Data anaysis and Unsupervised Learning

Clustering: distance-based methods

MAP 573, 2020 – Julien Chiquet

École Polytechnique, Autumn semester, 2020

https://jchiquet.github.io/MAP573

Packages required for reproducing the slides

```
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(FactoMineR) # PCA and oter linear method for dimension reduction
library(factoextra) # fancy plotting for FactoMineR output
library(kernlab)    # Kernel-based methods, among which spectral-clustering
library(aricode)    # fast computation of clustering measures
library(animation)  # kmeans animation slides
library(igraph)     # graph manipulation
theme_set(theme_bw()) # plots themes
```

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.

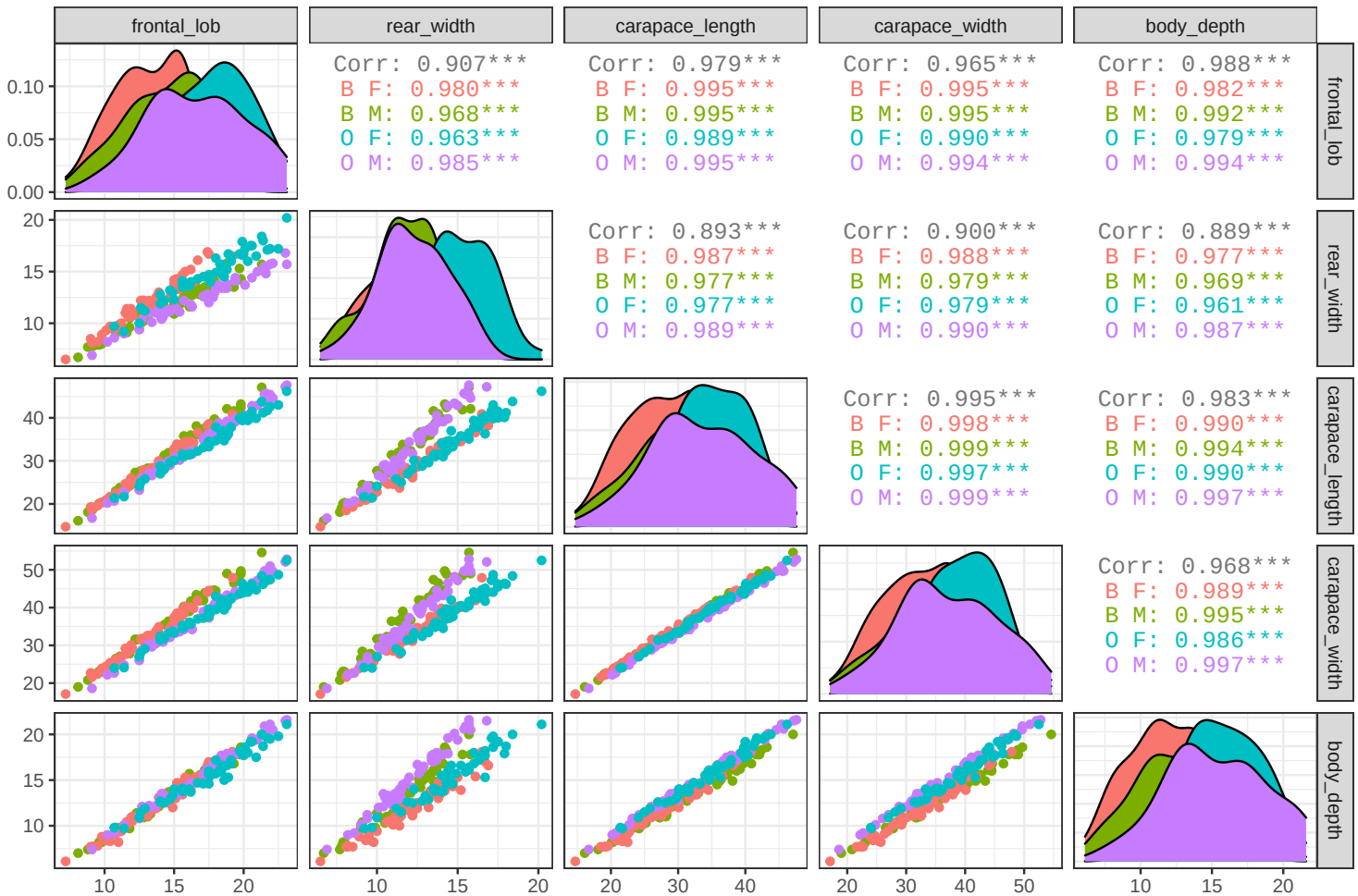
```
crabs <- MASS::crabs %>% select(-index) %>%
  rename(sex = sex,
         species          = sp,
         frontal_lob      = FL,
         rear_width       = RW,
         carapace_length = CL,
         carapace_width   = CW,
         body_depth       = BD)
crabs %>% select(sex, species) %>% summary()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

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

Companion data set II

Pairs plot of attributes

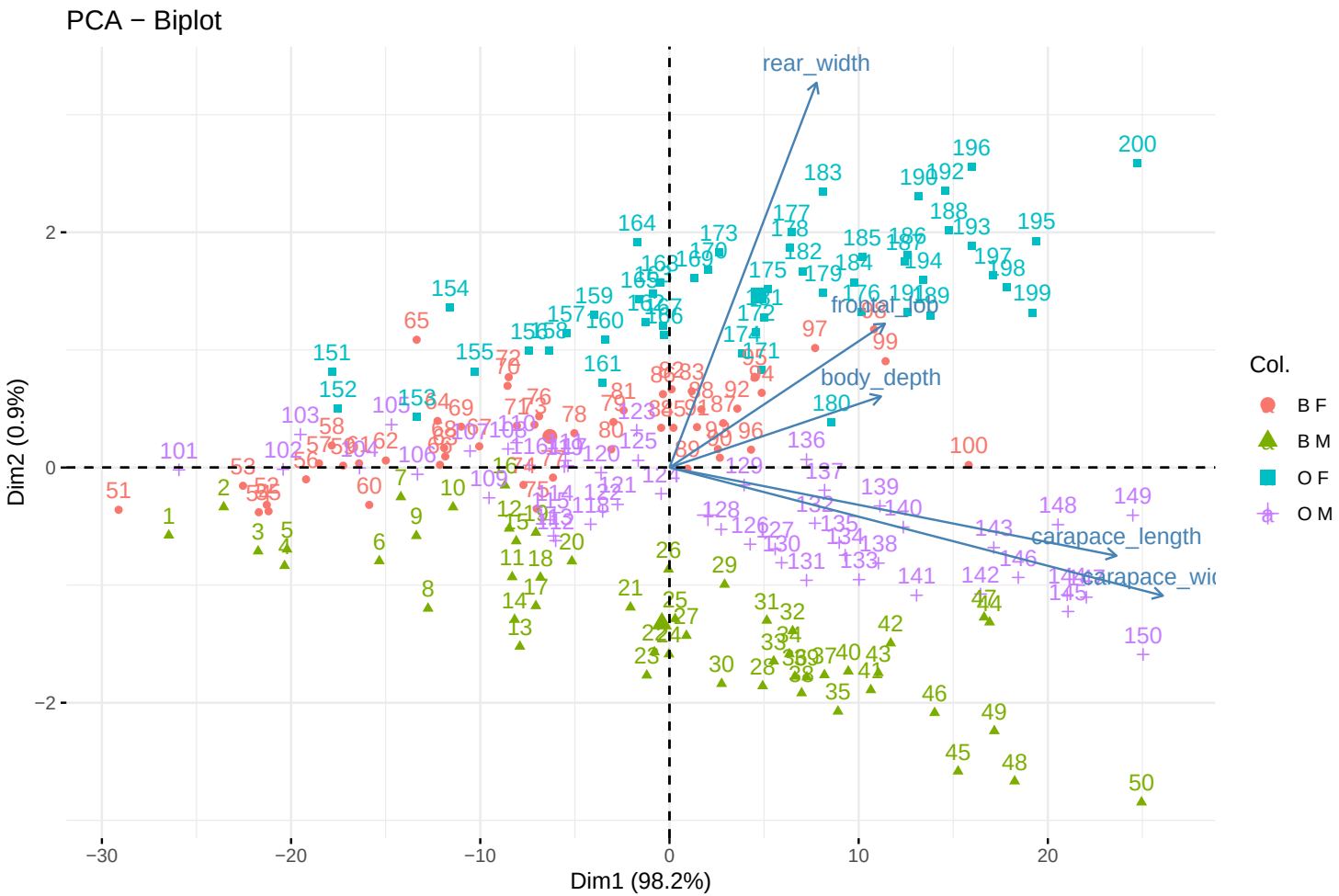
```
ggpairs(crabs, columns = 3:7, aes(colour = paste(crabs$species, crabs$sex)))
```



Companion data set III

PCA on the attributes

