: Heuristic

Idea

1. Start with small clusters (*e.g.* one cluster $\equiv$ one individual)
2. Merge the most similar clusters sequentially (and greedily)
3. Stops when all individuals are in the same groups

Ingredients

1. a dissimilarity measure (distance between individuals)
2. a merging criterion Δ (dissimilarity between clusters)

+ Generates a hierarchy of clustering instead of a single partition

– Need to select the number of cluster afterwards

Agglomerative Clustering: general algorithm

Algorithm

1. Start with $(\mathcal{C}_k^{(0)}) = (\{\mathbf{x}_i\})$ the collection of all singletons.
2. At step s, we have $n - s$ clusters $(\mathcal{C}_k^{(s)})$:
   - Find the two most similar clusters according to a criterion Δ:

$$(k, \ell) = \arg\min_{(k',\ell')} \Delta(\mathcal{C}_{k'}^{(s)}, \mathcal{C}_{ell'}^{(s)})$$

   - Merge $\mathcal{C}_k^{(s)}$ and $\mathcal{C}_\ell^{(s)}$ into $\mathcal{C}_k^{(s+1)}$
   - Update the distances between $\mathcal{C}_k^{(s+1)}$ and the remaining clusters
3. Repeat until there is only one cluster.

Complexity

- In general $O(n^3)$
- Can be reduced to $O(n^2)$ if boundering the number of merges

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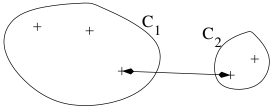
2. At step s, we have $n - s$ clusters $(\mathcal{C}_k^{(s)})$:
   - Find the two most similar clusters according to a criterion Δ:

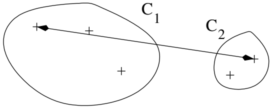
   $$(k, \ell) = \arg\min_{(k', \ell')} \Delta(\mathcal{C}_{k'}^{(s)}, \mathcal{C}_{ell'}^{(s)})$$

   - Merge $\mathcal{C}_k^{(s)}$ and $\mathcal{C}_\ell^{(s)}$ into $\mathcal{C}_k^{(s+1)}$
   - Update the distances between $\mathcal{C}_k^{(s+1)}$ and the remaining clusters
3. Repeat until there is only one cluster.

Complexity

- In general $O(n^3)$
- Can be reduced to $O(n^2)$ if boundering the number of merges





Merging criterion based on the distance between points

- Single linkage (or minimum linkage):

$$\Delta(\mathcal{C}_k, \mathcal{C}_\ell) = \min_{\mathbf{x}_i \in \mathcal{C}_k, \mathbf{x}_j \in \mathcal{C}_\ell} d(\mathbf{x}_i, \mathbf{x}_j)$$

- Complete linkage (or maximum linkage):

$$\Delta(\mathcal{C}_k, \mathcal{C}_\ell) = \max_{\mathbf{x}_i \in \mathcal{C}_k} \max_{\mathbf{x}_j \in \mathcal{C}_\ell} d(\mathbf{x}_i, \mathbf{x}_j)$$

- Average linkage (or group linkage):

$$\Delta(\mathcal{C}_k, \mathcal{C}_\ell) = \frac{1}{|\mathcal{C}_k||\mathcal{C}_\ell|} \sum_{\mathbf{x}_i \in \mathcal{C}_k} \sum_{\mathbf{x} \in \mathcal{C}_\ell} d(\mathbf{x}_i, \mathbf{x}_j)$$

Ward's criteria

Merging criterion based on distance to the mean

Ward's criterion:

$$\begin{aligned}\Delta(\mathcal{C}_k, \mathcal{C}_\ell) = &\sum_{\mathbf{x}_i \in \mathcal{C}_k} \left(d^2(\mathbf{x}_i, \boldsymbol{\mu}_{\mathcal{C}_k \cup \mathcal{C}_\ell}) - d^2(\mathbf{x}_i, \boldsymbol{\mu}_{\mathcal{C}_k})\right) \\ &+ \sum_{\mathbf{x}_j \in \mathcal{C}_\ell} \Big(d^2(\mathbf{x}_j, \boldsymbol{\mu}_{\mathcal{C}_j \cup \mathcal{C}_\ell}) - d^2(\mathbf{x}_j, \boldsymbol{\mu}_{\mathcal{C}_\ell})\Big)\end{aligned}$$

