

Data Wrangling and Data Analysis Clustering:

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This week

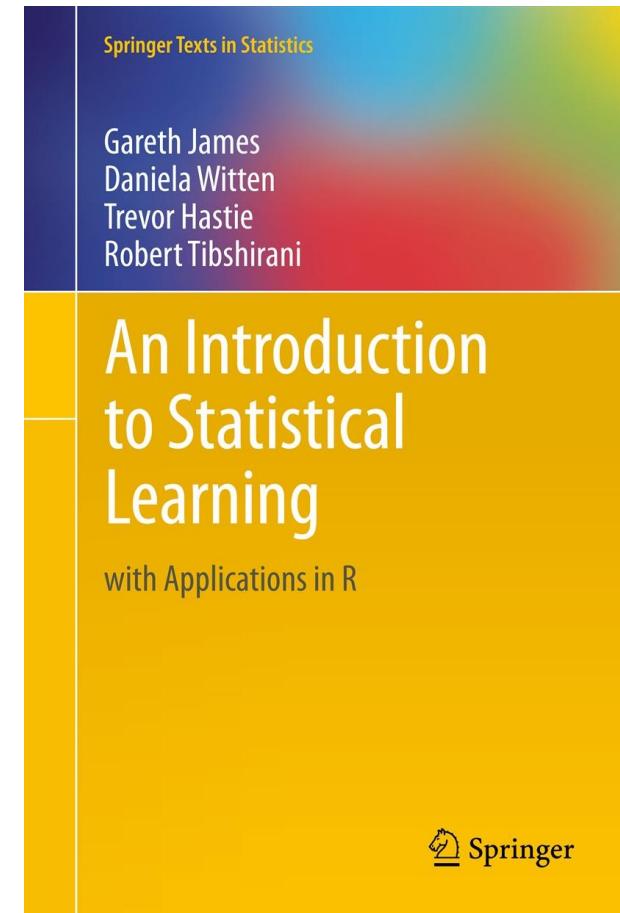
- *Hierarchical* and *partitional* clustering
- The K-means clustering algorithm
- (*tomorrow*) Model-based clustering

Goal of the week: *understand, apply, and evaluate* clustering methods



Reading materials for this week

- Selected paragraphs from **Introduction to Statistical Learning (ISLR)** §10.3
- <https://faculty.marshall.usc.edu/gareth-james/ISL/>
- “Mixture models: latent profile and latent class analysis” [Oberski, 2016] §1, §2
- <http://daob.nl/wp-content/papercite-data/pdf/oberski2016mixturemodels.pdf>



Optional, much more in-depth material

“Cluster validation: how to think and what to do”

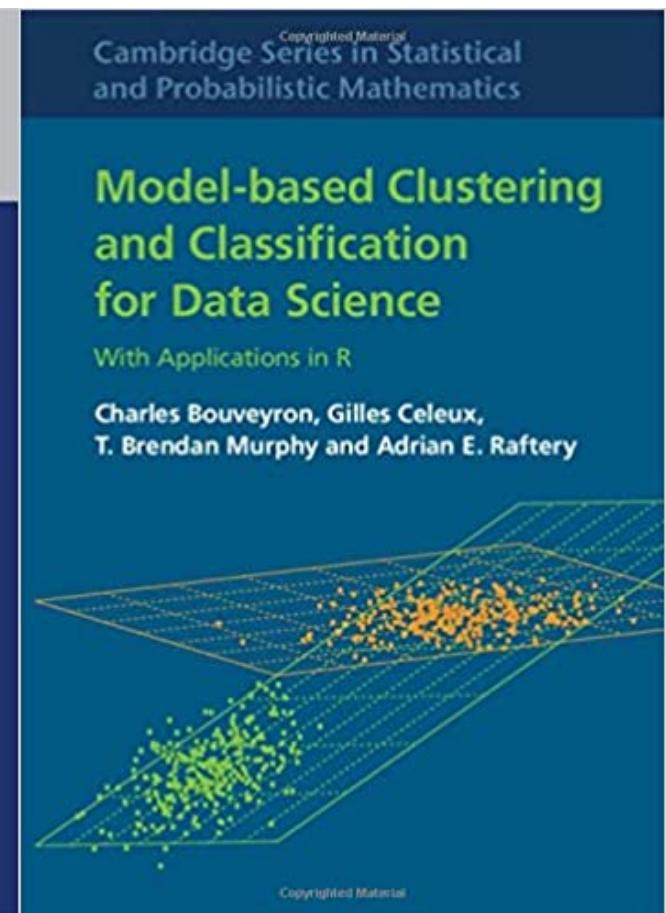
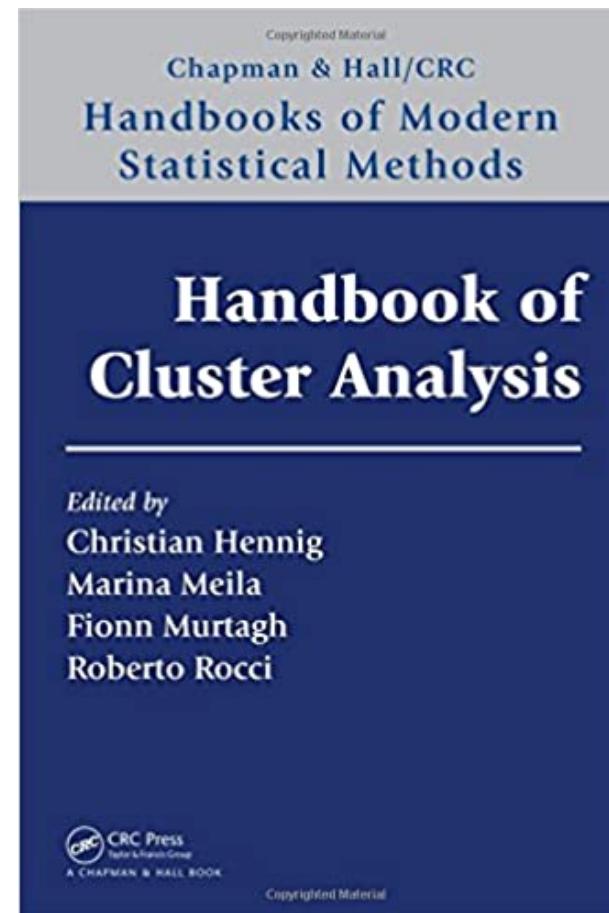
– presentation by Hennig

Handbook of Cluster Analysis

Hennig et al. (2016)

Model-based Clustering and Classification for Data Science

Bouveyron et al. (2018)



Assignments this week

- Monday: R assignment on hierarchical and k-means clustering
- Tuesday: R assignment with `mclust`
- Thursday: either (a) resit for the test, or (b) programming k-medoids clustering from scratch



Clustering

Find subgroups (clusters) of similar examples in a database



Why clustering?

- Unsupervised: expect groups in our data, but were not able to measure them
 - potential new subtypes of cancer tissue
- We want to summarize features into a categorical feature to use in further decisions/analysis
 - subgrouping customers by their spending types



Some applications of clustering

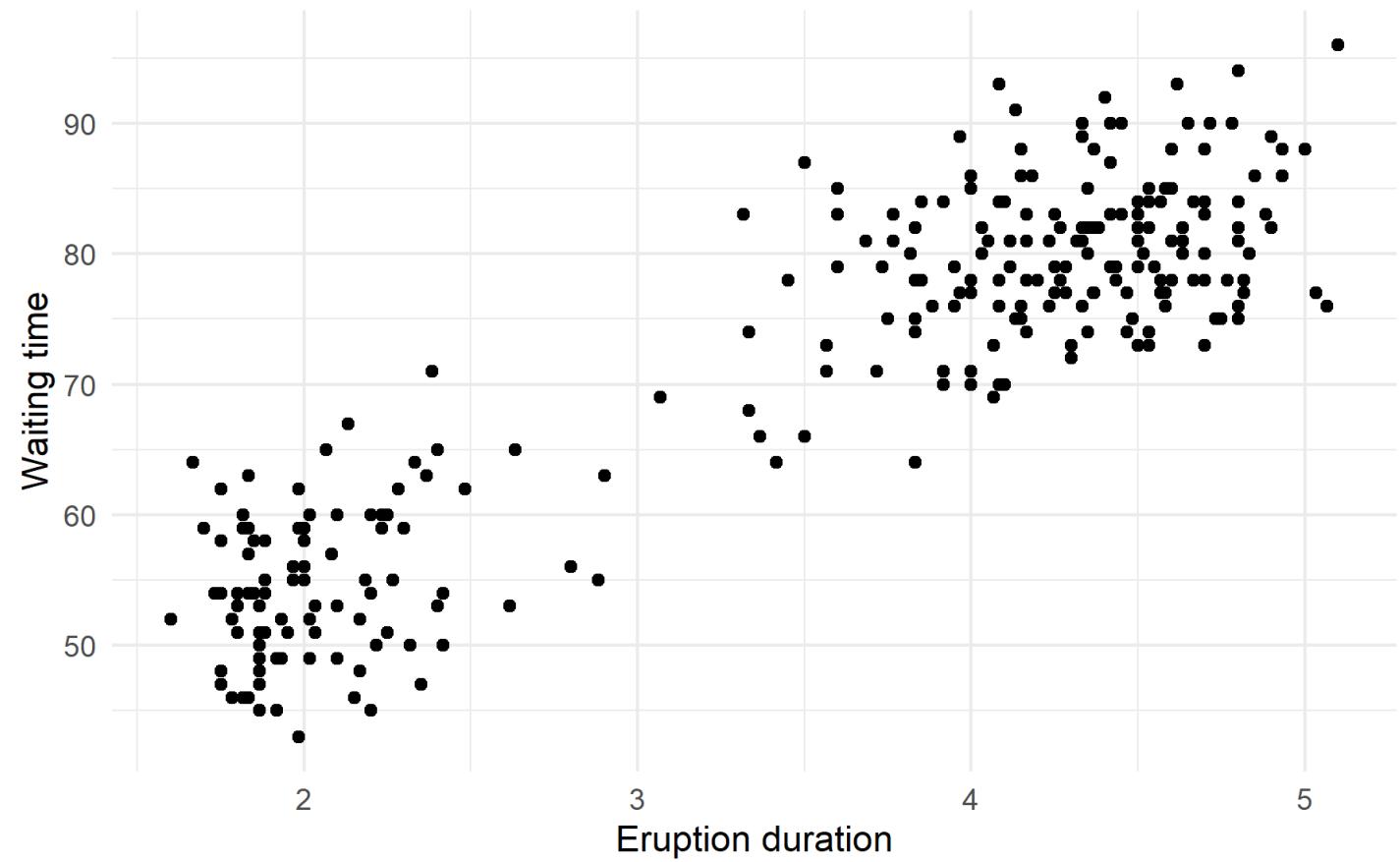
- Intermediate step for other fundamental data mining problems
- Collaborative filtering
- Customer segmentation
- Data summarization
- Dynamic trend detection
- Multimedia data analysis
- Biological data analysis
- Social network analysis





Old Faithful: two types of eruption?