```
select(crabs, -species, -sex) %>% PCA(scale.unit = FALSE, graph = FALSE) %>%
  fviz_pca_biplot(axes = c(1,2), col.ind = paste(crabs$species, crabs$sex))
```



Remove size effect I

Carried by the 1st principal component

First component

$$\mathbf{f}_1 = \mathbf{X}^c \mathbf{u}_1.$$

We extract the best rank-1 approximation of $\mathbf{X}$ to remove the *size effect*, carried by the first axis, and return to the original space,

$$\tilde{\mathbf{X}}^{(1)} = \mathbf{f}_1 \mathbf{u}_1^\top.$$

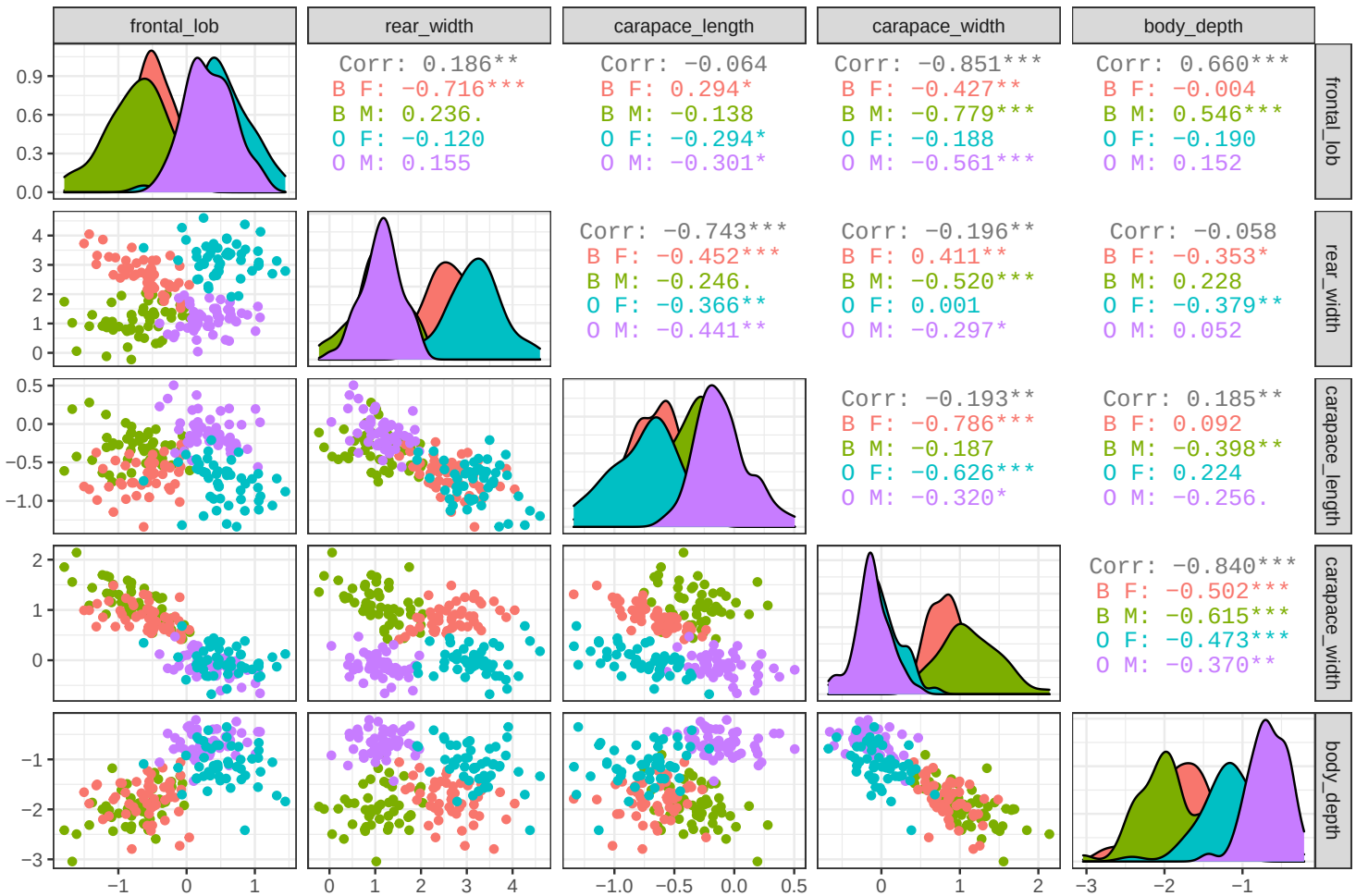
```
attributes <- select(crabs, -sex, -species) %>% as.matrix()
u1 <- eigen(cov(attributes))$vectors[, 1, drop = FALSE]
attributes_rank1 <- attributes %*% u1 %*% t(u1)
crabs_corrected <- crabs
crabs_corrected[, 3:7] <- attributes - attributes_rank1
```

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

Remove size effect II

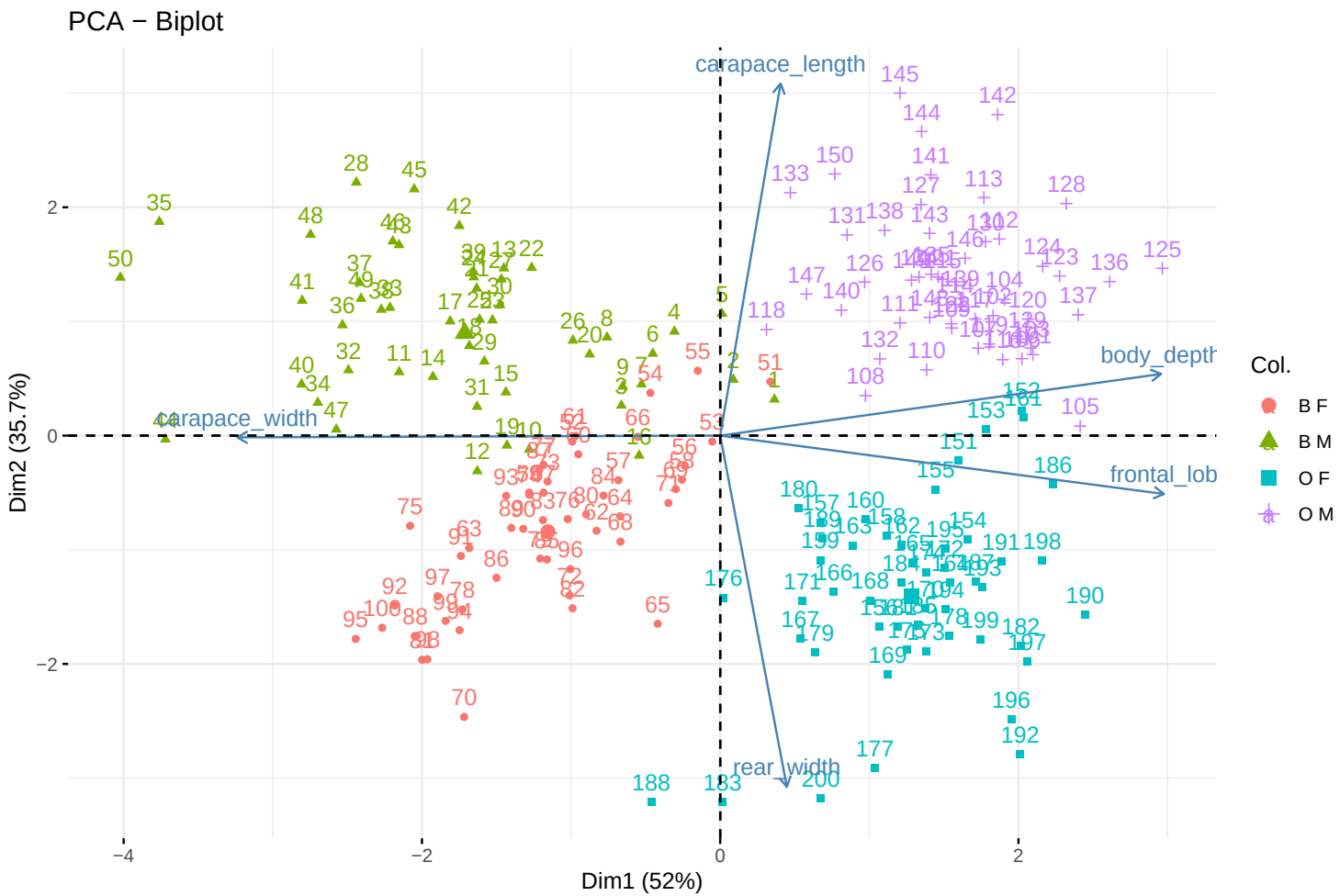
Carried by the 1st principal component

```
ggpairs(crabs_corrected, columns = 3:7, aes(colour = paste(crabs$species, crabs$sex
```



PCA on corrected data