Inertia Intra-cluster

If d is the Euclidean distance, then

$$\Delta(\mathcal{C}_k, \mathcal{C}_\ell) = \frac{2|\mathcal{C}_k||\mathcal{C}_\ell|}{|\mathcal{C}_k| + |\mathcal{C}_\ell|} d^2(\boldsymbol{\mu}_{\mathcal{C}_k}, \boldsymbol{\mu}_{\mathcal{C}_\ell})$$

Ward's criteria: details

Recall that the intra-class inertia measures the homogenity of th size-K clustering

$$I_W = \sum_{k=1}^{K} \sum_{\mathbf{x}_i \in \mathcal{C}_k} \|\mathbf{x}_i - \boldsymbol{\mu}_{\mathcal{C}_k}\|_2^2$$

Consider the following two partitions

- $\mathcal{P} = (\mathcal{C}_1, \dots, \mathcal{C}_K)$ at one level of the hierarchy Ω
- $\mathcal{P}'$ is $\mathcal{P}$ once $\mathcal{C}_k, \mathcal{C}_\ell$ merged

Then

$$I_W(\mathcal{P}) - I_W(\mathcal{P}') = \frac{|\mathcal{C}_k||\mathcal{C}_\ell|}{|\mathcal{C}_k| + |\mathcal{C}_\ell|} d^2(\boldsymbol{\mu}_{\mathcal{C}_k}, \boldsymbol{\mu}_{\mathcal{C}_\ell}) = \frac{1}{2}\Delta(\mathcal{C}_k, \mathcal{C}_\ell).$$

$\rightsquigarrow$ At each step, Ward limits the increase of the intra class variance

$\rightsquigarrow$ Defines an indexed hierarchy (height of the dendrogram)

$\rightsquigarrow$ Same criteria as in the K-means algorithm

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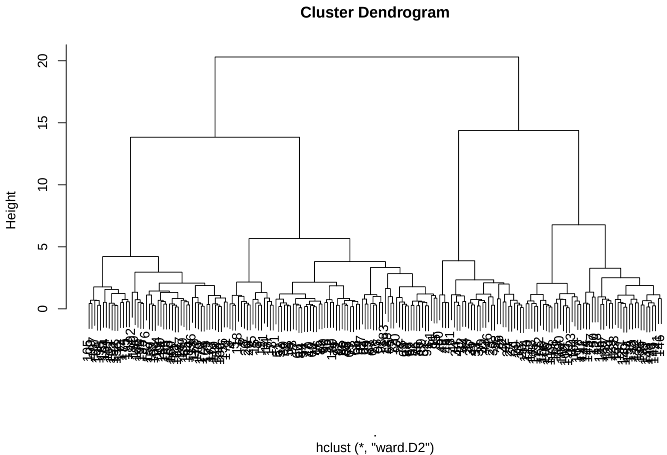
$\leadsto$ Defines an indexed hierarchy (height of the dendrogram)

$\leadsto$ Same criteria as in the K-means algorithm

Ward agglomerative clustering in R

```
Ward <- crabs_corrected %>%
  select(-sex, -species) %>%
  dist(method = "euclidean") %>%
  hclust(method = "ward.D2")
plot(Ward)
```



Ward agglomerative clustering in R: comparison I

Compare with out reference classification and k-means

```
aricode::ARI(cutree(Ward, 4), classes)

## [1] 0.6829729

aricode::ARI(cutree(Ward, 4), clusters)

## [1] 0.7999974
```

```
knitr::kable(table(clusters, cutree(Ward,4)),
caption = "k-means vs Ward")
```

Table: k-means vs Ward

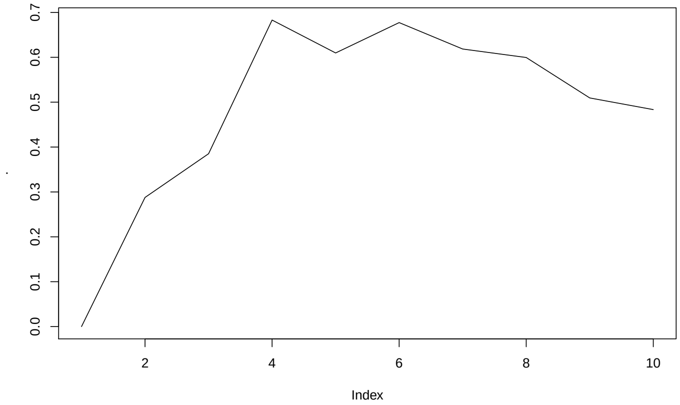
1	2	3	4
2	0	49	8
1	0	0	40
65	0	0	0
5	30	0	0