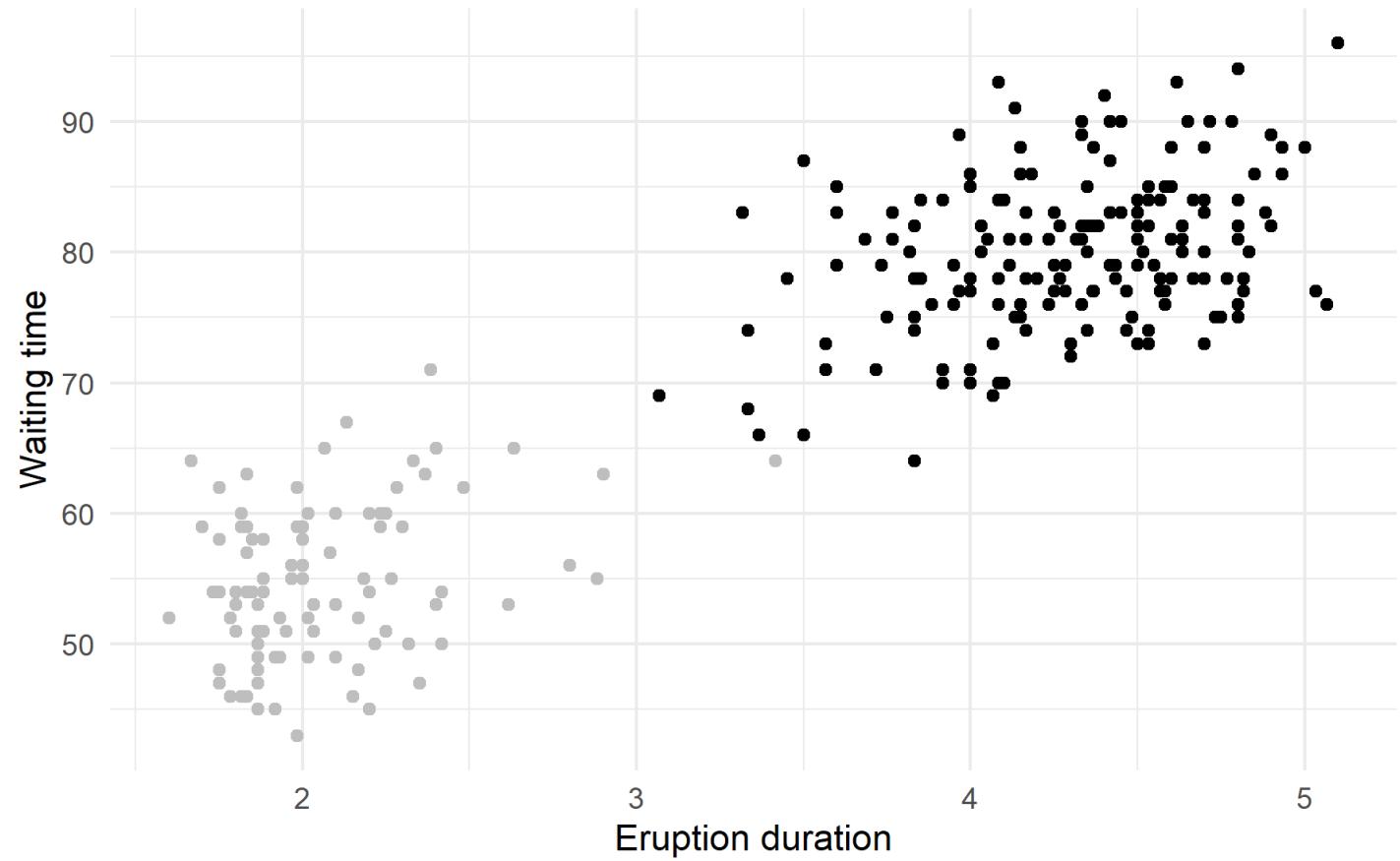
Old faithful geyser eruptions





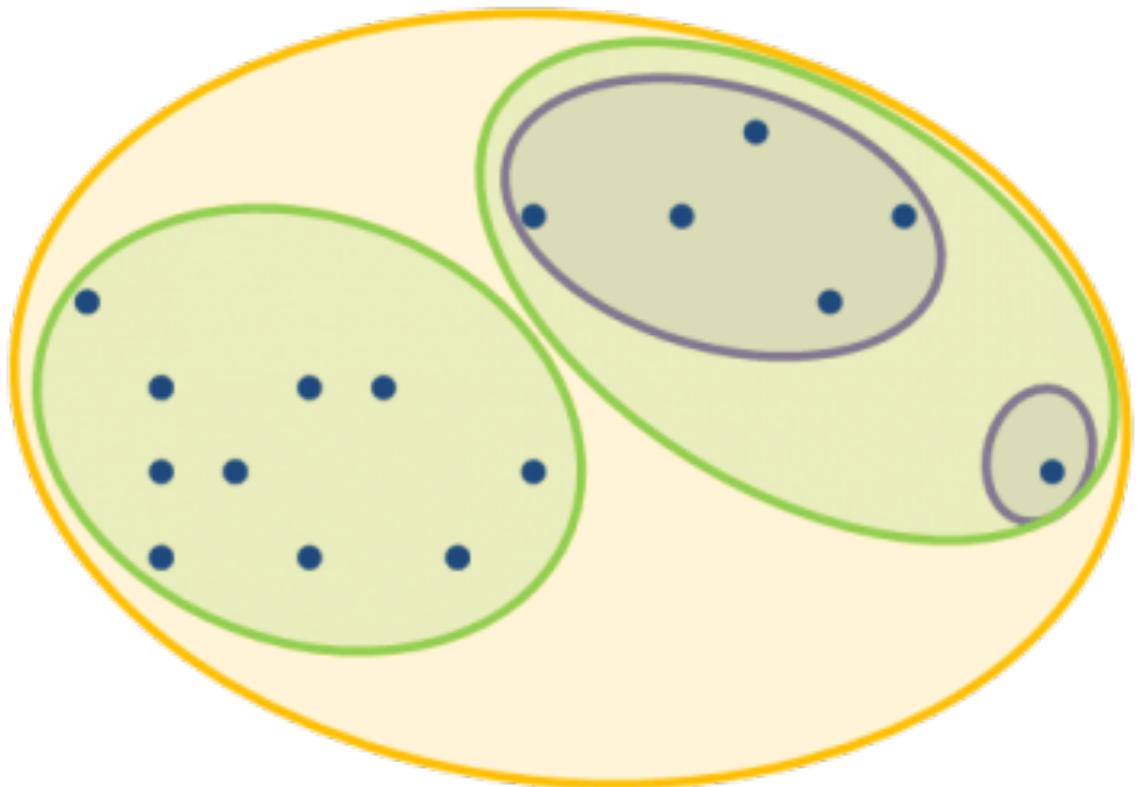
Old Faithful: two types of eruption?

Old faithful geyser eruptions (clustered)

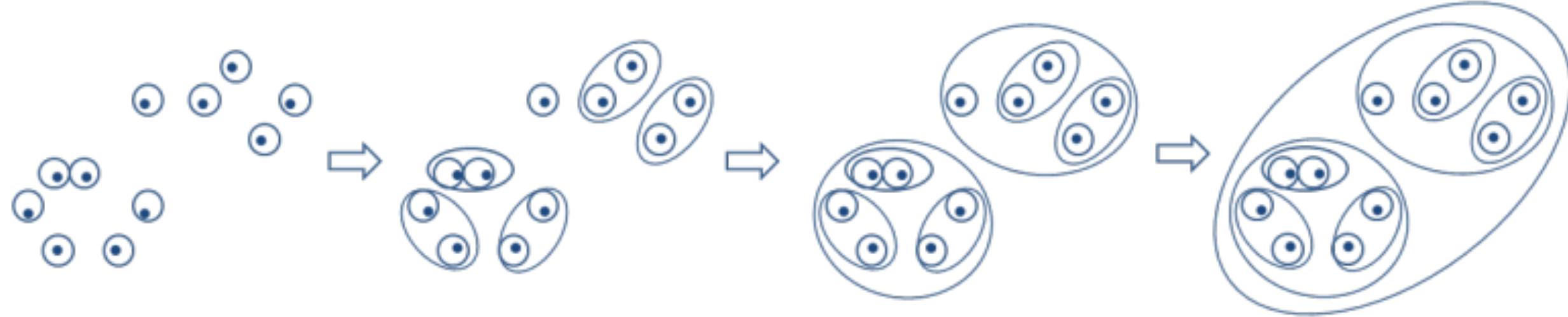


Clustering types

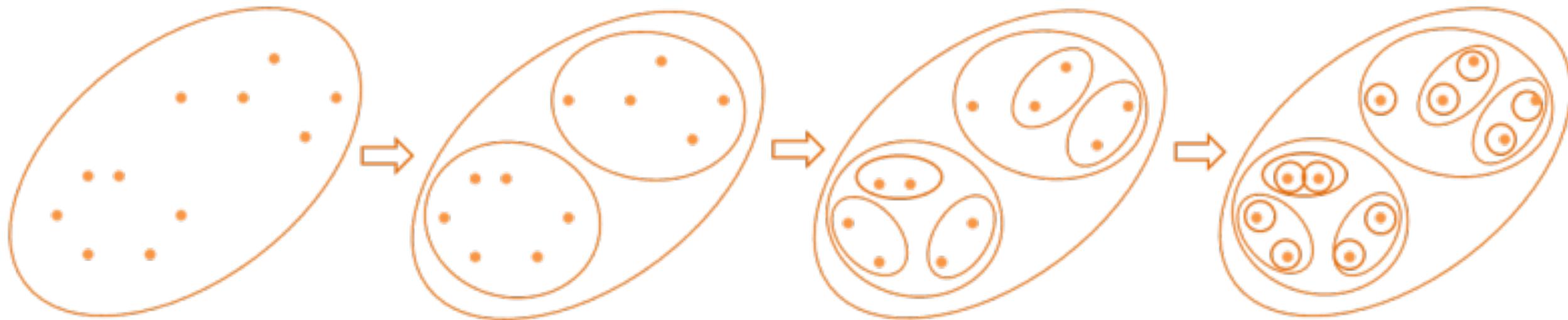
Hierarchical Clustering



Agglomerative Hierarchical Clustering



Divisive Hierarchical Clustering



Source: T. Fuertes

<https://quantdare.com/hierarchical-clustering/>

Hierarchical clustering

Bottom-up agglomerative clustering

- For each observation, compute the *distance* to all other observations
- Assign all examples to their individual cluster
- Combine *most similar* clusters
- Keep combining clusters until there is only one cluster left
- Select number of clusters for the final solution

*(Divisive: start with *one* cluster and keep splitting *most different*)*



Hierarchical clustering

In R:

```
distances <- dist(faithful, method = "euclidean")
result     <- hclust(distances, method = "average")
```

Then we can plot the dendrogram with `plot()` or `ggdendrogram`

```
library(ggdendro)
ggdendrogram(result)
```

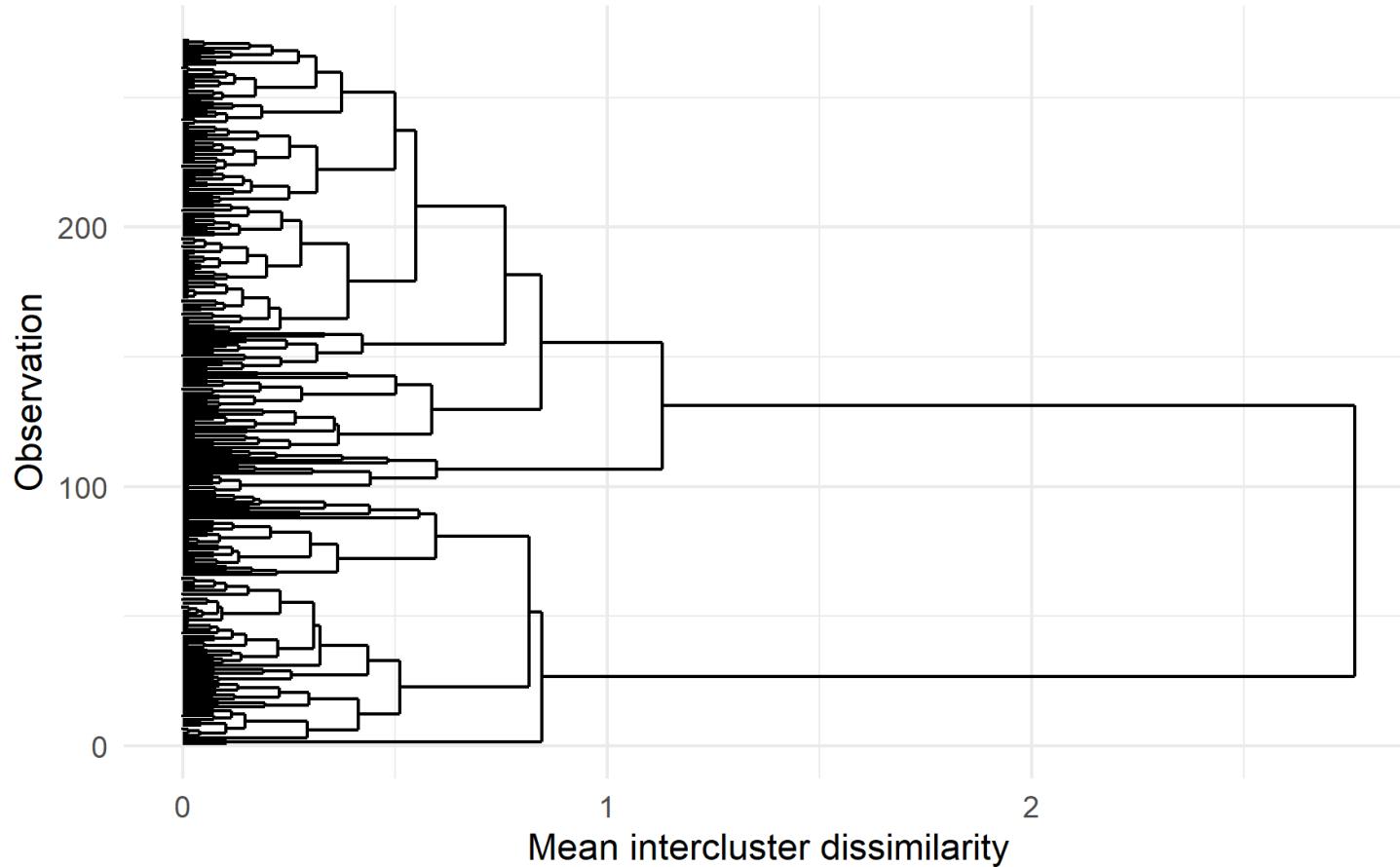
Then, select the number of clusters using a cutoff point

```
cutree(result, h = 2)
```