```
select(crabs_corrected, -species, -sex) %>% FactoMineR::PCA(graph = FALSE) %>%
fviz_pca_biplot(col.ind = paste(crabs_corrected$species, crabs_corrected$sex))
```



Questions

1. Could we automatically identify some grouping (clustering) between samples?
2. Would this clustering correspond to some known labels (sex, species)?
3. Do we need to transform the data before we perform clustering?

Clustering: general goals

Objective: construct a map

$$f : \mathcal{D} = \{1, \ldots, n\} \mapsto \{1, \ldots, K\}$$

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 $\mathbb{P}$

Part II

Distance-based method

Outline

Distance-based method

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.

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

Dissimilarity and Distance

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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 $\mathcal{P} = \{P_1, \ldots, P_K\}$ 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 $\Omega = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ 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;*
- $\{\Omega, P_1, \ldots, P_K, \mathbf{x}_1, \ldots, \mathbf{x}_n\}$ *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	$\dots$	$V_{\|V\|}$	Sums
U_1	n_{11}	n_{12}	$\dots$	$n_{1\|V\|}$	$n_{1.}$
U_2	n_{21}	n_{22}	$\dots$	$n_{2\|V\|}$	$n_{2.}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$U_{\|U\|}$	$n_{\|U\|1}$	$n_{\|U\|2}$	$\dots$	$n_{\|U\|\|V\|}$	$n_{\|U\|.}$
Sums	$n_{.1}$	$n_{.2}$	$\dots$	$n_{.\|V\|}$	$n_{..} = n$

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

Distance-based method

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

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

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

K-means algorithm (Loyds)

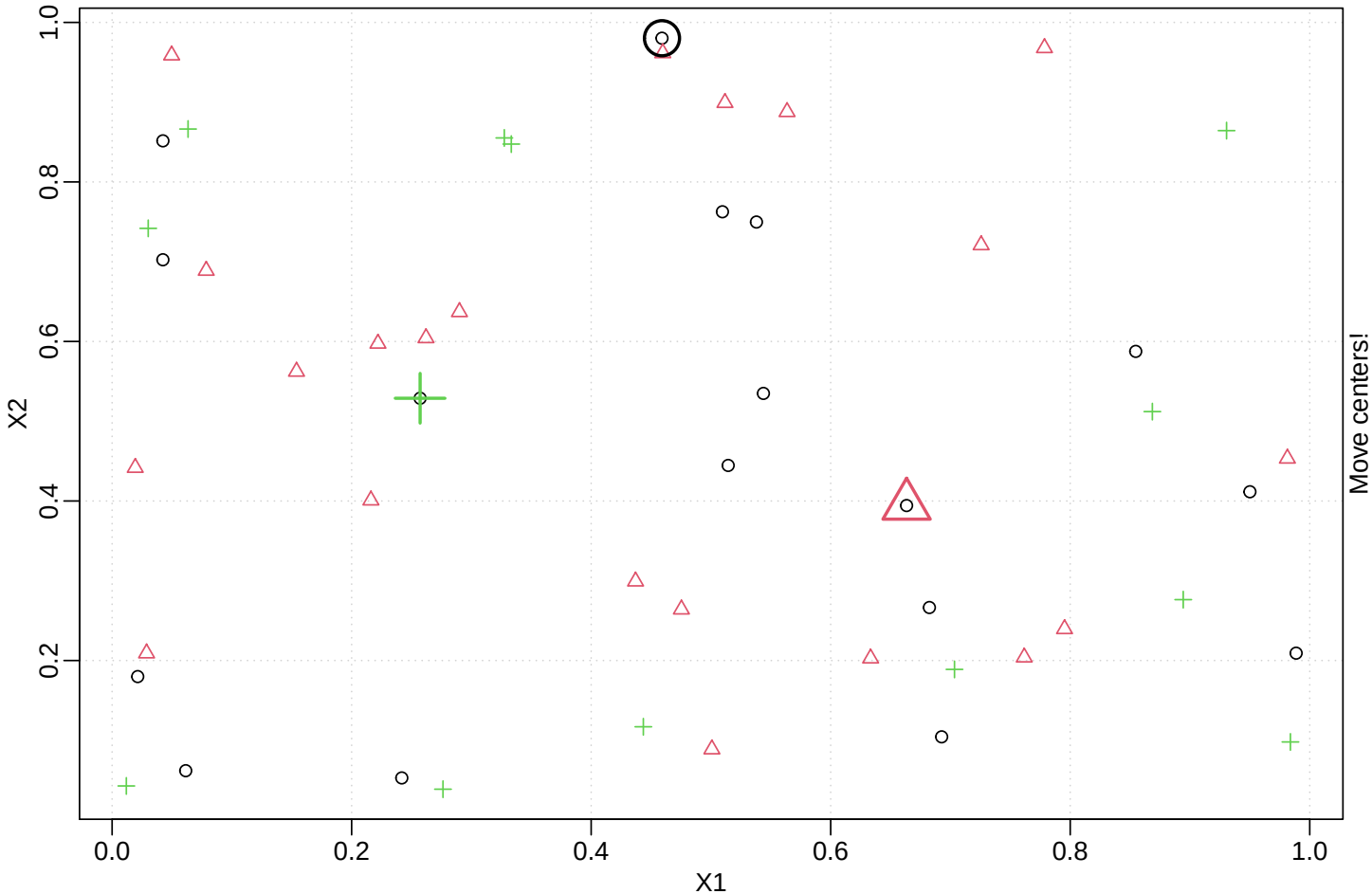
Initialization start by a (pseudo) random choice for the centers $\boldsymbol{\mu}_k$

Alternate until convergence

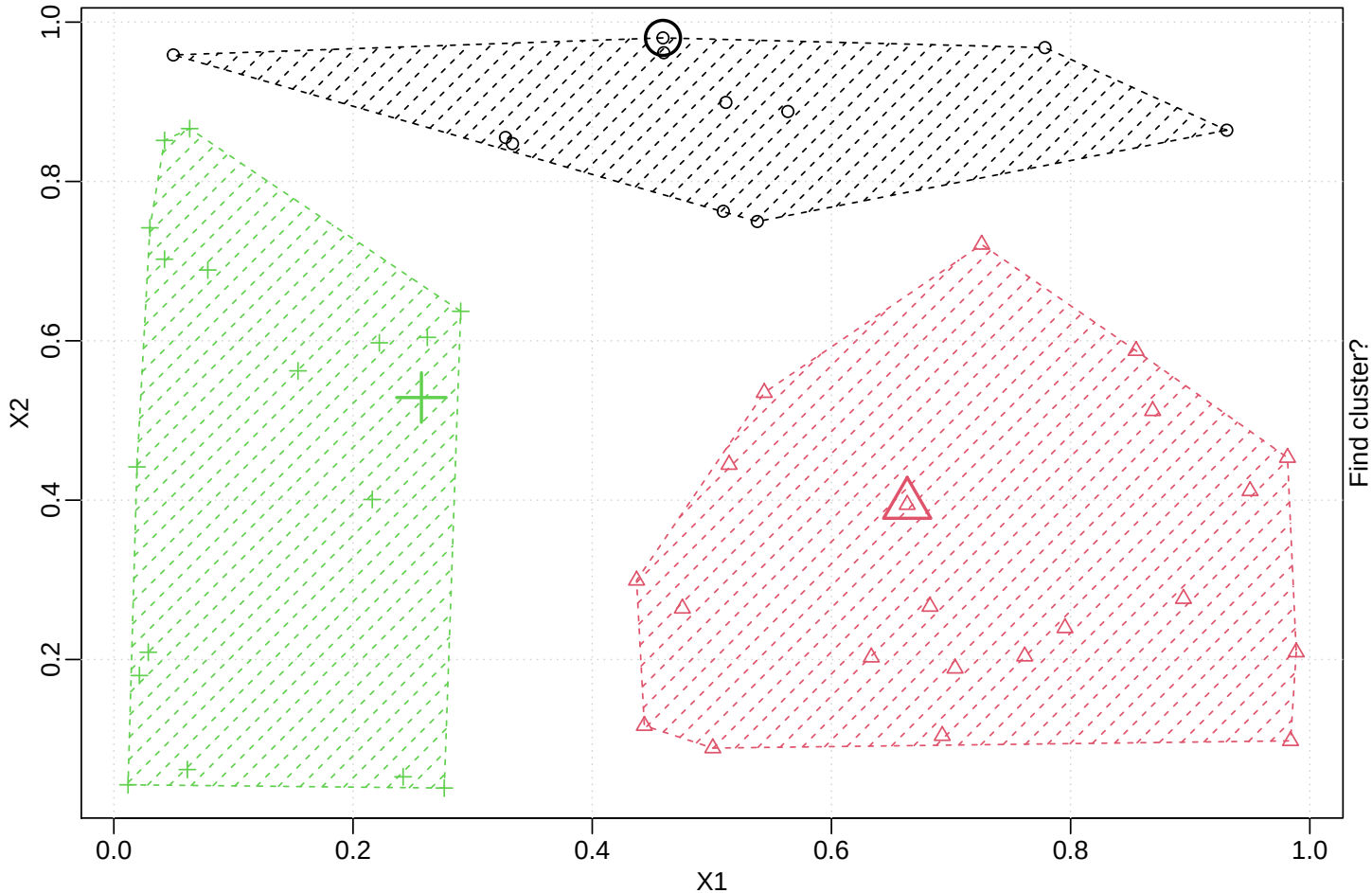
step 1 given $\boldsymbol{\mu}$, chose $\mathbf{c}$ minimizing $I_w \equiv$ assign $\mathbf{x}_i$ to the nearest prototype

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

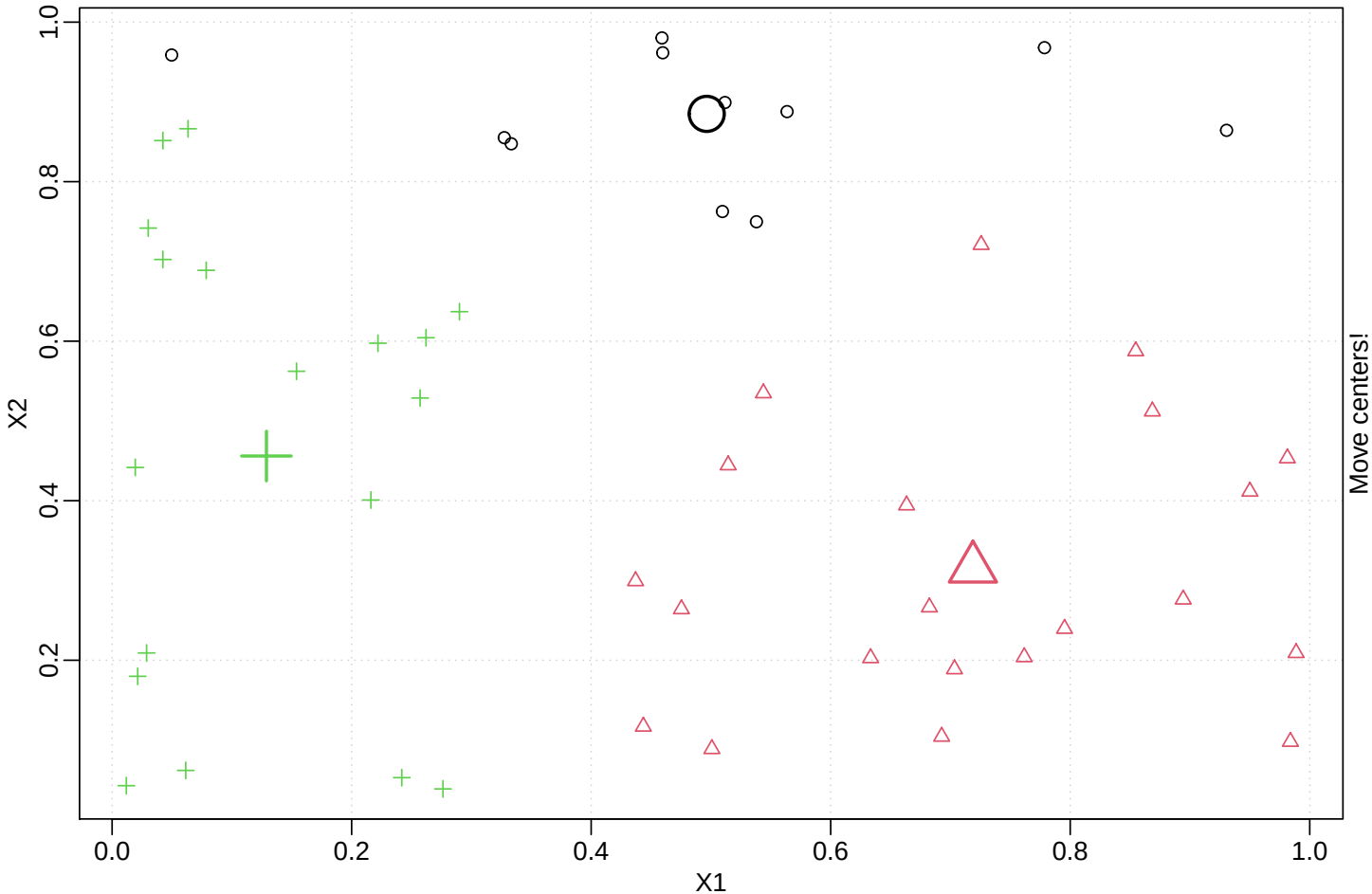
K-means in action I



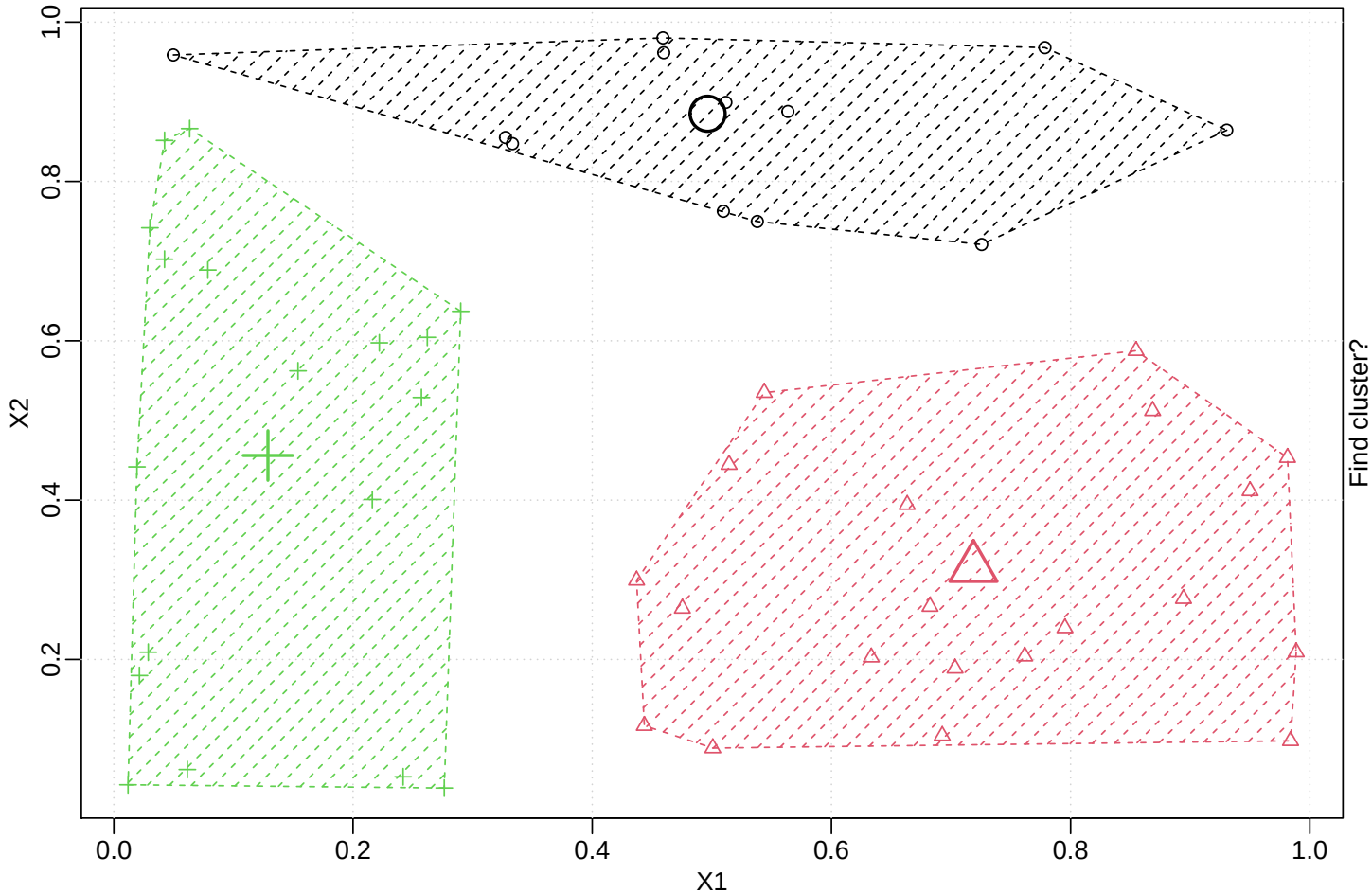
K-means in action II



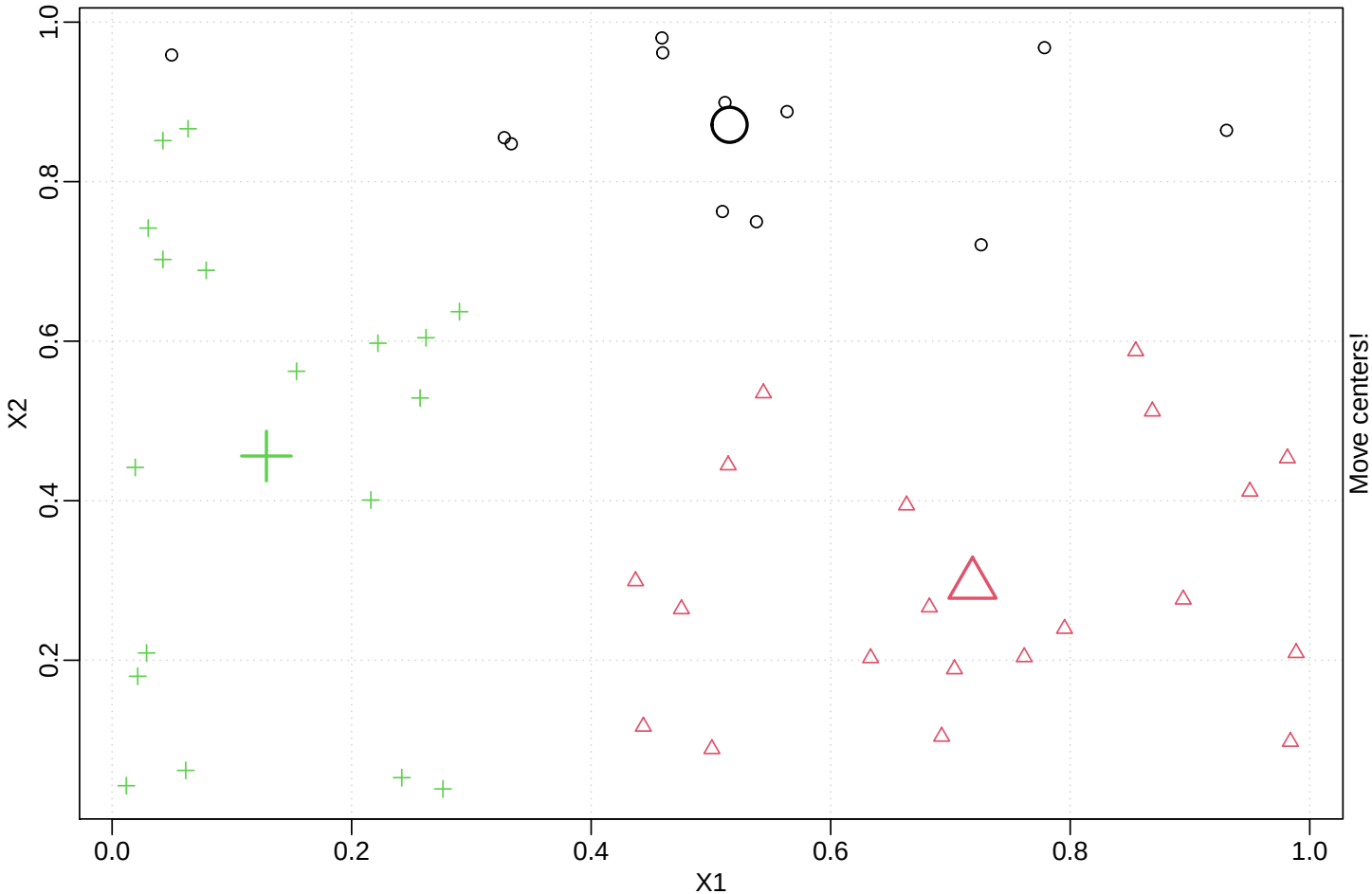
K-means in action III



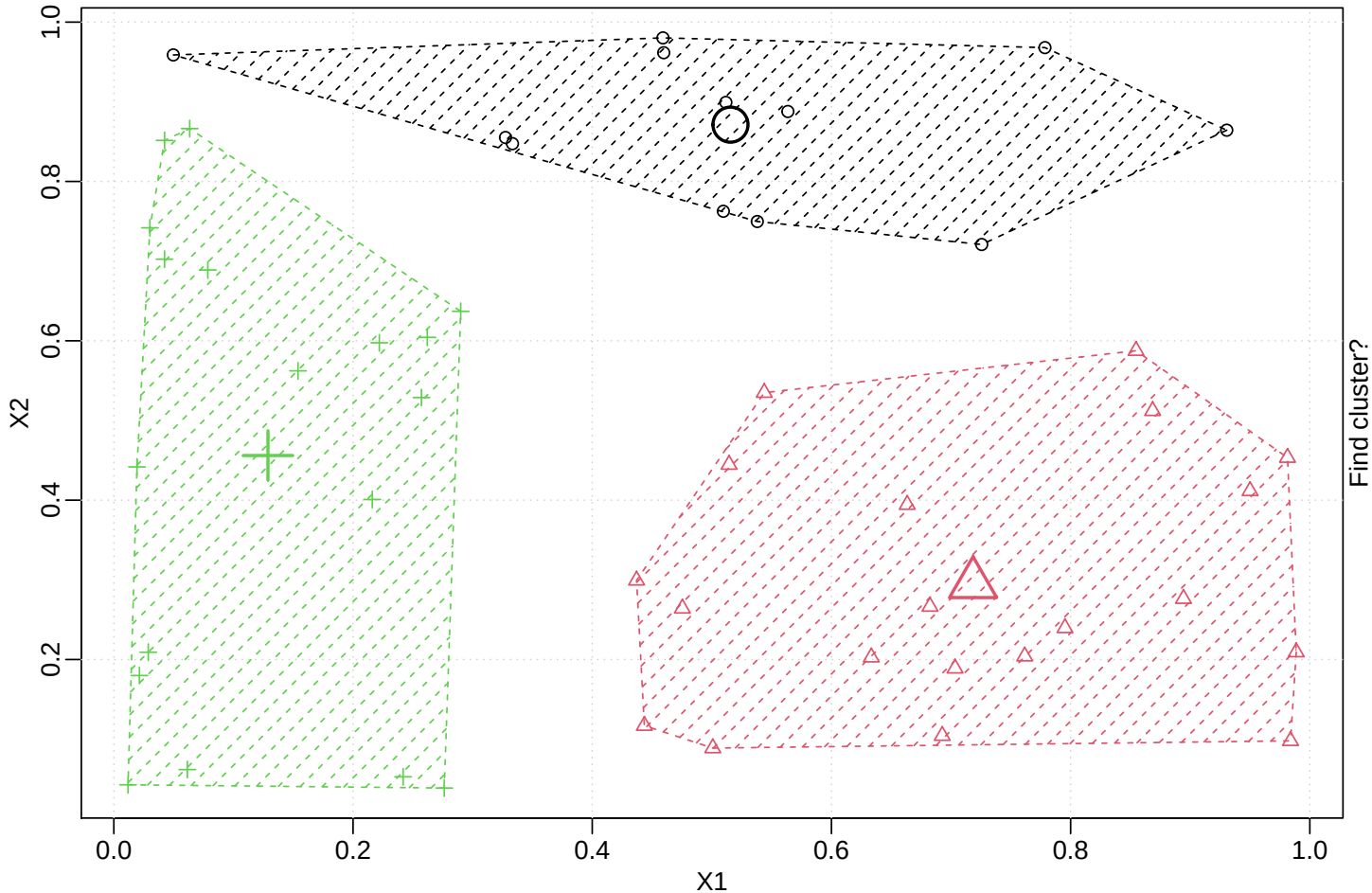
K-means in action IV



K-means in action V



K-means in action VI



K-means: 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

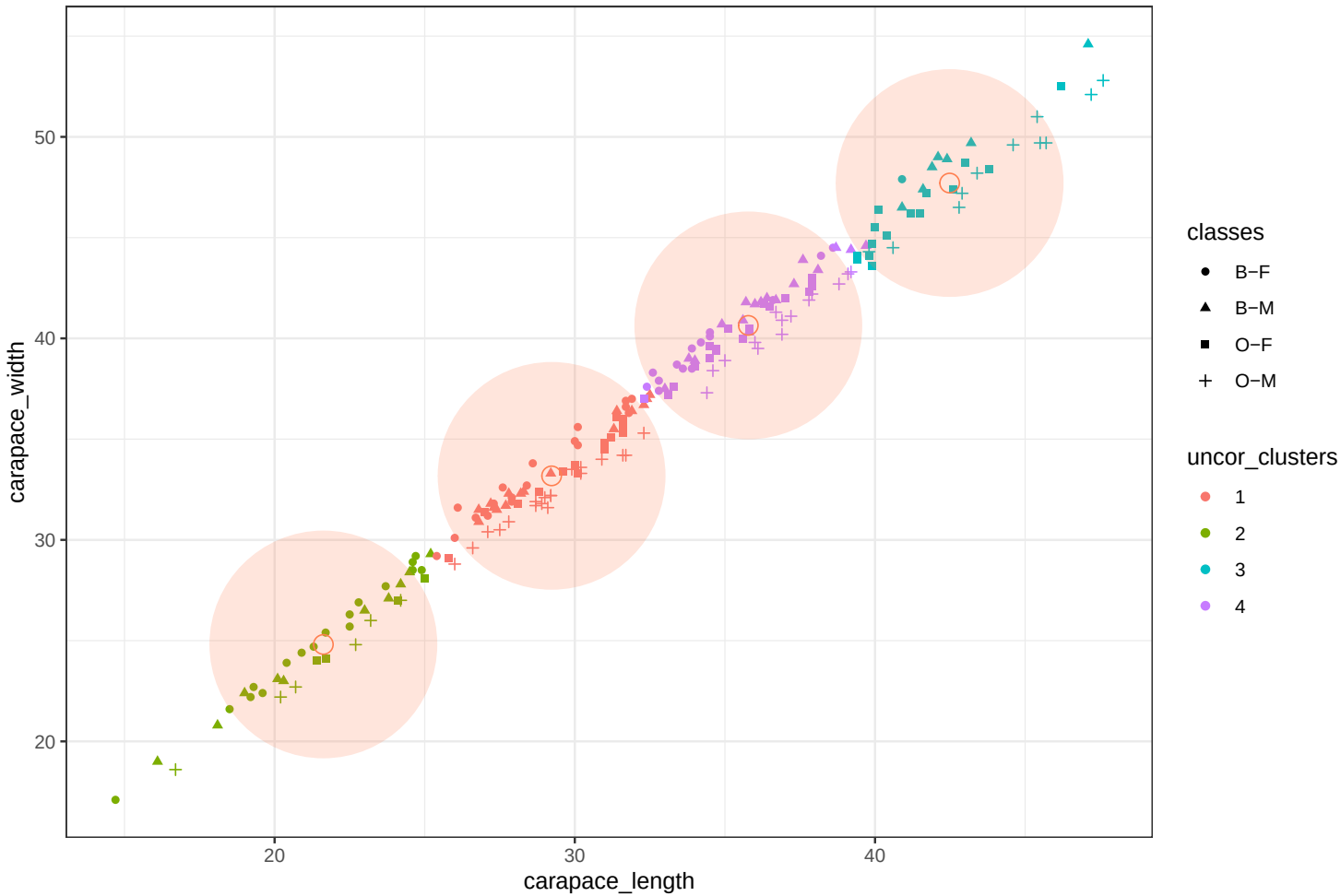
$O(nKT)$ where T is the number of step in the algorithm.

K-means in R on uncorrected data set I