Ward agglomerative clustering in R: comparison II

Optimize over a range of values

```
Ward %>%  cutree(k = 1:10) %>%  as.data.frame() %>% as.list() %>%
  sapply(aricode::ARI, classes) %>% plot(type = "l")
```

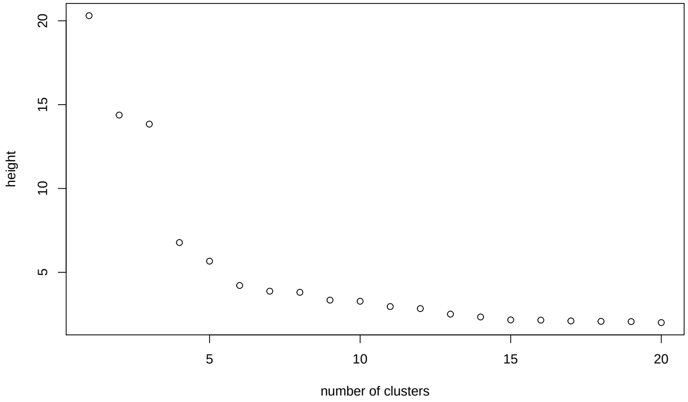
Ward agglomerative clustering in R: comparison III



Look at Ward intra-class variance

Ward agglomerative clustering in R: comparison IV

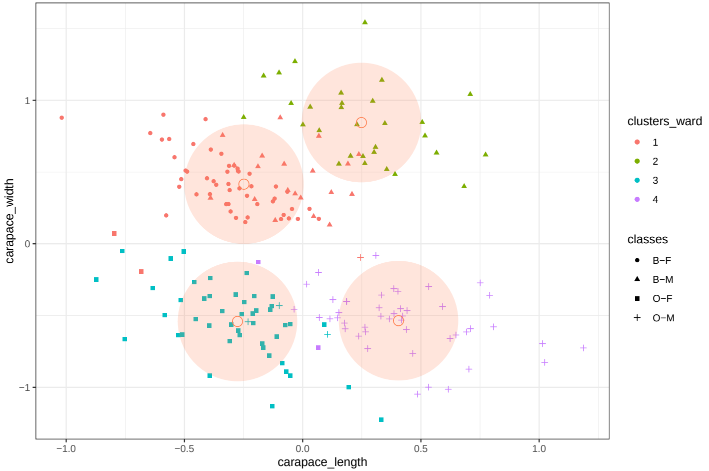
```r
plot(rev(Ward$height)[1:20], xlab = "number of clusters", ylab = "height")
```



Ward agglomerative clustering in R: projection I

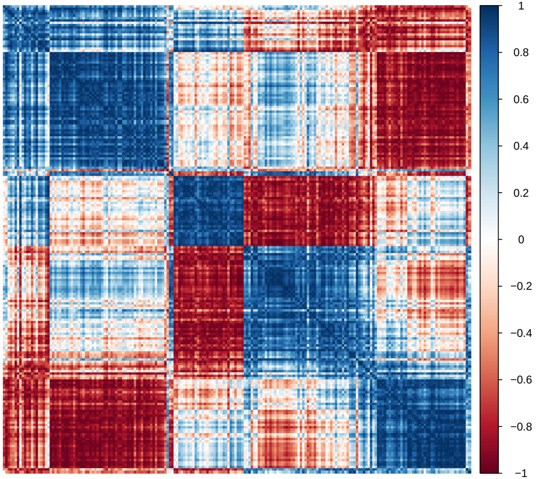
```r
clusters_ward <- as.factor(cutree(Ward, 4))
centers_ward  <- select(crabs_corrected, -sex, -species) %>%
  aggregate(list(cutree(Ward, 4)), mean) %>% as_tibble() %>% select(-Group.1)

crabs_corrected %>%
  ggplot(aes(x = carapace_length, y = carapace_width, color = clusters_ward)) +
  geom_point(aes(shape = classes)) +
  geom_point(data = centers_ward, color = 'coral', size = 4 , pch = 21) +
  geom_point(data = centers_ward, color = 'coral', size = 50, alpha = 0.2)
```