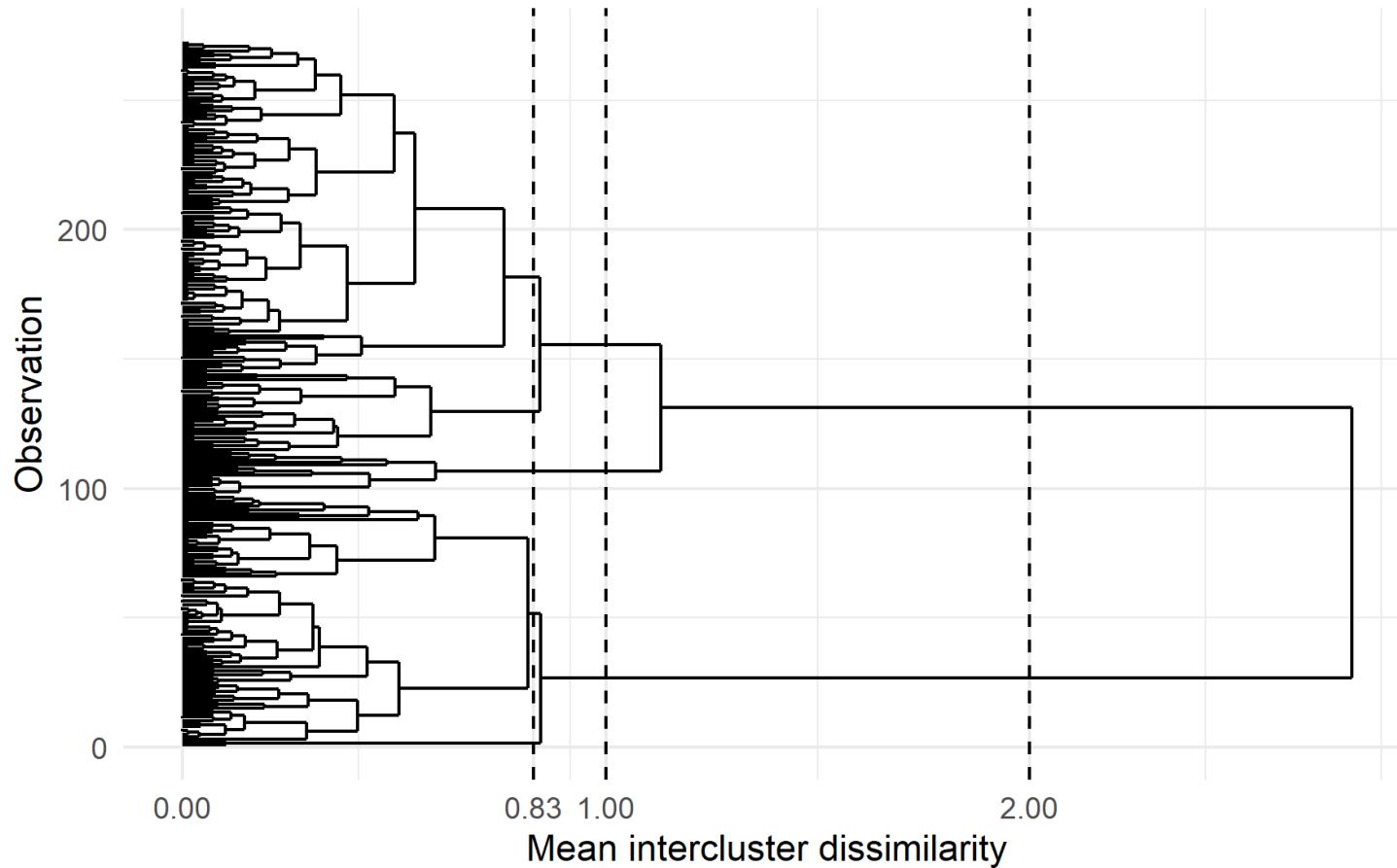
Hierarchical clustering

Old faithful hierarchical clustering with average linkage

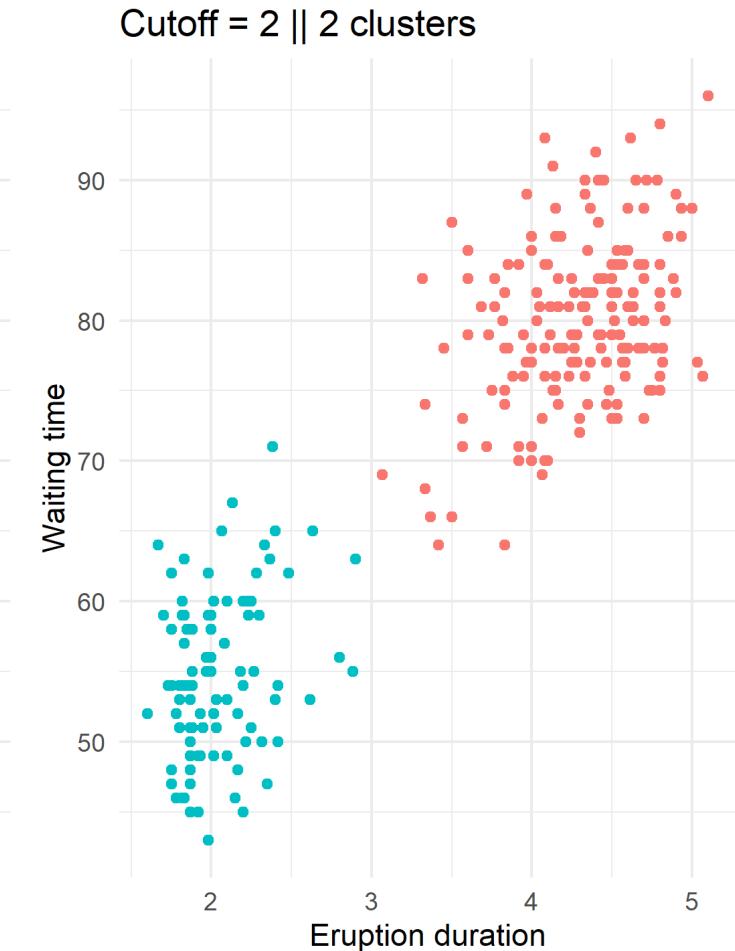
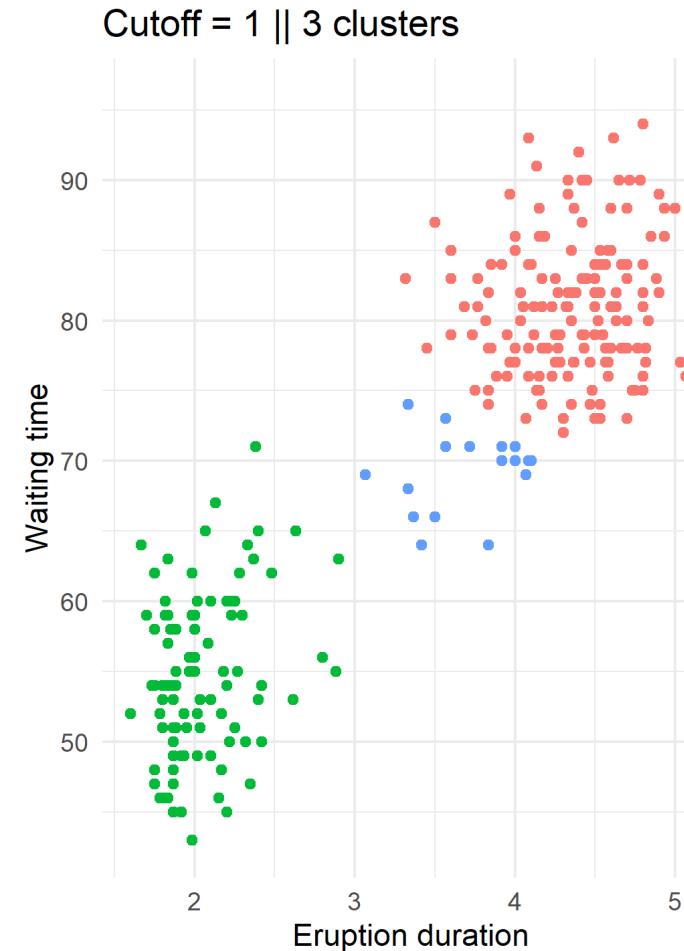
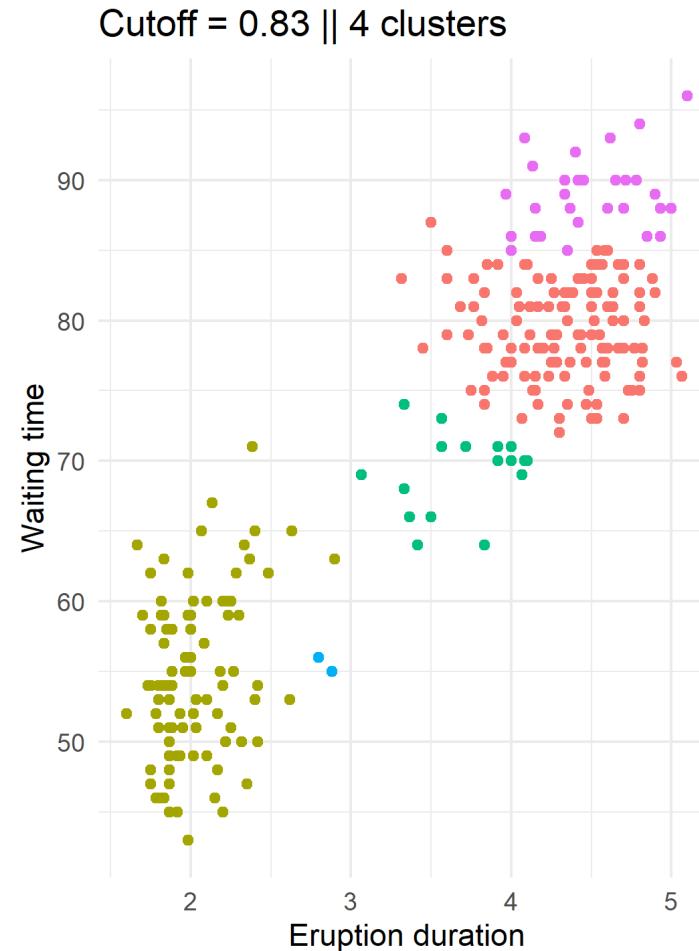


Hierarchical clustering

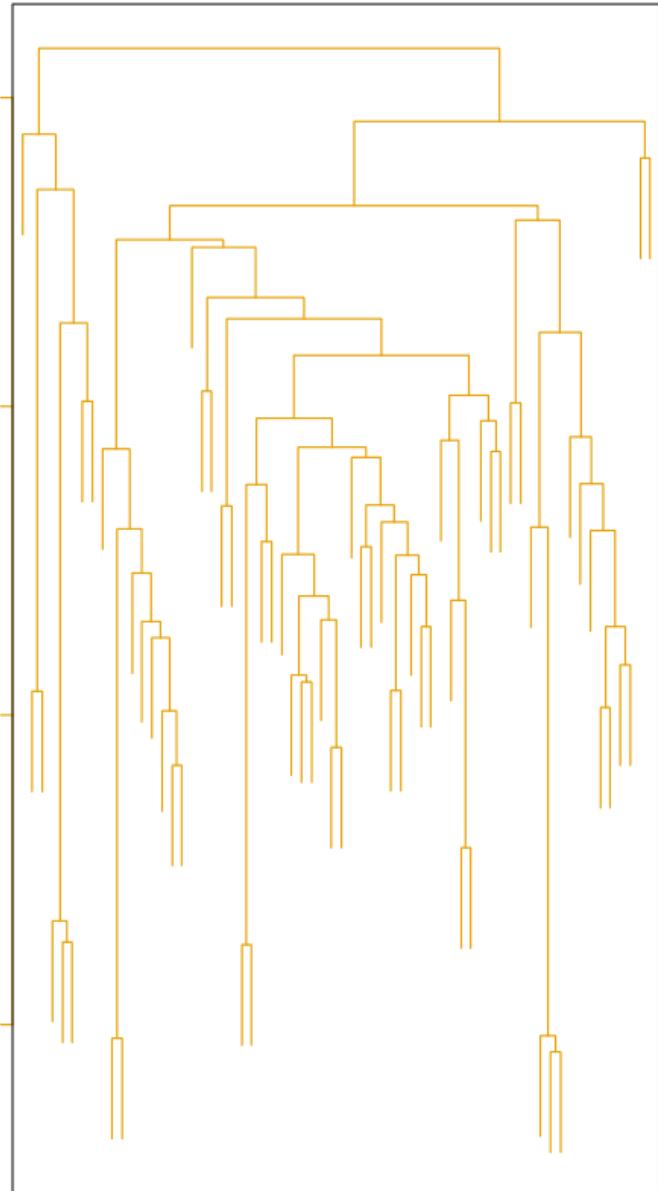
Old faithful hierarchical clustering with average linkage