```
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

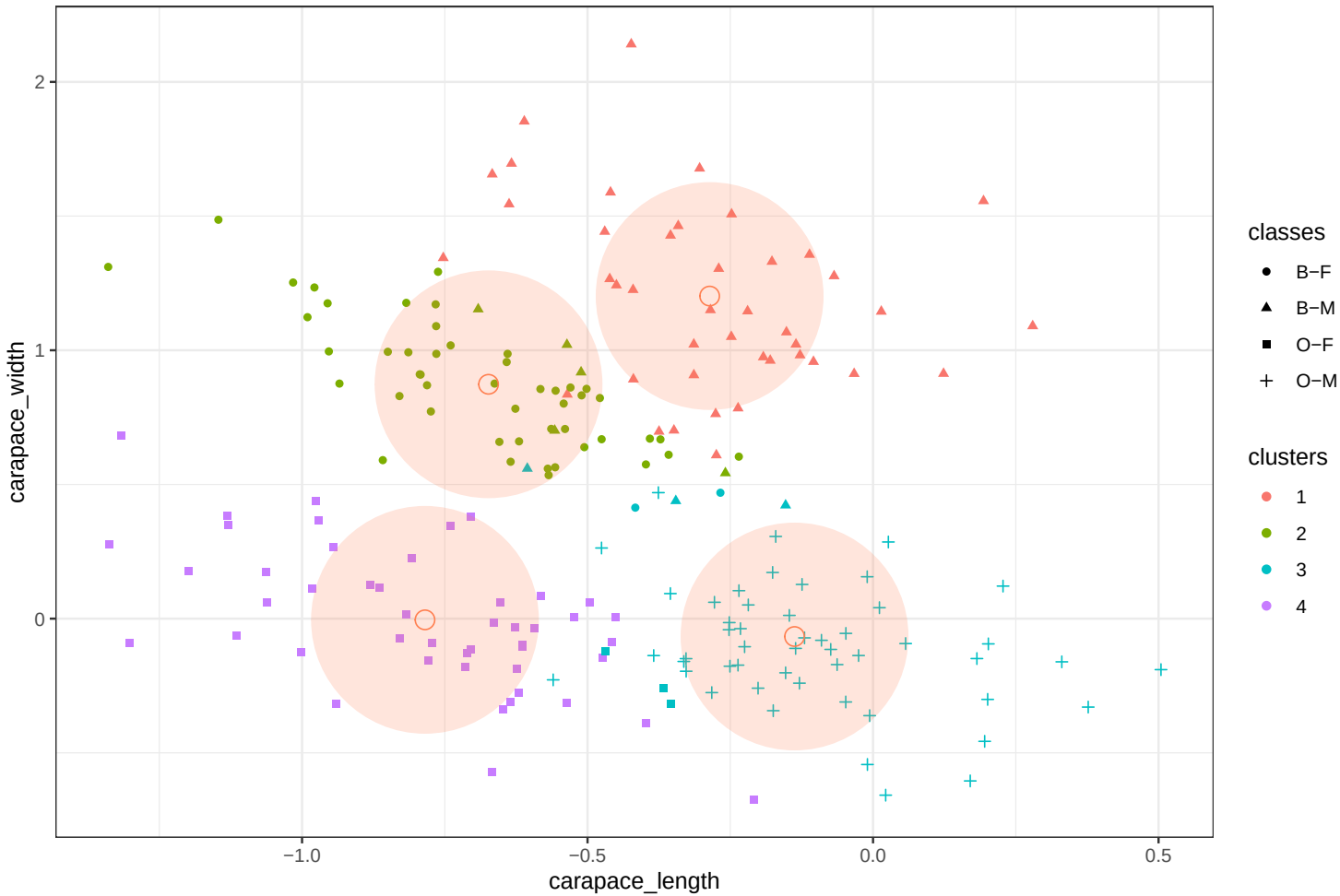


K-means in R on corrected crabs data set I

```
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) +
  geom_point(data = centers, color = 'coral', size = 50, alpha = 0.2)
```

K-means in R on corrected crabs data set II



Clustering comparison

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

## [1] 0.8317615

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	42	0	0
48	5	0	0
2	3	3	50
0	0	47	0