Ward agglomerative clustering in R: projection II



Reordered correlation matrix between individuals

```
C <- cor(t(select(crabs_corrected, -sex, -species)))
C <- C[order(clusters_ward),order(clusters_ward)]
  corrplot(C, method = "color", tl.pos = "n")
```



Outline

References

- Pattern recognition and machine learning,
  Christopher Bishop
  Chapter 9: Mixture Models and EM
  http://users.isr.ist.utl.pt/~wurmd/Livros/school/
- Models with Hidden Structure with Applications in Biology and Genomics,
  Stéphane Robin
  Master MathSV Course
  https://www6.inra.fr/mia-paris/content/download/4587/42934/version/1/file/ModelsHiddenStruct-Biology.pdf
- Classification non-supervisées,
  É. Lebarbier, T. Mary-Huard
  Chapitre 3 - méthode probabiliste: le modèle de mélange
  https://www.agroparistech.fr/IMG/pdf/ClassificationNonSupervisee-AgroParisTech.pdf

Outline

Latent variables models

Definition

A latent variable model is a statistical model that relates, for $i = 1, \dots, n$ individuals,

- a set of manifest (observed) variables $\mathbf{X} = (X_i, i = 1, \dots, n)$ to
- a set of latent (unobserved) variables $\mathbf{Z} = (Z_i, i = 1, \dots, n)$.

Common assumption: conditional independence

$$\mathbb{P}((X_1, \dots, X_n)|(Z_1, \dots, Z_n)) = \prod_{i=1}^{n} \mathbb{P}(X_i|Z_i).$$

Famous examples

- $(Z_i, i \geq 1)$ is Markov chain: Markov models
- Z_i categorical and independent: mixture models

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Mixture models: the latent variables

When $(Z_1, \ldots, Z_n)$ are independent categorical variables, they give a natural (latent) classification of the observations $(X_1, \ldots, X_n)$ – or labels.

Notations

Let $(Z_1, \ldots, Z_n)$ be *iid* categorical variables with distribution

$$\mathbb{P}(i \in q) = \mathbb{P}(Z_i = q) = \alpha_q, \quad \text{s.t.} \sum_{q=1}^{Q} \alpha_q = 1.$$

Alternative (equivalent) notation

Let $Z_i = (Z_{i1}, \ldots, Z_{iq})$ be an indicator vector of label for i:

$$\mathbb{P}(i \in q) = \mathbb{P}(Z_{iq} = 1) = \alpha_q, \quad \text{s.t.} \sum_{q=1}^{Q} \alpha_q = 1.$$

By definition, $Z_i \sim \mathcal{M}(1, \boldsymbol{\alpha})$, with $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_Q)$.

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Mixture models: the manifest variables

A mixture model represents the presence of subpopulations within an overall population as follows:

$$\mathbb{P}(X_i) = \sum_{z_i \in \mathcal{Z}_i} \mathbb{P}(X_i, Z_i) = \sum_{Z_i \in \mathcal{Z}_i} \mathbb{P}(X_i | Z_i) \mathbb{P}(Z_i).$$

Conditional distribution of the manifest variables

We assume a parametric distribution of X in each subpopulation

$$X_i | \{Z_i = q\} \sim \mathbb{P}_{\theta_q} \qquad \left(\Leftrightarrow X_i | \{Z_{iq}\} = 1 \sim \mathbb{P}_{\theta_q} \right)$$

The specificity of each class is handled by $\{\boldsymbol{\theta}_q\}_{q=1}^{Q}$.