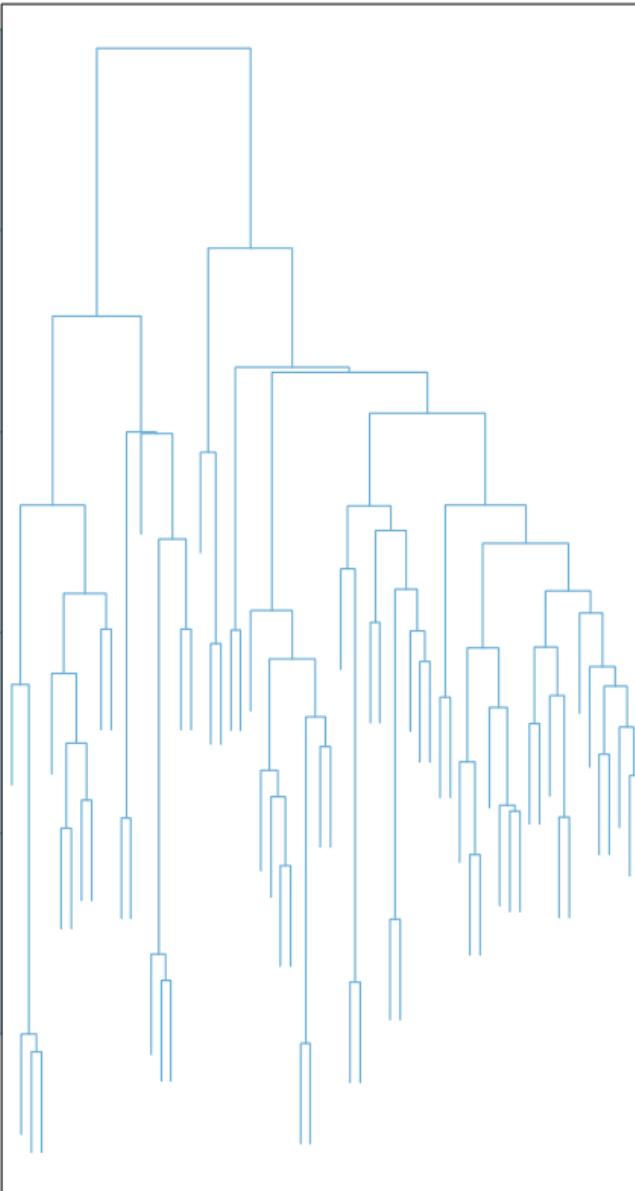
Hierarchical clustering



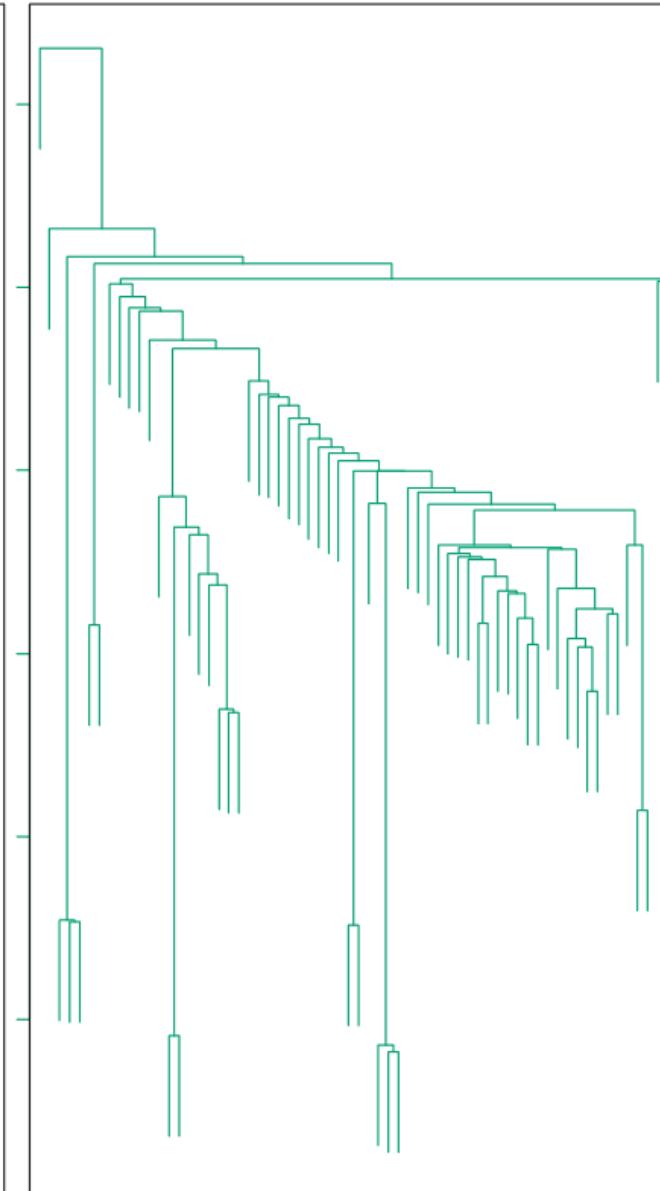
Average Linkage



Complete Linkage



Single Linkage



See *ISLR*, Table 10.2 for explanation of “linkage” options

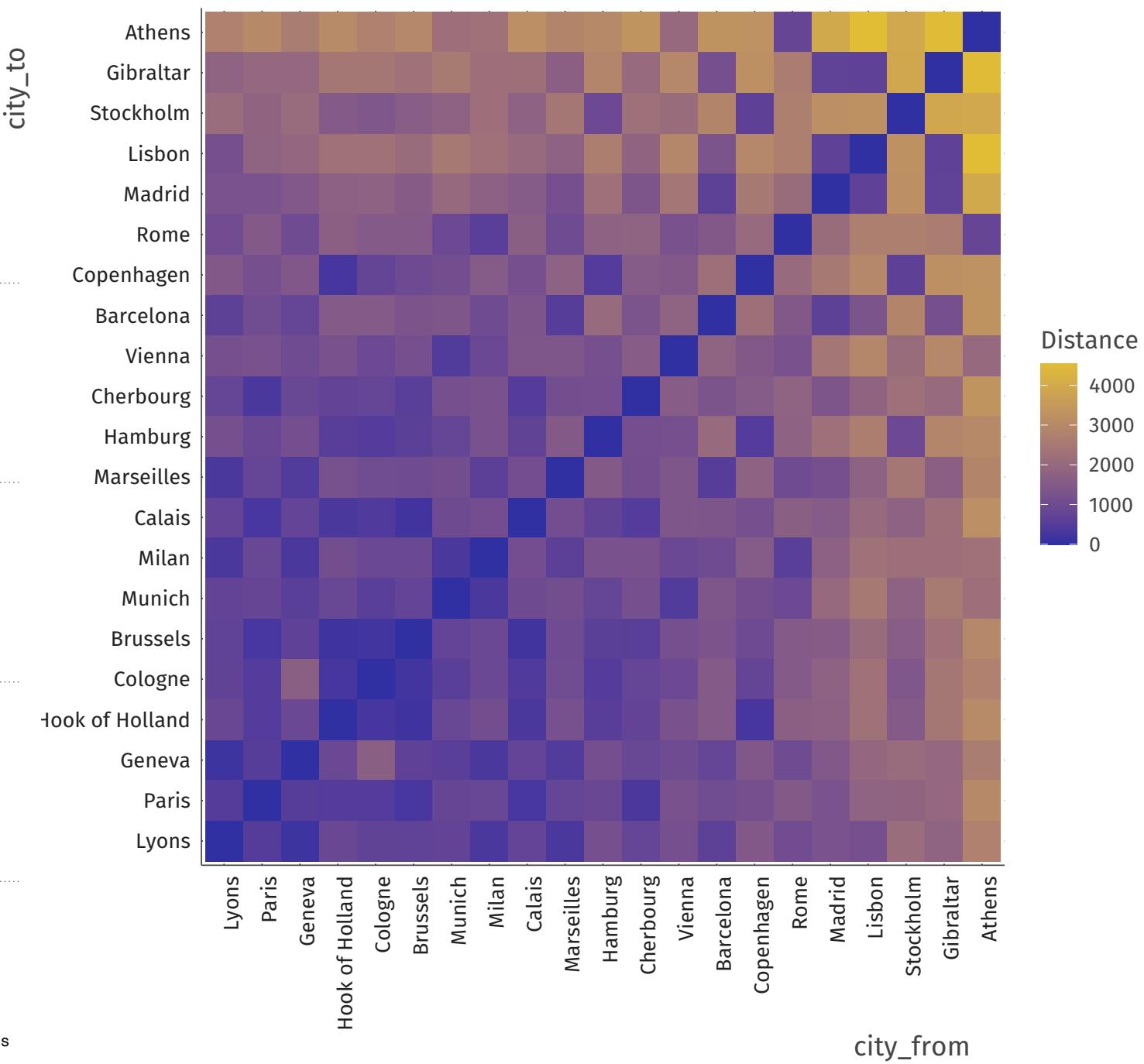
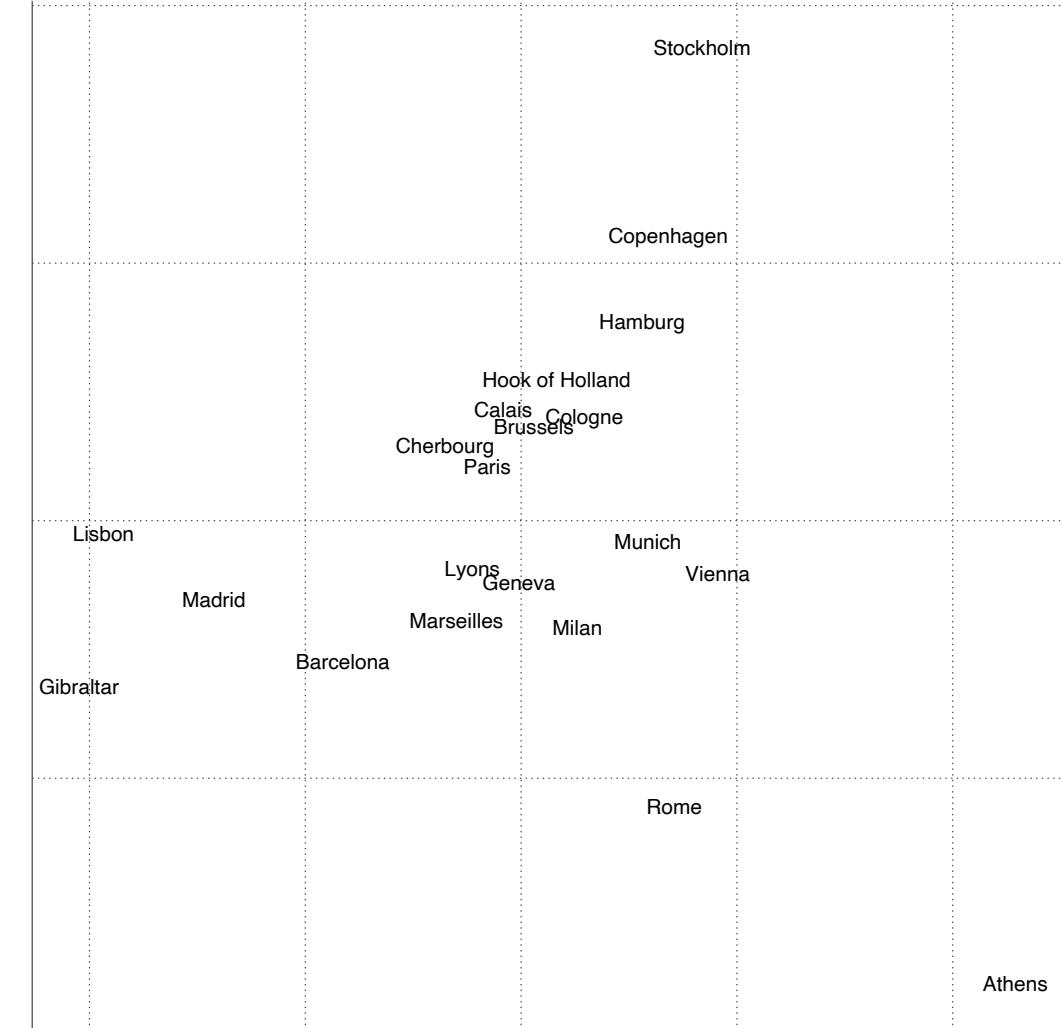


Note: scaling

- It is generally a good idea to measure your features in the same scale before entering them into a clustering algorithm
- Otherwise, height in **cm** will be more important in the distance computation than width in **m**
- Generally, you want the features to have a similar scale
- This can be done by **standardization**, or z-transformation: subtract the mean from each feature and divide by its observed standard deviation
- Changes the interpretation of the values, but not their association

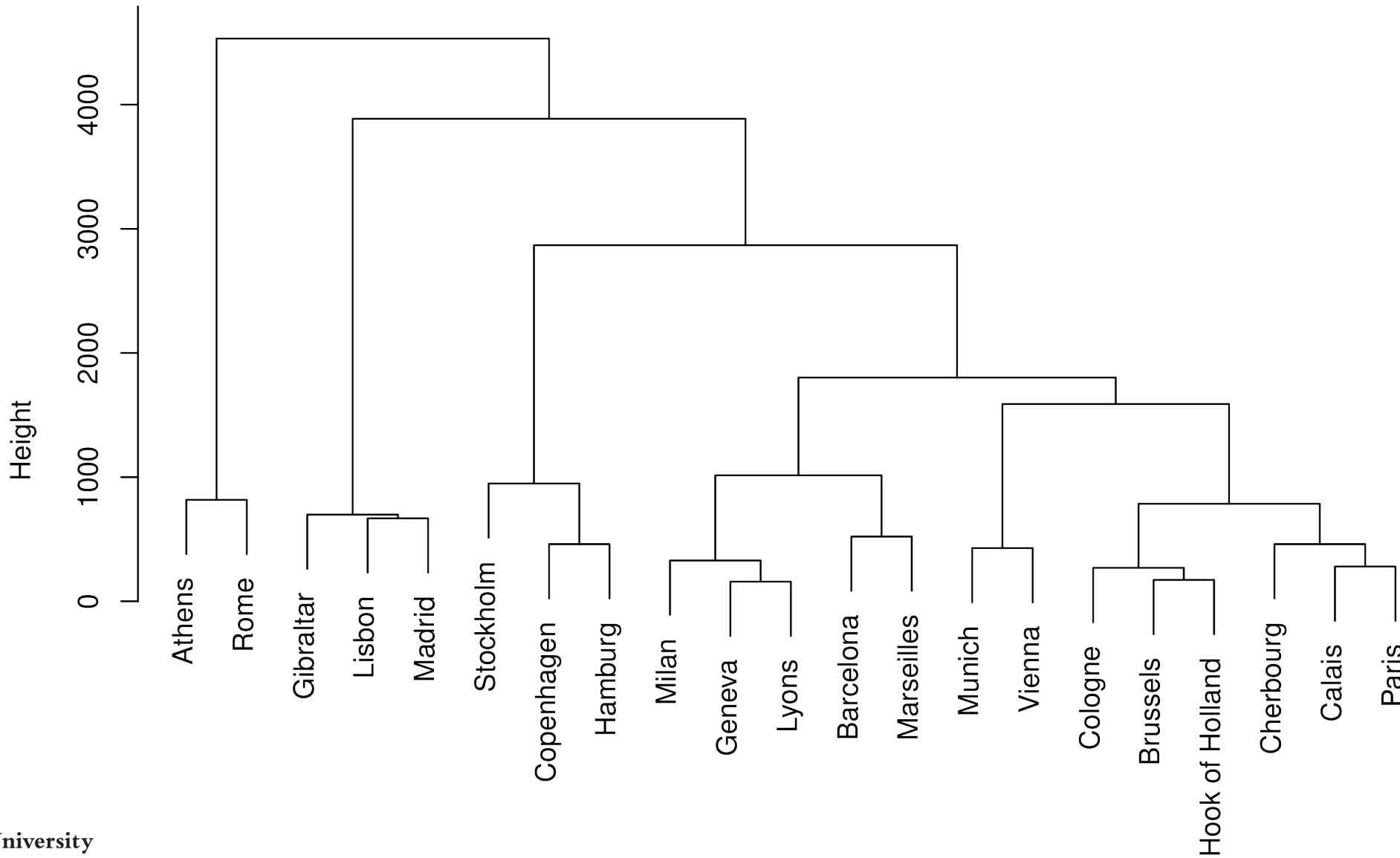


“Distance” matrix



```
plot(hclust(eurodist))
```

Cluster Dendrogram



“Distance” can mean lots of things

- **Continuous:** Euclidean, maximum, Manhattan, Minkowski, ...
- Time series: “Dynamic time warping”, Fréchet, cross-corr., wavelets, ...
- Networks: Modularity, Shortest path, ...
- Text/DNA: Edit distance, Hamming distance, TF-IDF distance, ..
- Images: “Structural similarity”, GAN loss...



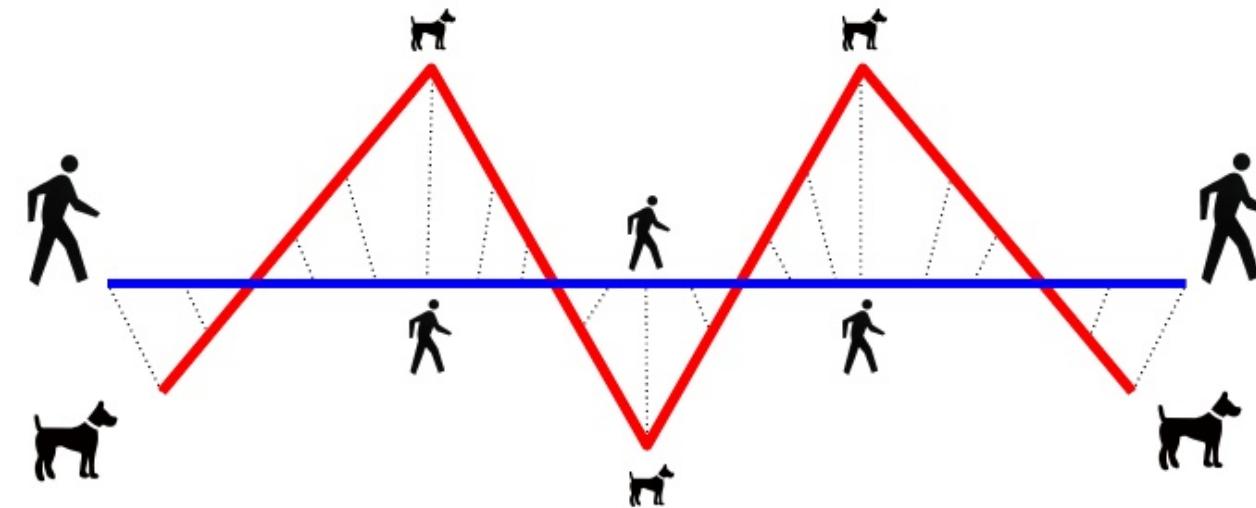
Buchin et al. 2019

Figure 1: Example of a (k, ℓ) -clustering for the flight paths of a pigeon with the number of clusters k increasing from 2 (left) until 5 (right) and the complexity of the clusters being $\ell = 10$. Trajectories belonging to the same cluster are shown in the same color. For each cluster, a center trajectory generated by the algorithm is shown using thick lines of the same color.