How about a "spectral" k-means? I

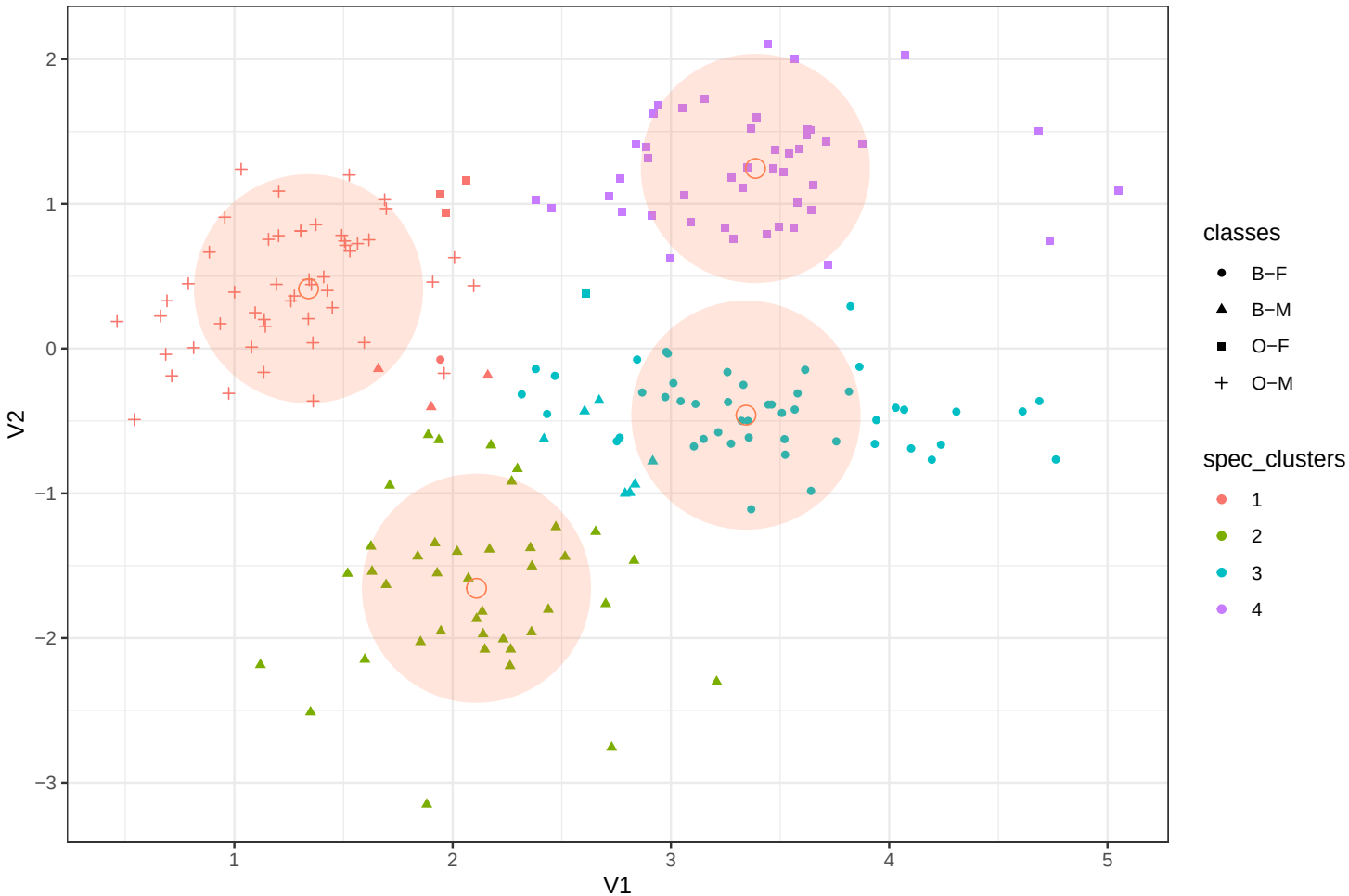
PCA + k-means

```
SVD <- svd(select(crabs_corrected, -species, -sex))
spec_crabs <- as.tibble(SVD$u[,1:2] %*% diag(SVD$d[1:2]))
spec_kmeans_res <- spec_crabs %>%
  kmeans(4, nstart = 10)
spec_clusters <- as.factor(spec_kmeans_res$cluster)
spec_centers  <- as.tibble(spec_kmeans_res$centers)
classes <- paste(crabs_corrected$species, crabs_corrected$sex, sep = "-")

ggplot(spec_crabs, aes(V1, V2, color = spec_clusters)) +
  geom_point(aes(shape = classes)) +
  geom_point(data = spec_centers, color = 'coral', size = 4 , pch = 21) +
  geom_point(data = spec_centers, color = 'coral', size = 50, alpha = 0.2)
```

How about a "spectral" k-means? II

PCA + k-means



How about a "spectral" k-means? III

PCA + k-means

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

## [1] 0.8090372
```

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

Table: Estimating structure with spectral k-means

B-F	B-M	O-F	O-M
1	3	3	50
0	40	0	0
49	7	1	0
0	0	46	0

Outline

Distance-based method

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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- In general $O(n^3)$
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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:

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

Euclidean case

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 inertia measures the homogenity of th size-K clustering

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

Consider the following two partitions

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

Then

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

$\rightsquigarrow$ At each step, Ward limits the loss (increase) of the intra (inter) class variance

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

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

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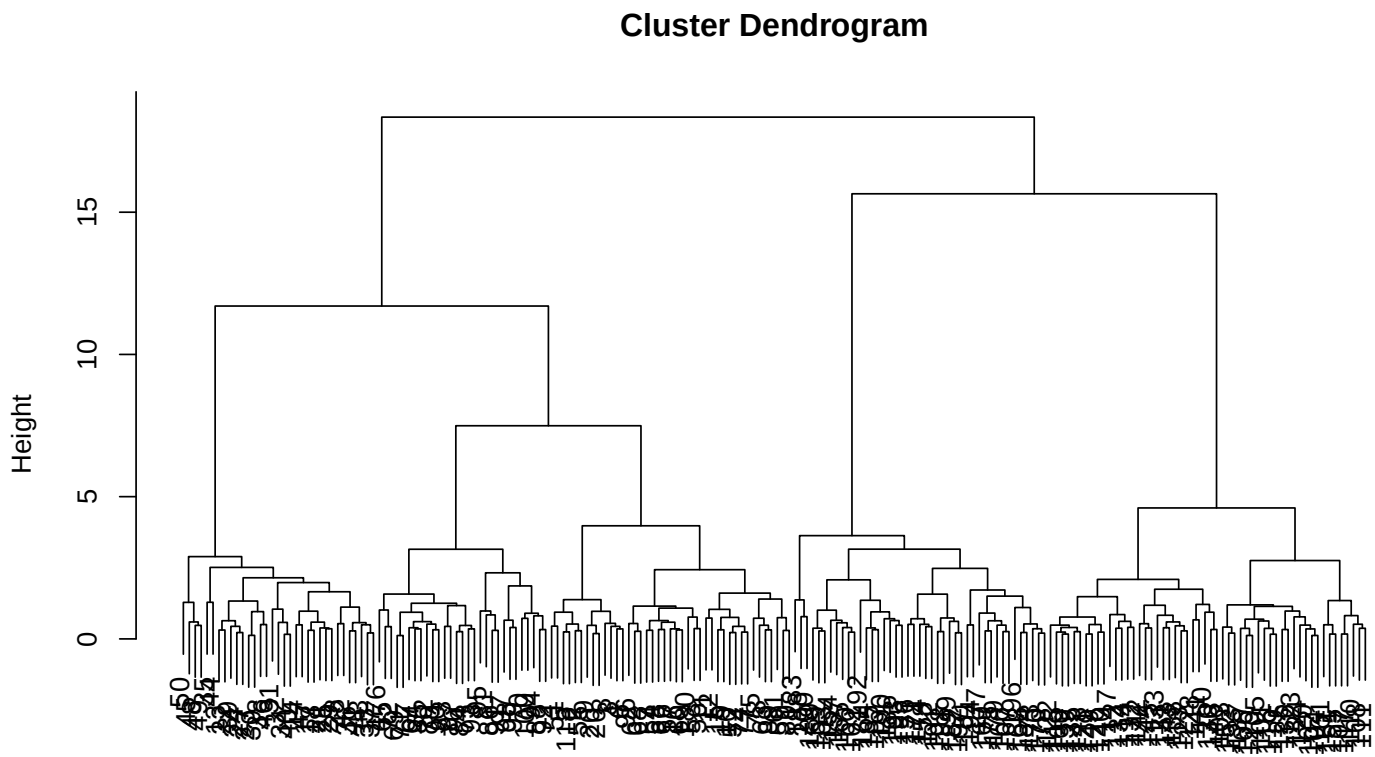
Ward agglomerative clustering in R

```
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] 0.7071894

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

## [1] 0.7538279
```

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

Table: k-means vs Ward

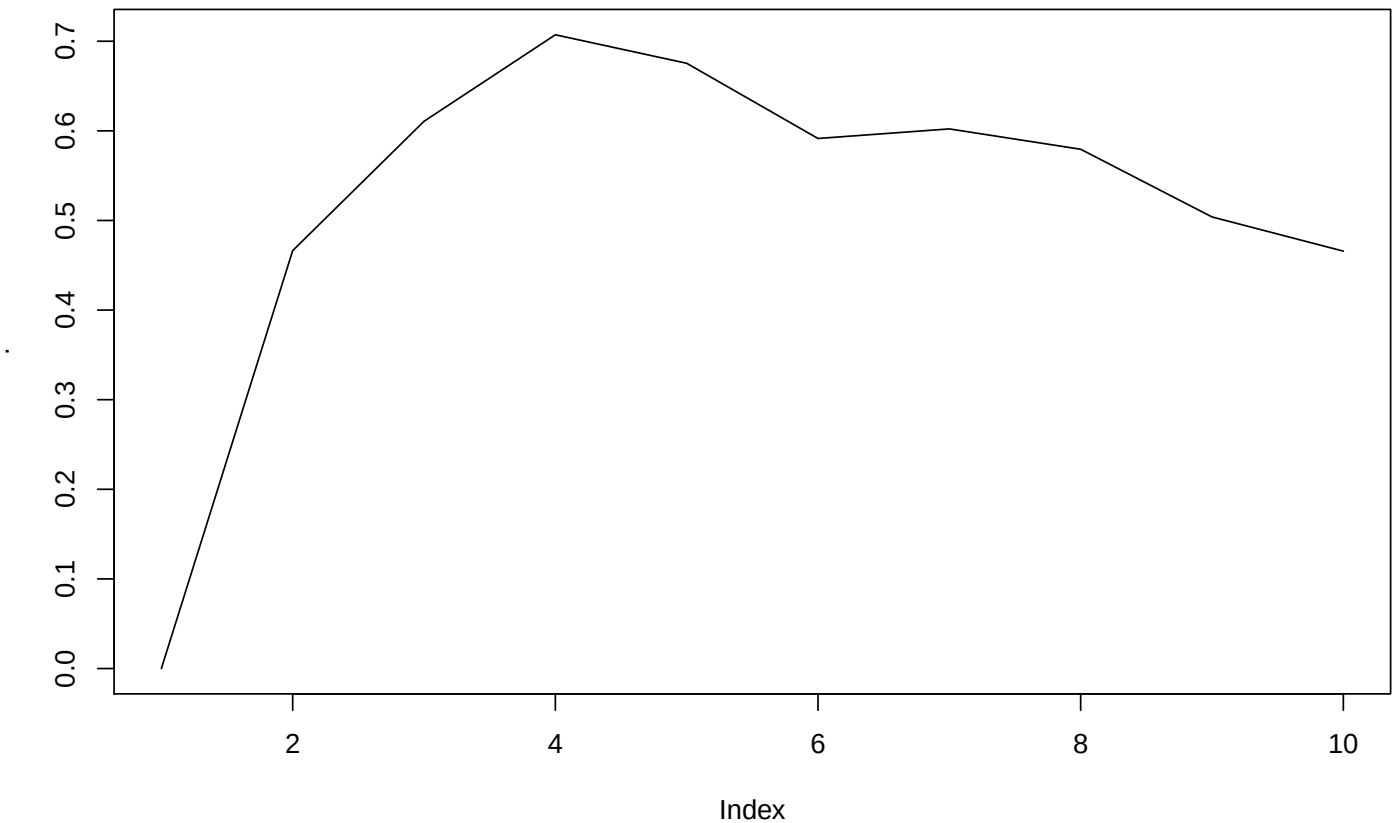
1	2	3	4
9	33	0	0
53	0	0	0
6	0	52	0
2	0	2	43

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")
```