Mixture models: likelihoods

The complete-data likelihood

It is the join distribution of (X_i, Z_i):

$$\mathbb{P}(X_i, Z_i) = \alpha_{Z_i} \mathbb{P}_{\boldsymbol{\theta}_{Z_i}}(X_i)$$

The incomplete-data likelihood

It is the marginal distribution of X_i once Z_i integrated:

$$\mathbb{P}(X_i) = \sum_{q=1}^{Q} \mathbb{P}(X_i, Z_i = q) = \sum_{q=1}^{Q} \alpha_q \mathbb{P}_{\boldsymbol{\theta}_q}(X_i)$$

$\rightsquigarrow$ A mixture model is a sum of distributions weigthed by the proportion of each subpopulation.

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Outline

Intractability of the Likelihood

Maximum Likelihood Estimator

The MLE aims to maximize the (marginal) likehood of the observations:

$$L(\boldsymbol{\theta}; \mathbf{X}) = \mathbb{P}_{\boldsymbol{\theta}}((X_1, \dots, X_n)) = \int_{\mathbf{Z} \in \mathcal{Z}} \mathbb{P}_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{Z}) \mathrm{d}\mathbf{Z}$$

Integrations are summation over $\{1, \dots, Q\}$: we have Q^n terms !

Intractable summation

With mixture models, for $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_Q)$ we have

$$\log L(\boldsymbol{\theta}; \mathbf{X}) = \sum_{i=1}^{n} \log \left\{ \sum_{q=1}^{Q} \alpha_q \mathbb{P}_{\boldsymbol{\theta}_q}(X_i) \right\}.$$

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$\rightsquigarrow$ Direct maximization of the likelihood is impossible in practice

Bayes decision rule / Maximum *a posteriori*

Principle

Affect an individual i to the subpopulation which is the most likely according to the data:

$$\tau_{iq} = \mathbb{P}(Z_{iq} = 1 | X_i = x_i)$$

This is the posterior probability for $i \in q$.

Application of the Bayes Theorem

It is straightforward to show that

$$\tau_{iq} = \frac{\alpha_q \mathbb{P}_{\theta_q}(x_i)}{\sum_{q=1}^{Q} \alpha_q \mathbb{P}_{\theta_q}(x_i)}$$

Principle of the EM algorithm

If $\boldsymbol{\theta}$ were known

…estimating the posterior probability $\mathbb{P}(Z_i|\mathbf{X})$ of $\mathbf{Z}$ should be easy
By means of the Bayes decision rule

If $\mathbf{Z}$ were known…

…estimating the best set of parameter $\boldsymbol{\theta}$ should be easy
This is close to usual maximum likelihood estimation

EM principle

Maximize the marginal likelihood iteratively:

1. Initialize θ
2. Compute the probability of $\mathbf{Z}$ given θ
3. Get a better θ with the new $\mathbf{Z}$
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Formal algorithm

Initialization: start from a good guess either of $\mathbf{Z}$ or $\boldsymbol{\theta}$, then iterate 1-2

1. Expectation step

Calculate the expected value of the loglikelihood under the current $\boldsymbol{\theta}$

$$Q\left(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}\right) = \mathbb{E}_{\mathbf{Z}|\mathbf{X};\boldsymbol{\theta}^{(t)}}\big[\log L(\boldsymbol{\theta};\mathbf{X},\mathbf{Z})\big] \qquad (\textit{needs } \mathbb{P}_{\boldsymbol{\theta}^{(t)}}(\mathbf{Z}|\mathbf{X}))$$

2. Maximization step

Find the parameters that maximize this quantity

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} Q\left(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}\right)$$

Stop when $\|\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\| < \varepsilon$ or $\|Q^{(t+1)} - Q^{(t)}\| < \varepsilon$

(Basic) Convergence analysis

Theorem

At each step of the EM algorithm, the loglikelihood increases. EM thus reaches a local optimum.

Proof.

On board. □

Choosing the number of component

Reminder: Bayesian Information Criterion

The BIC is a model selection criterion which penalizes the adjustement to the data by the number of parameter in model $\mathcal{M}$ as follows:

$$\mathrm{BIC}(\mathcal{M}) = \log L(\hat{\boldsymbol{\theta}}; \mathbf{X}) - \frac{1}{2}\log(n)\mathrm{df}(\mathcal{M}).$$

Integrated Classification Criterion

It is an adaptation working with the complete-data likelihood:

$$\begin{aligned}\mathrm{ICL}(\mathcal{M}) &= \log L(\hat{\boldsymbol{\theta}}; \mathbf{X}, \hat{\mathbf{Z}}) + \frac{1}{2}\log(n)\mathrm{df}(\mathcal{M}) \\ &= \mathrm{BIC} - \mathcal{H}(\mathbb{P}(\hat{\mathbf{Z}}|\mathbf{X}),\end{aligned}$$

where the entropy $\mathcal{H}$ measures the separability of the subpopulations.