Some example distances that aren't Euclidean but useful for specific data types

Fréchet distance for time series/curves

Walking your dog



The **Fréchet distance** between the curves is the minimum leash length that permits such a walk

Minimum edit distance for text/DNA

I	N	T	E	*	N	T	I	O	N
*	E	X	E	C	U	T	I	O	N

(edit distance = 5)

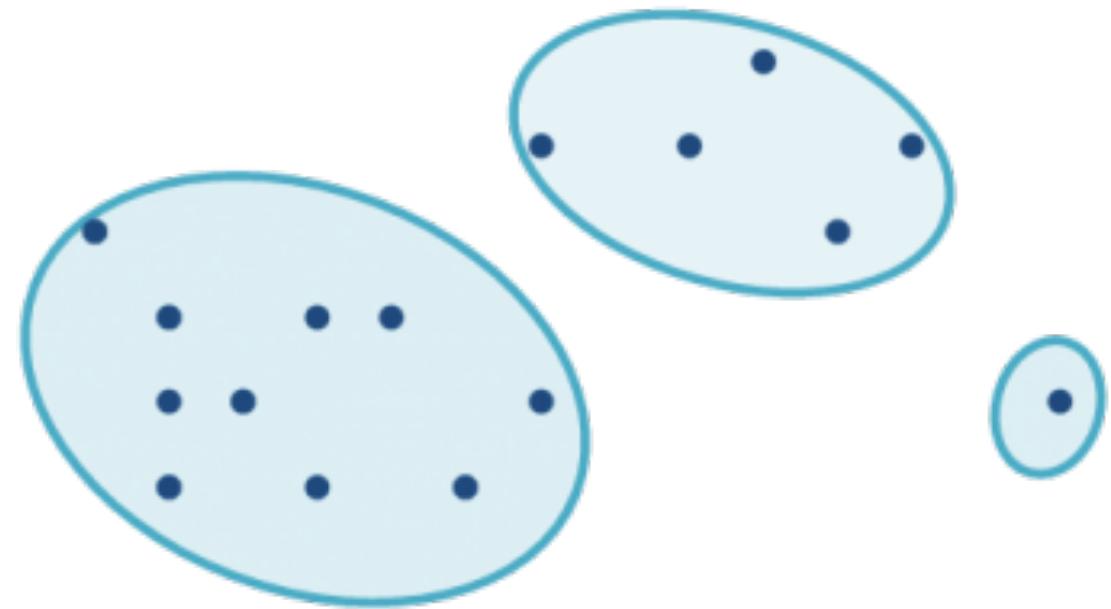
Hierarchical clustering: conclusion

- Tree-based representation - dendrogram
- Determine number of clusters afterwards
- Different distance metrics possible
- Different agglomeration methods (“linkage” rules) possible
- Taking distance matrix as input → very flexible technique
- Distance matrix $N \times N \rightarrow$ can be tricky when N is large (esp. divisive)



Clustering types

Partitional Clustering



Source: T. Fuertes

<https://quantdare.com/hierarchical-clustering/>

K-means clustering algorithm

1. Randomly assign examples to K clusters
- 2a. Calculate the **centroid** (per-feature mean) for each cluster

```
faithful %>% group_by(cluster) %>% summarize_all(mean)

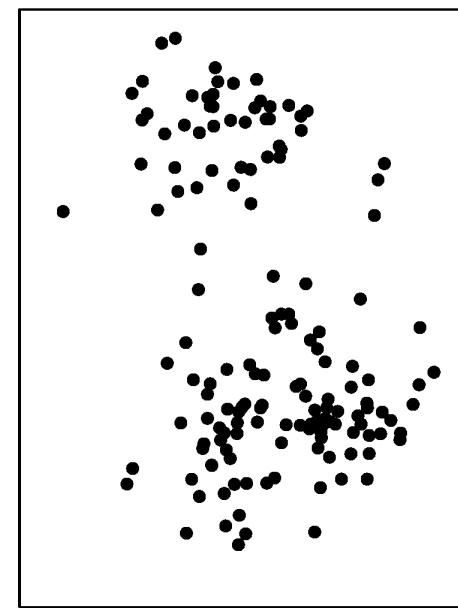
#> #>   cluster eruptions waiting
#> #>   <int>      <dbl>     <dbl>
#> 1    1          3.69      73.4
#> 2    2          3.30      68.6
```

- 2b. Assign each example to the cluster belonging to its **closest** centroid
3. If the assignments changed, go to step 2a, else stop

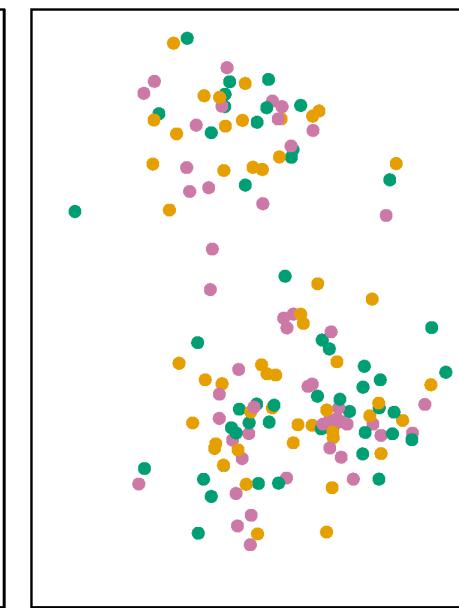


K-means clustering

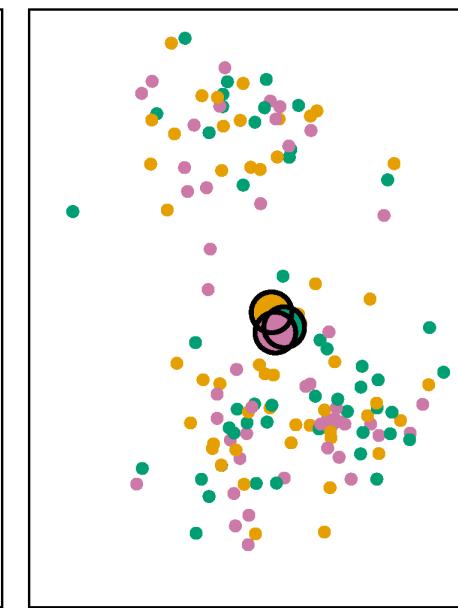
Data



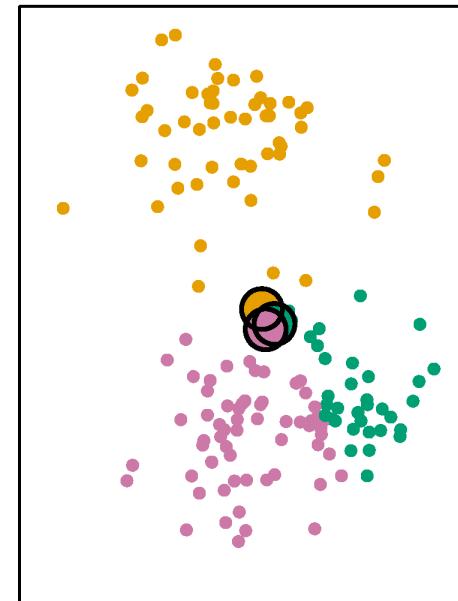
Step 1



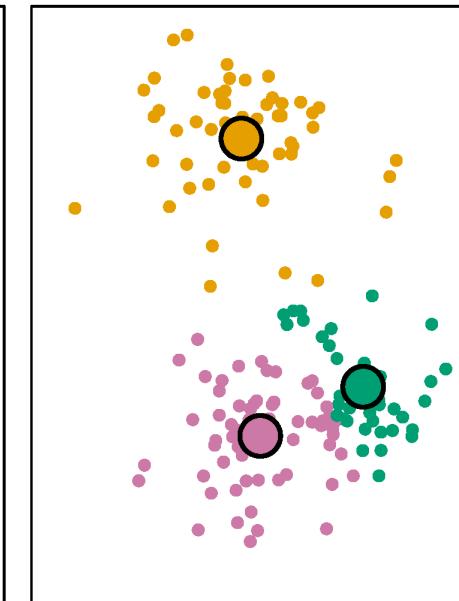
Iteration 1, Step 2a



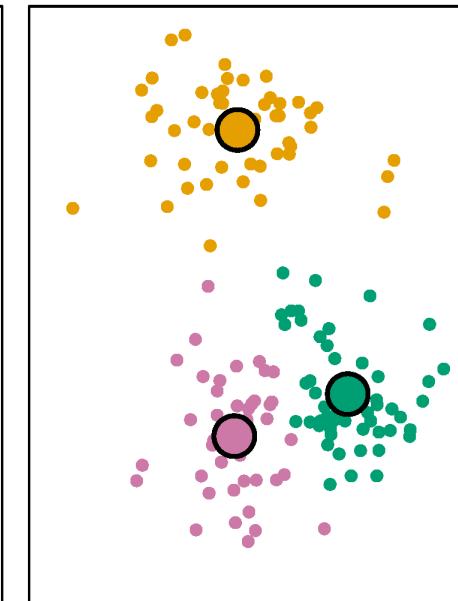
Iteration 1, Step 2b



Iteration 2, Step 2a



Final Results



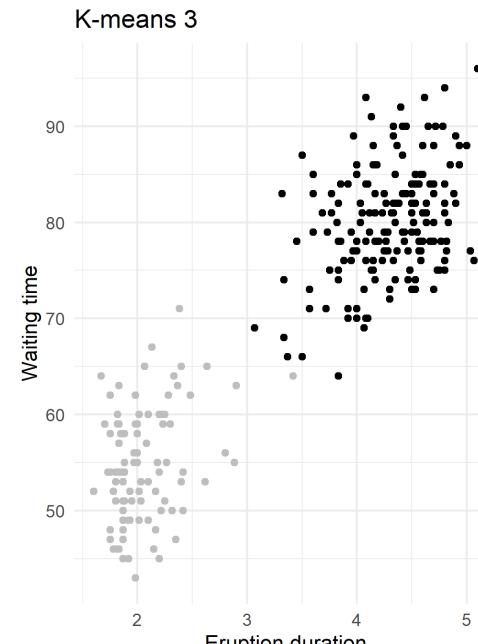
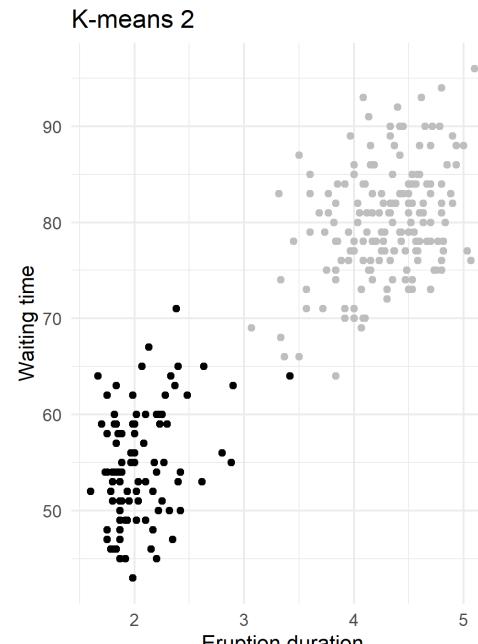
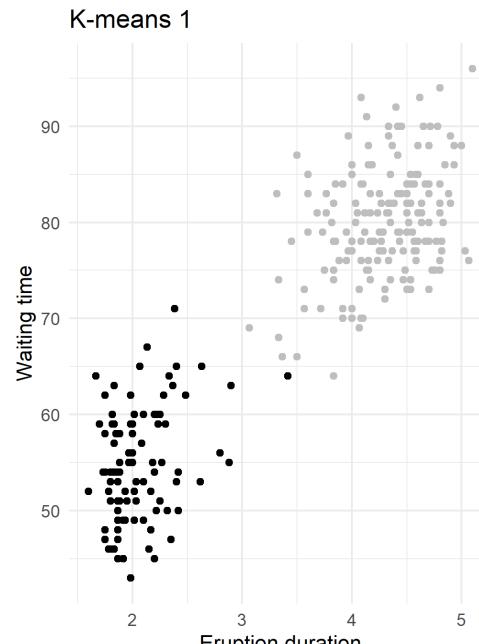
K-means clustering

- K (and, in theory, the distance metric) are hyperparameters (ISLR Sec 10.3)
(in practice, distance is almost always Euclidean (sum of squares criterion))
- K is determined in advance by the analyst
- Could be based on knowledge about the data or the goal of the analysis
 - Perhaps there are generally 2 types of geyser eruption because of physics
 - We may have resources to approach customers in at most 3 different ways
- Other criteria discussed later.