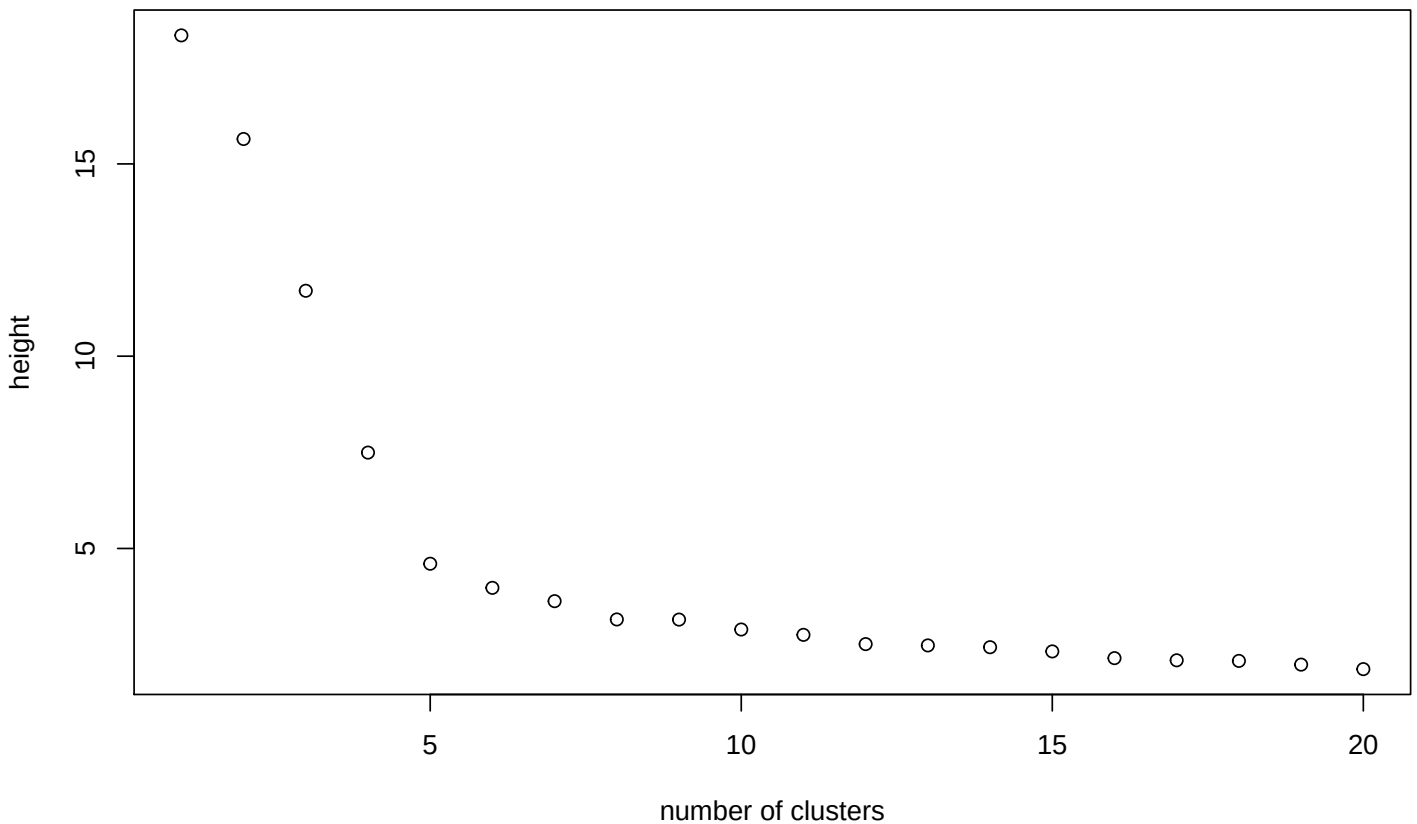
Ward agglomerative clustering in R: comparison III