$\rightsquigarrow$ We choose $\mathcal{M}(Q)$ that maximizes either BIC or ICL

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Popular model: Gaussian Multivariate mixture models

The distribution of X_i conditional on the label of i is assumed to be a multivariate Gaussian distribution with unknown parameters:

$$X_i | i \in q \sim \mathcal{N}(\boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q)$$

Complete Likelihood $(\mathbf{X}, \mathbf{Z})$

The model complete loglikelihood is

$$\log L(\boldsymbol{\mu}, \boldsymbol{\Sigma}; \mathbf{X}, \mathbf{Z}) = \sum_{i=1}^{n} \sum_{q=1}^{Q} Z_{iq} \left(\log \alpha_q - \frac{1}{2} \log \det(\boldsymbol{\Sigma}_q) - \frac{1}{2} \|\mathbf{x}_i - \boldsymbol{\mu}_q\|^2_{\boldsymbol{\Sigma}_q^{-1}} \right) + c$$

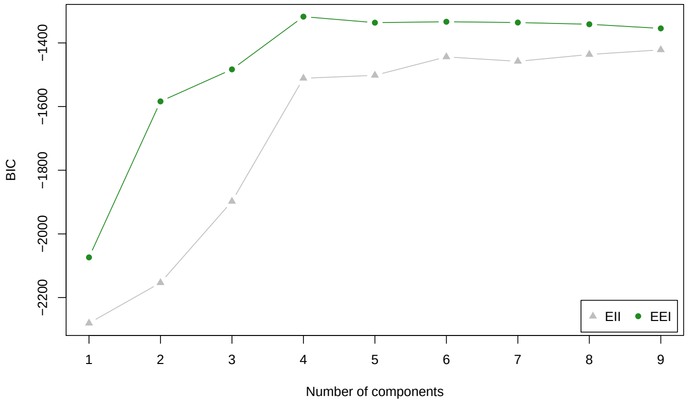
$\rightsquigarrow$ Implementation of the univariate case during the labs.

Gaussian mixture model in R I

The package Mclust is a great reference
See https://cran.r-project.org/web/packages/mclust/vignettes/mclust.html

```
GMM <- crabs_corrected %>%
  select(-sex, -species) %>%
  Mclust(modelNames = c("EII", "EEI"))
plot(GMM, 'BIC')
```

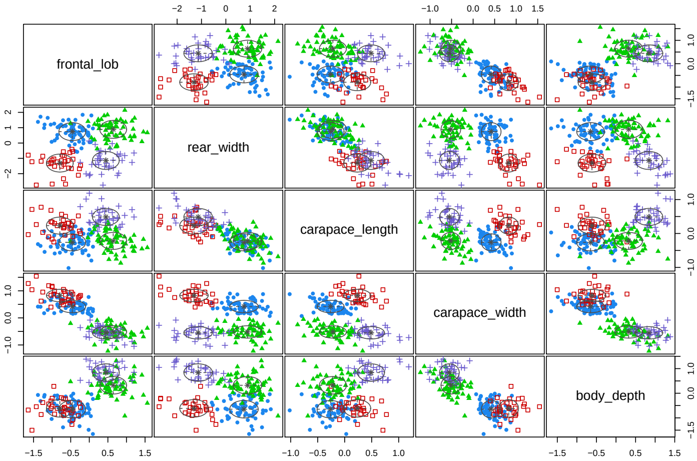
Gaussian mixture model in R II



Gaussian mixture model in R III

```
aricode::ARI(GMM$classification, classes)

## [1] 0.6451662

aricode::ARI(GMM$classification, clusters)

## [1] 0.8746812

aricode::ARI(GMM$classification, clusters_ward)

## [1] 0.8209783

plot(GMM, 'classification')
```

Gaussian mixture model in R IV


frontal_lob
rear_width
carapace_length
carapace_width
body_depth