K-means clustering

- Because the initialization is random, the result is random
 - Label switching: cluster 1, 2, 3 may end up in each other's locations
 - Some examples at the boundary may end up in different clusters altogether
 - Use **multiple starts** to obtain the best solution



K-means clustering

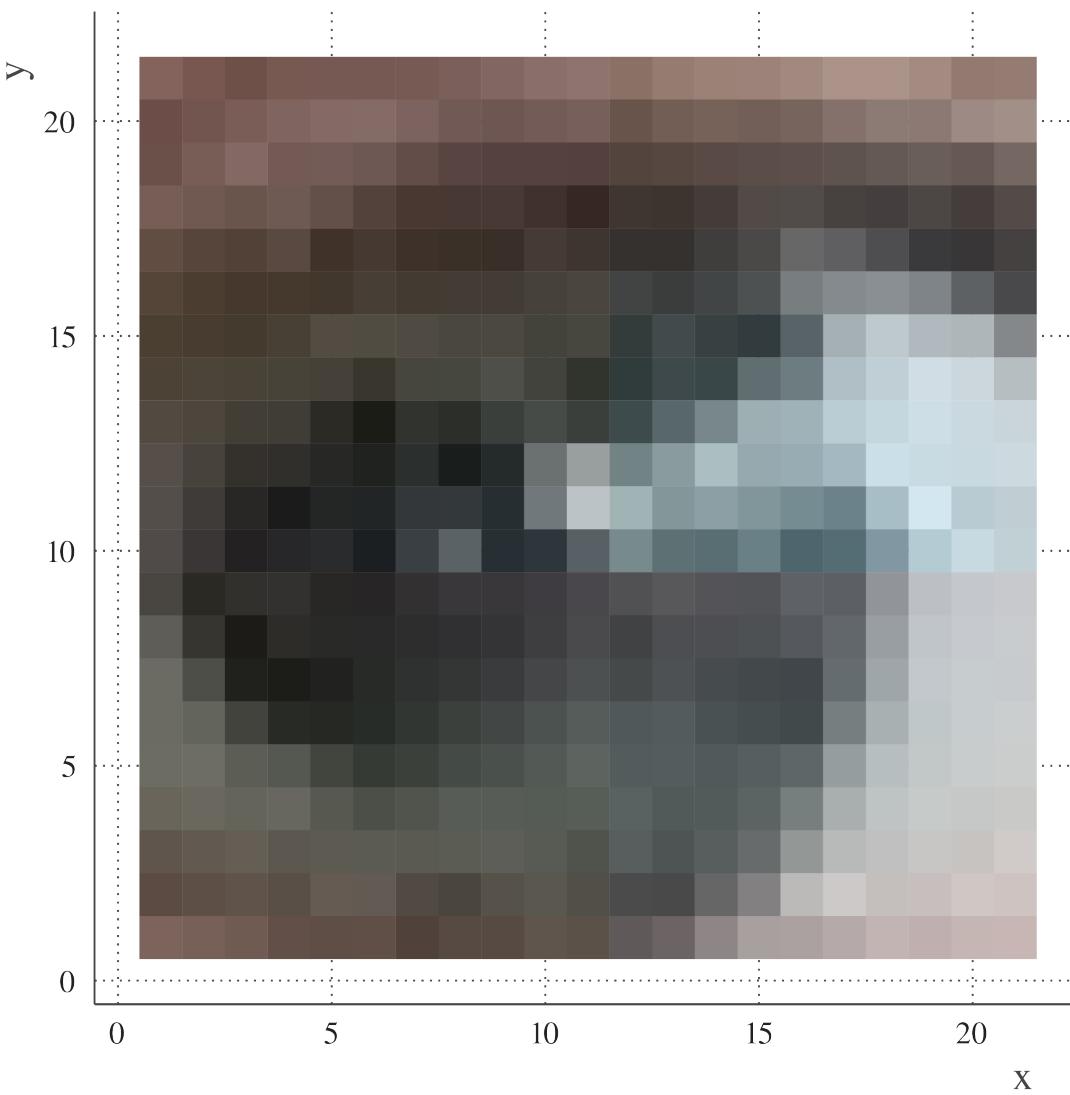
K-means clustering applied to images is called “*vector quantization*”

Goal: image compression → less storage!

Cluster pixels, then replace them by their cluster centroid



r, g, b



0.49, 0.39, 0.36
0.34, 0.29, 0.26
0.66, 0.63, 0.62
0.36, 0.29, 0.26
0.29, 0.27, 0.24
0.51, 0.50, 0.51
0.37, 0.33, 0.30
0.36, 0.36, 0.33
0.40, 0.42, 0.42
0.41, 0.40, 0.35
0.34, 0.36, 0.34
0.36, 0.39, 0.39
0.42, 0.42, 0.38
0.27, 0.29, 0.27
0.33, 0.37, 0.38
0.42, 0.42, 0.39
0.23, 0.25, 0.24
0.27, 0.30, 0.31
0.42, 0.42, 0.39
0.20, 0.21, 0.21
0.26, 0.28, 0.29
0.37, 0.36, 0.35
0.19, 0.19, 0.20
0.30, 0.32, 0.33
0.29, 0.27, 0.25
0.22, 0.22, 0.23
0.32, 0.33, 0.34
0.31, 0.29, 0.28
0.35, 0.38, 0.40
0.41, 0.50, 0.53
0.33, 0.31, 0.29



Original

671 kB



$K = 100$

419 kB



Original

671 kB



$K = 10$

126 kB



Original

671 kB



$K = 9$

117 kB



Original

671 kB



$K = 8$

101 kB



Original

671 kB



$K = 7$

93 kB



Original

671 kB



$K = 6$

79 kB



Original

671 kB



$K = 5$

65 kB



Original

671 kB



$K = 4$

57 kB



Original

671 kB



$K = 3$

36 kB



Original

671 kB



$K = 2$

18 kB



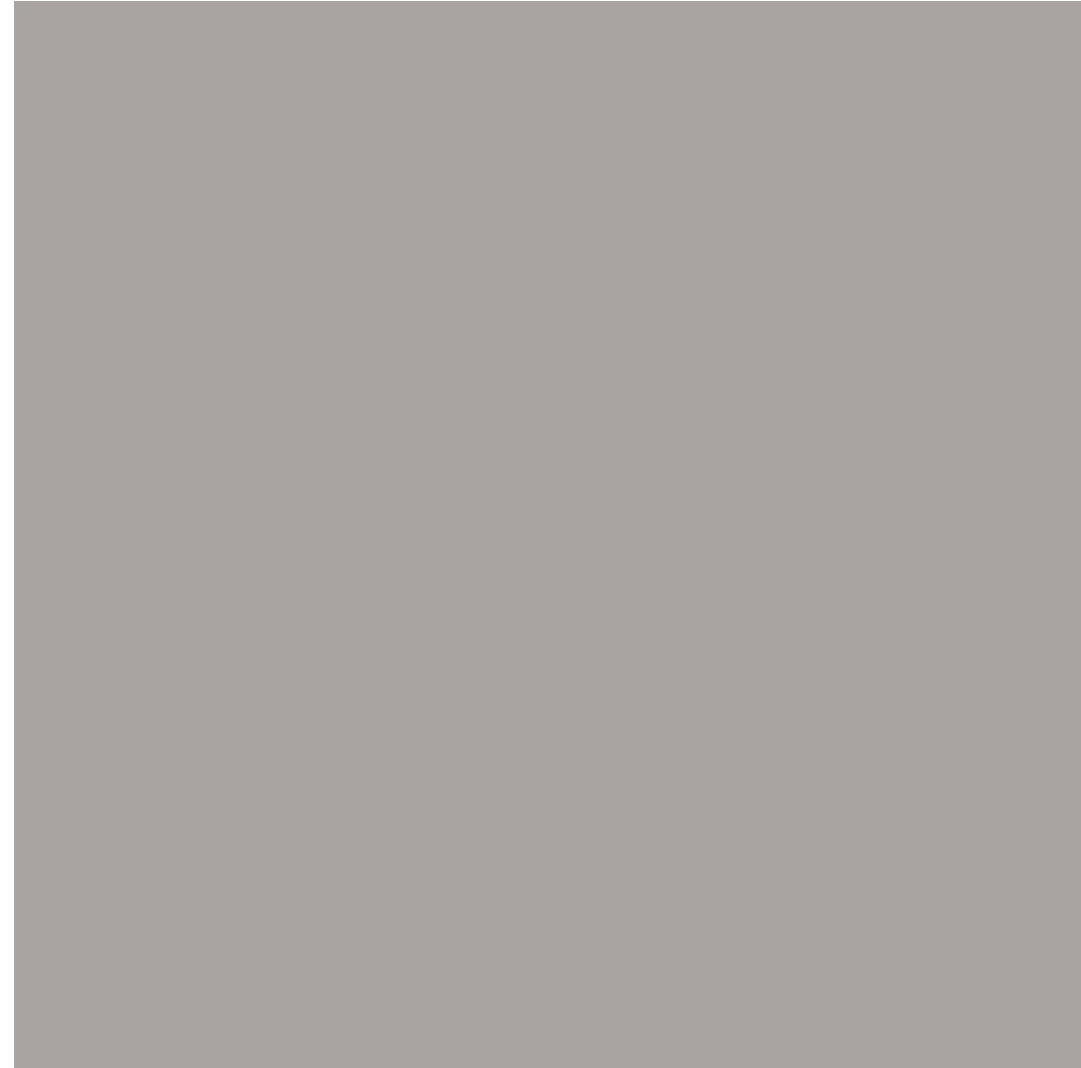
Original

671 kB



$K = 1$

4 kB



File size increases with number clusters

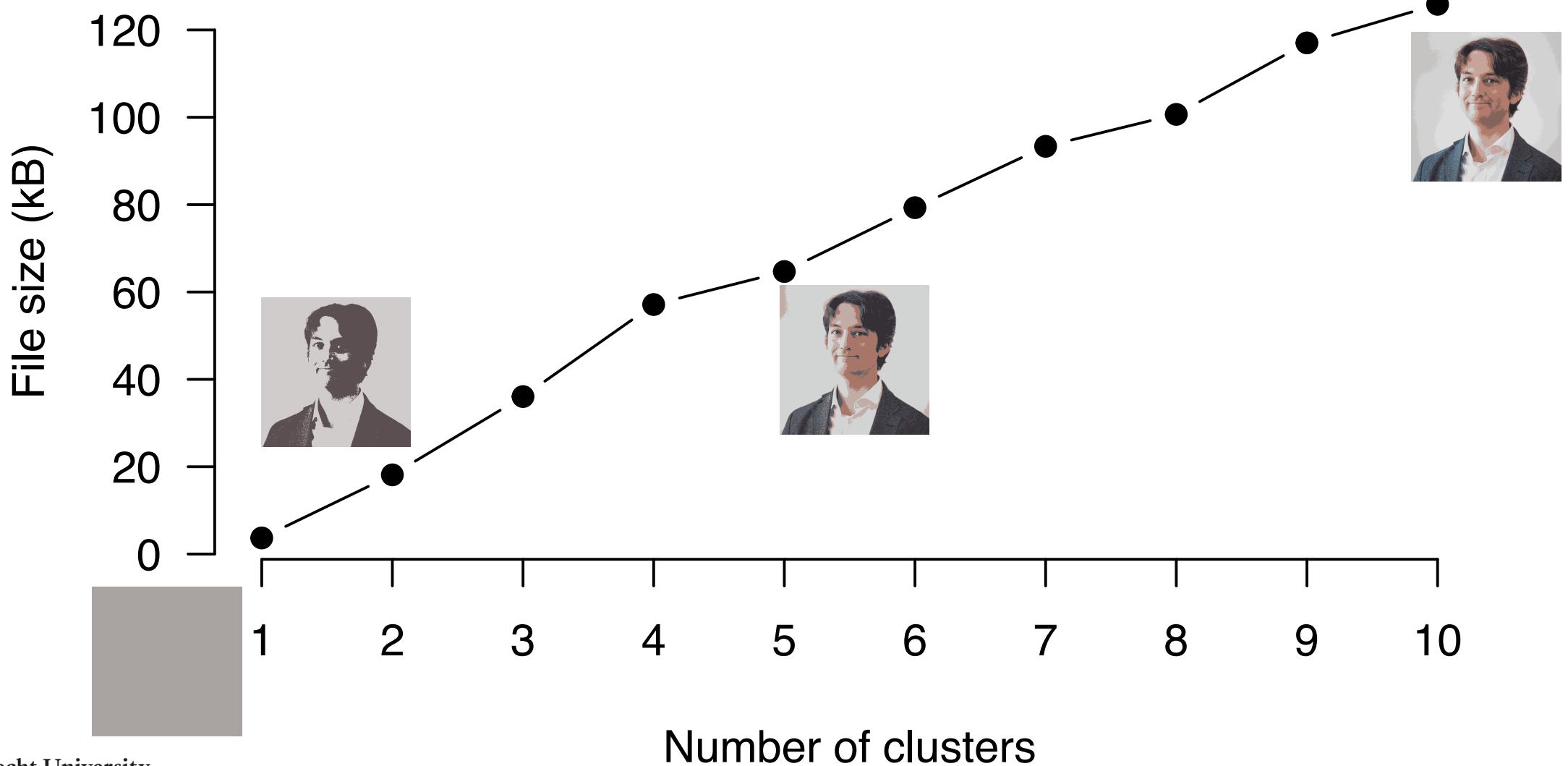
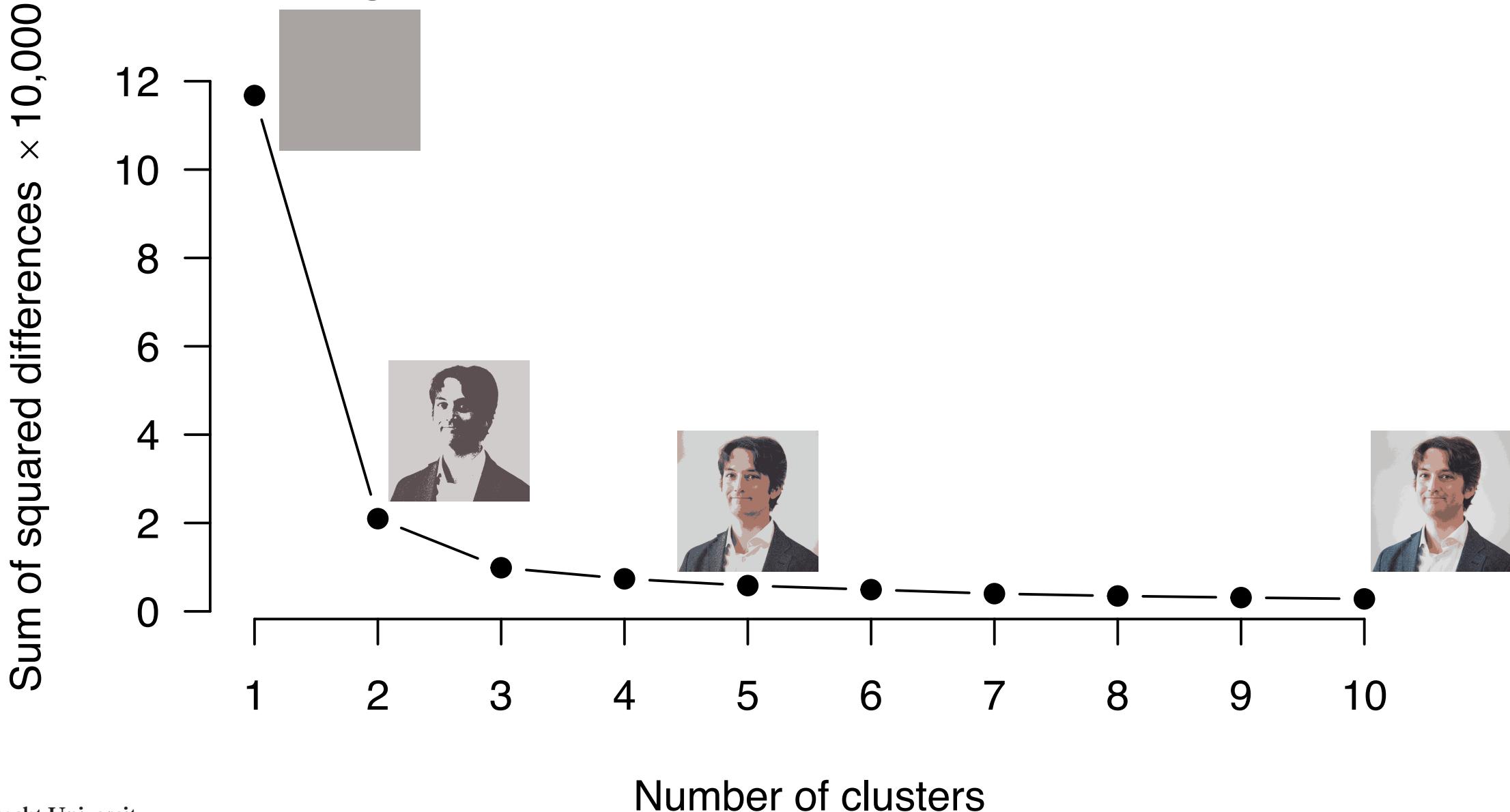