Look at Ward intra-class variance

Ward agglomerative clustering in R: comparison IV

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

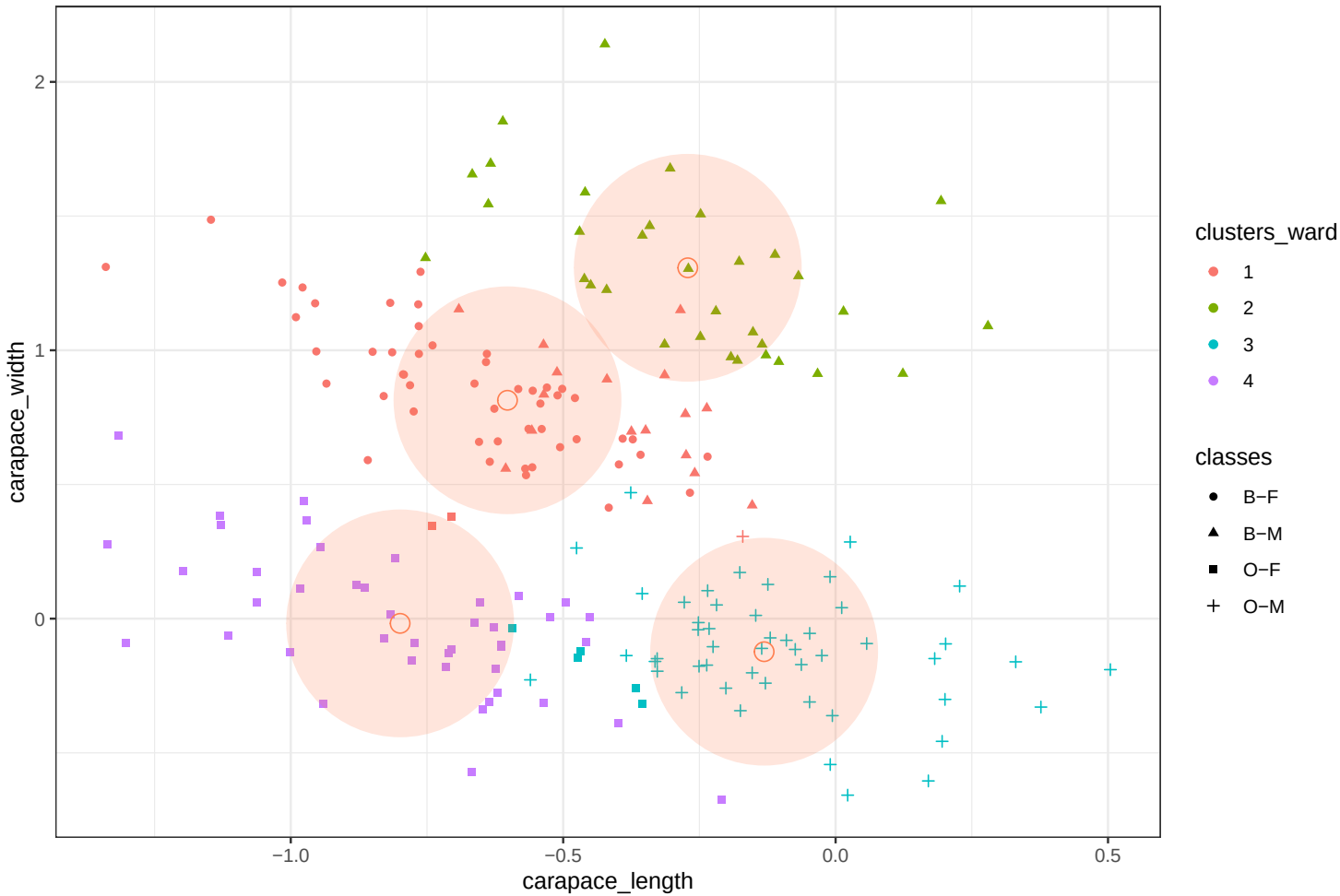


Ward agglomerative clustering in R: projection I

```
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



Outline

Distance-based method

References

- DS David Sontag's Lecture
  `http://people.csail.mit.edu/dsontag/courses/ml13/slides/lecture16.pdf`
- A Tutorial on Spectral Clustering,
  Ulrike von Luxburg

Spectral Clustering

Principle: graph-based transformation prior to clustering

1. Build a similarity with a weighted graph of the data
2. Use the spectral property of this similarity ($\rightsquigarrow$ kernel)
3. Apply clustering (e.g., k-means) to the projected data

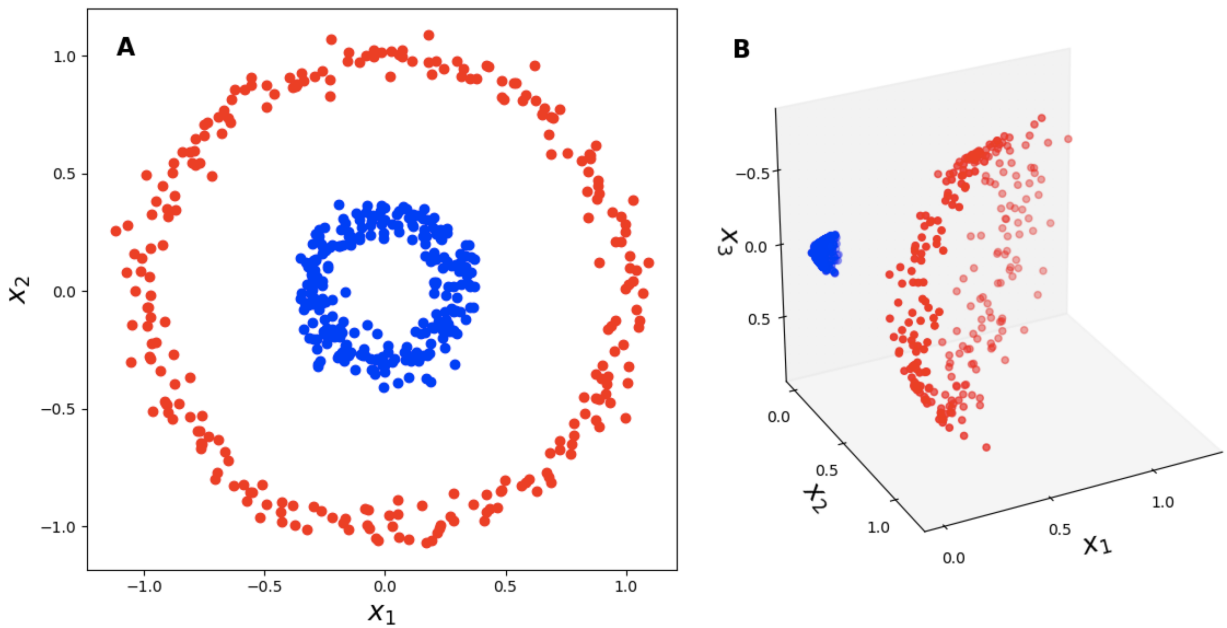


Figure: Performing clustering after transformation + dimension reduction of the data

Creating the graph

Many choices

- K-nearest neighbor graph
- any distance-based similarity (fully connected graph)
- any kernel-based similarity (e.g., Gaussian kernel)

The connectivity of $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is captured by the (weighted) adjacency matrix $\mathbf{A}$:

$$(\mathbf{A})_{ij} = \begin{cases} w_{ij} > 0 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

Proposition

The degrees of $\mathcal{G}$ are then simply obtained as the row-wise and/or column-wise sums of $\mathbf{A}$.

Incidence matrix

Definition (Incidence matrix)

The connectivity of $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is captured by the $|\mathcal{V}| \times |\mathcal{E}|$ matrix $\mathbf{B}$:

$$(\mathbf{B})_{ij} = \begin{cases} \sqrt{w_{ij}} & \text{if } i \text{ is incident to edge } j, \\ 0 & \text{otherwise.} \end{cases}$$

Proposition (Relationship)

Let $\tilde{\mathbf{B}}$ be a modified signed version of $\mathbf{B}$ where $\tilde{B}_{ij} = +/- \sqrt{w_{ij}}$ if i is incident to j as tail/head. Then

$$\tilde{\mathbf{B}}\tilde{\mathbf{B}}^{\intercal} = \mathbf{D} - \mathbf{A},$$

where $\mathbf{D} = diag(\{d_i, i \in \mathcal{V}\})$ is the diagonal matrix of degrees.

Graph Laplacian

Definition ((Un-normalized) Laplacian)

The Laplacian matrix $\mathbf{L}$, resulting from the modified incidence matrix $\tilde{\mathbf{B}}$ $\tilde{B}_{ij} = 1/-1$ if i is incident to j as tail/head, is defined by

$$\mathbf{L} = \tilde{\mathbf{B}}\tilde{\mathbf{B}}^{\mathsf{T}} = \mathbf{D} - \mathbf{A},$$

where $\mathbf{D} = \text{diag}(d_i, i \in \mathcal{V})$ is the diagonal matrix of degrees.

Remark

- $\mathbf{L}$ is called the graph Laplacian (by analogy to continuous Laplacian).
- Spectrum of $\mathbf{L}$ has much to say about the structure of the graph $\mathcal{G}$.

Graph Laplacian: spectrum

Proposition (Spectrum of $\mathbf{L}$)

The $n \times n$ matrix $\mathbf{L}$ has the following properties:

$$\mathbf{x}^\top \mathbf{L}\mathbf{x} = \frac{1}{2}\sum_{i,j} A_{ij}(x_i - x_j)^2, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

- $\mathbf{L}$ *is a symmetric, positive semi-definite matrix,*
- *the smallest eigenvalue is* 0 *with associated eigenvector* $\mathbf{1}$*.*
- $\mathbf{L}$ *has* n *positive eigenvalues* $0 = \lambda_1 < \cdots < \lambda_n$*.*

Corollary (Spectrum and Graph)

- *The multiplicity of the first eigen value* (0) *of* $\mathbf{L}$ *determines the number of connected components in the graph.*
- *The larger the second non trivial eigenvalue, the higher the connectivity of* $\mathcal{G}$*.*

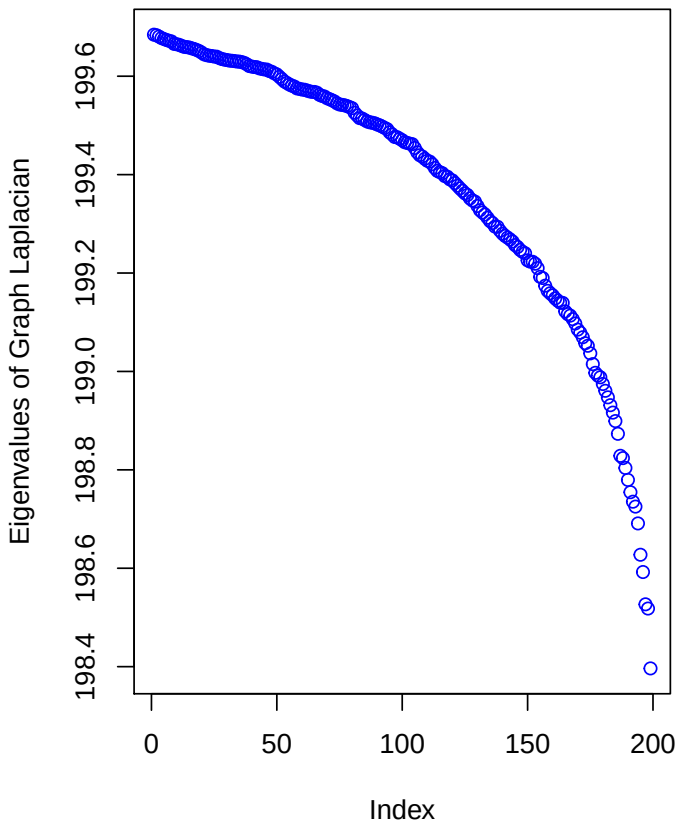
Crabs: Fielder vector and eigenvalue I

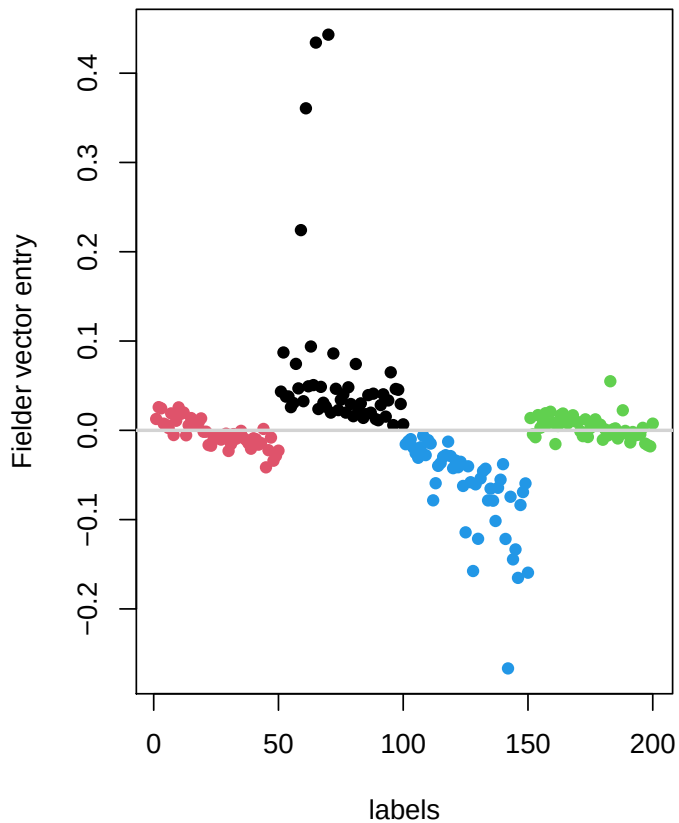
```
graph_crabs <- crabs %>% select(-species, -sex) %>%
  t() %>% cor() %>% graph_from_adjacency_matrix(weighted = TRUE)
eigen_crabs <- graph.laplacian(graph_crabs) %>% eigen()

fielder_vector <- eigen_crabs$vectors[, nrow(crabs) - 1]
faction <- factor(paste(crabs$species, crabs$sex, sep="-"))

par(mfrow = c(1,2))
plot(eigen_crabs$values[-nrow(crabs)], col = "blue", ylab = "Eigenvalues of Graph L
plot(fielder_vector, pch = 16, xlab = "labels",
   ylab = "Fielder vector entry", col = faction)
abline(0, 0, lwd = 2, col = "lightgray")
```

Crabs: Fielder vector and eigenvalue II





Some variants

Definition ((Normalized) Laplacian)

The normalized Laplacian matrix $\mathbf{L}$ is defined by

$$\mathbf{L}_N = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}.$$

Definition ((Absolute) Graph Laplacian)

The absolute Laplacian matrix $\mathbf{L}_{abs}$ is defined by

$$\mathbf{L}_{abs} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{L}_N,$$

with eigenvalues $1 - \lambda_n \leq \cdots \leq 1 - \lambda_2 \leq 1 - \lambda_1 = 1$, where $0 = \lambda_1 \leq \cdots \leq \lambda_n$ are the eigenvalues of $\mathbf{L}_N$.