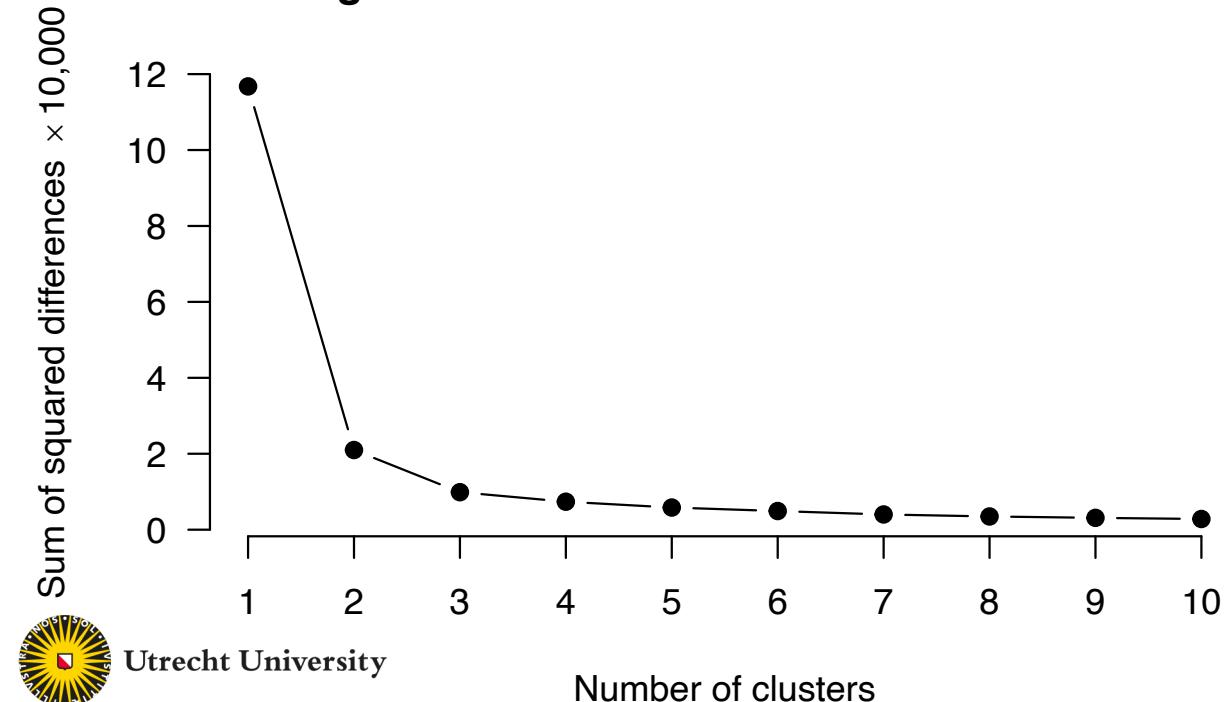
Image loss decreases with number of clusters



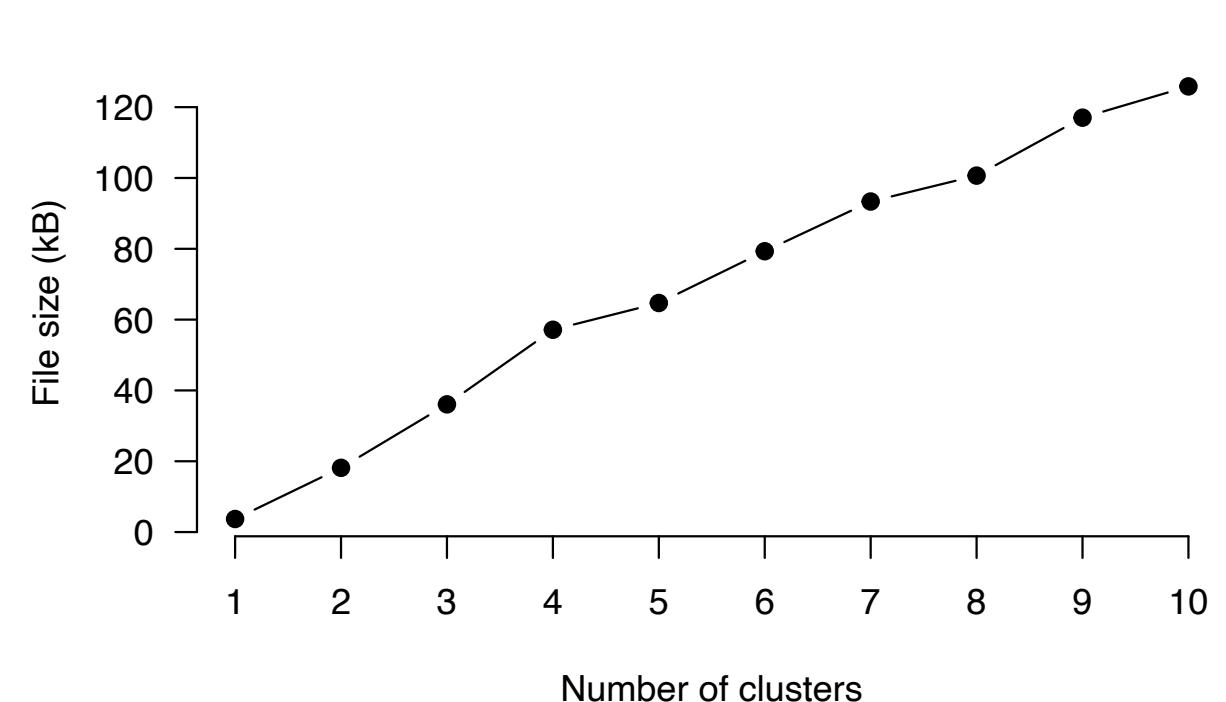
Which of these is the best and why?

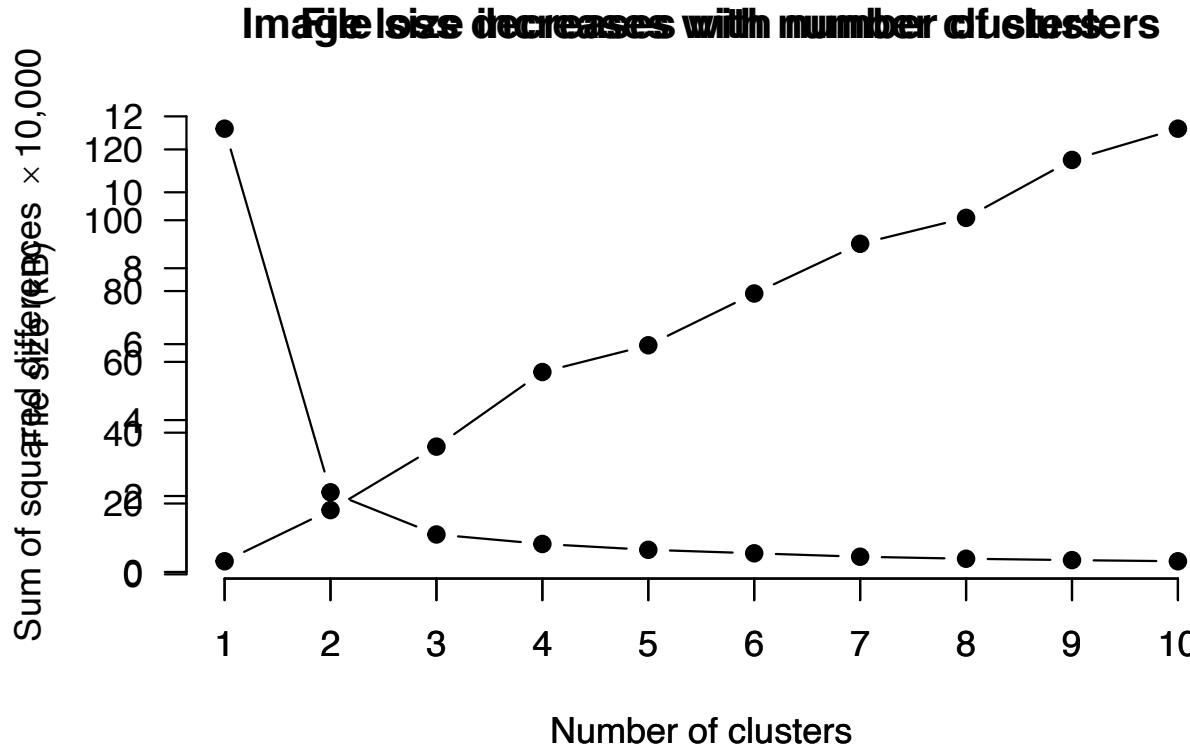


Image loss decreases with number of clusters



File size increases with number clusters





- More clusters gives **better “fit”** in terms of reconstruction of the image (compression is less “lossy”)
- More clusters gives **bigger file size** (solution is more complex, takes more bytes to store)
- So the **model loss and model complexity trade off against each other**
- This is a common theme in (unsupervised) machine learning and you should remember this for model-based clustering lecture

How to **evaluate** clustering results

1. Use of external information
2. Visual exploration
3. Stability assessment / sensitivity analysis
4. Internal validation indexes
5. (Testing for clustering structure)

*Much more info & helpful advice on Christian Hennig's homepage:
<http://www.homepages.ucl.ac.uk/~ucakche/presentations/compstatvalidation.pdf>*

1. External validation

Are the clusters associated with *external* feature Y?

“Making unsupervised supervised”

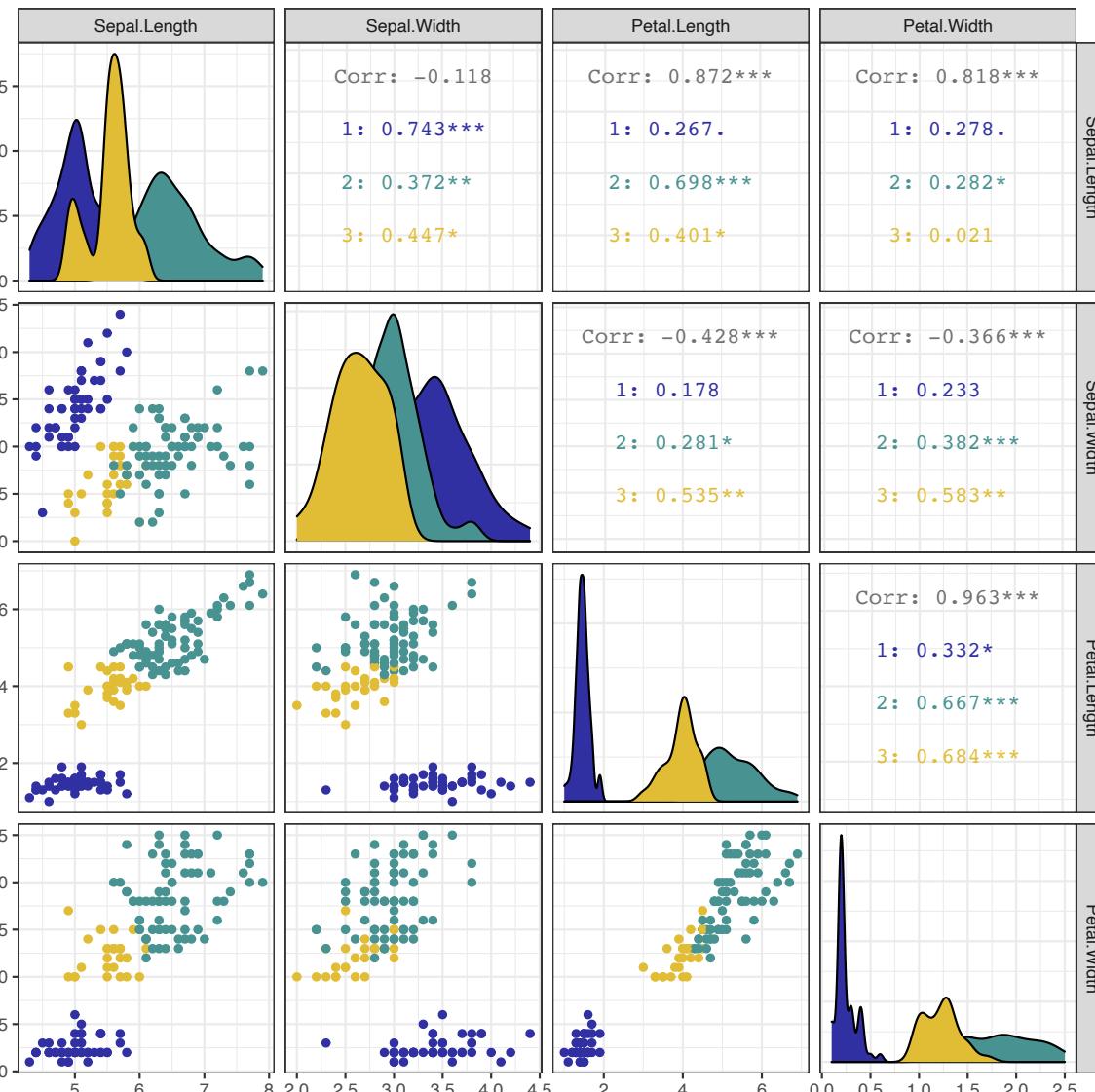
Examples:

- Are my customer segments based on spending associated with the demographics of the customers?
- Are the geyser eruption types strongly correlated with water pressure or temperature?
- Can I recognize the person in the vector quantized picture?



2. Visual exploration

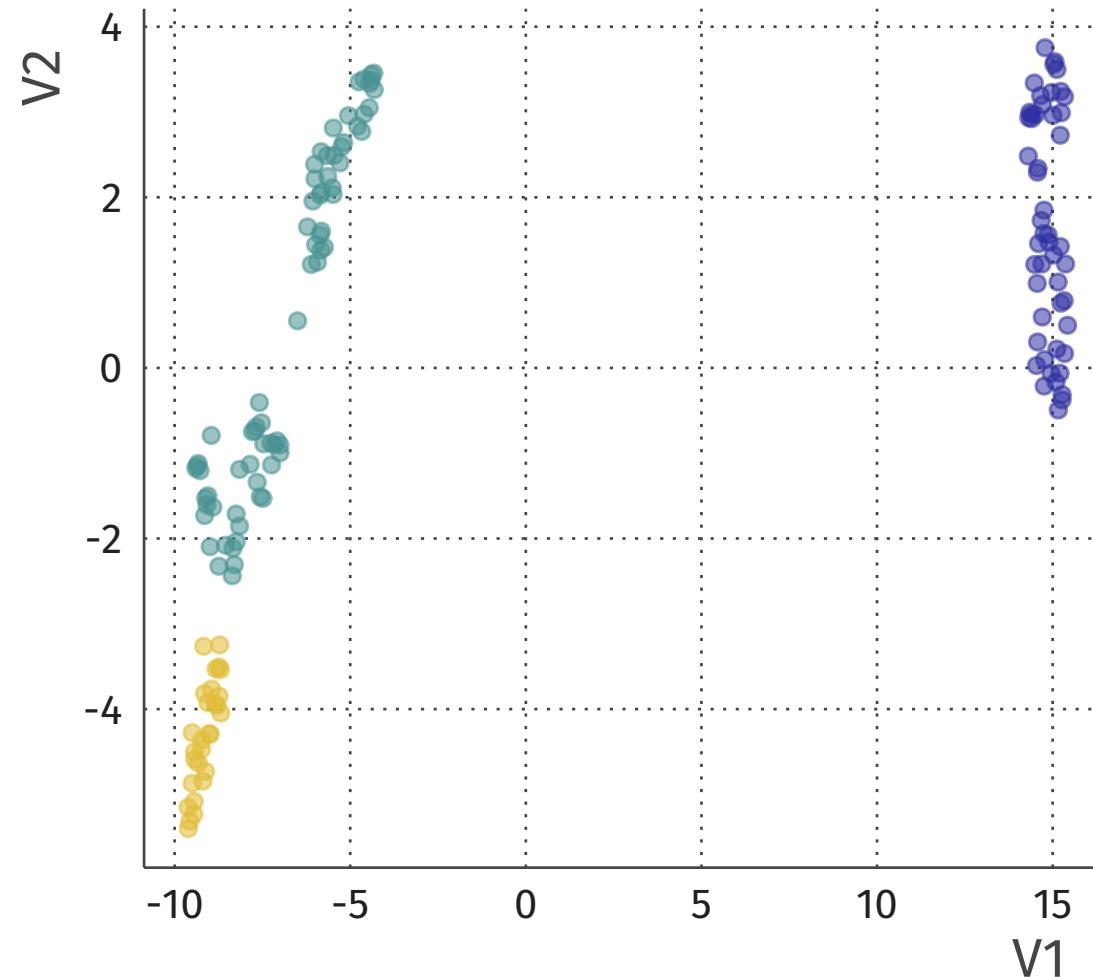
Iris: Scatterplot pairs



- **Problem:** Kind of hard to see already...
- Wait till you get 1000 variables!
- **New idea:** Reduce variables into 2D “manifold” for visualization
- Popular techniques: UMAP, t-SNE, MDS, Discriminant Coordinates, (PCA)

2. Visual exploration (using “manifold”)

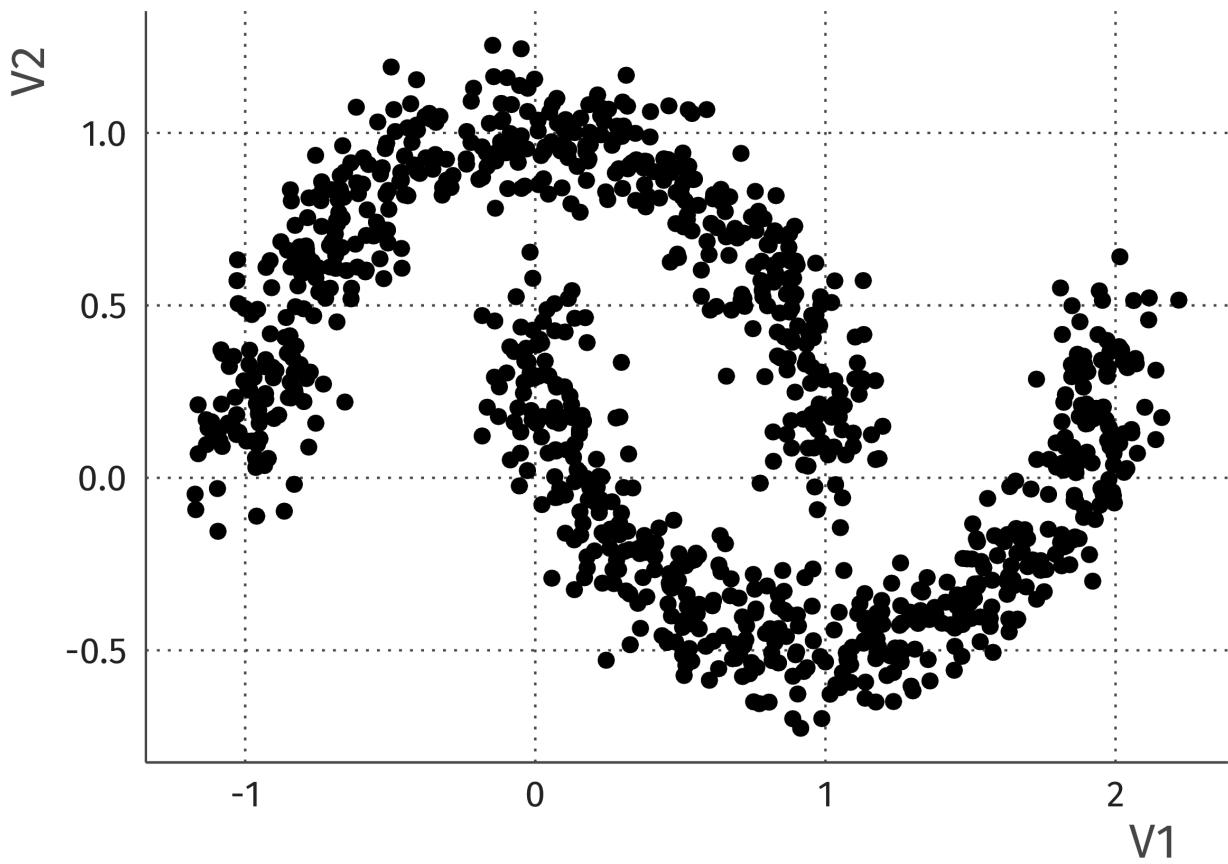
Iris: UMAP representation



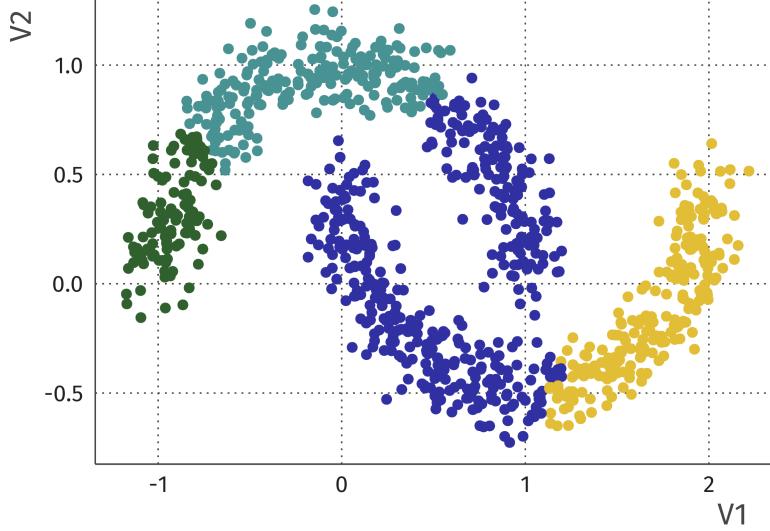
3. Stability assessment

A.k.a.: Clustering can be fiddly

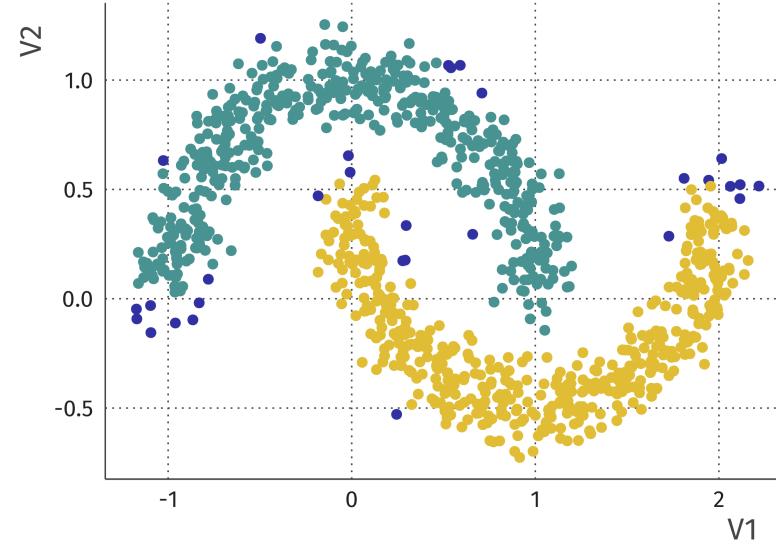
Toy dataset 'moons'



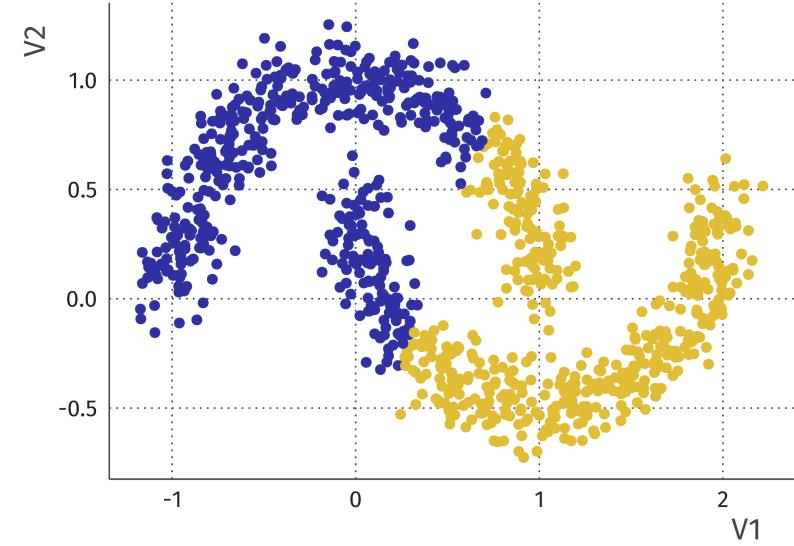
`hclust` [default settings, 2 cluster cutoff]



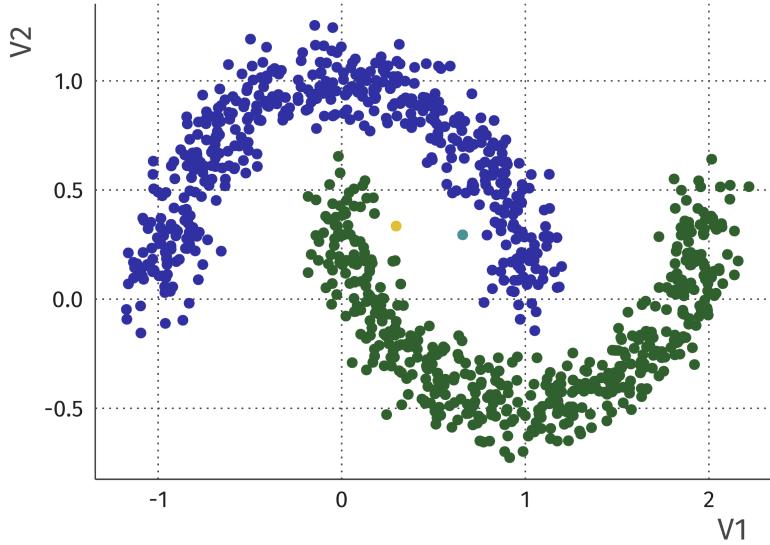
`dbSCAN` [noise set to true level, 0.1]



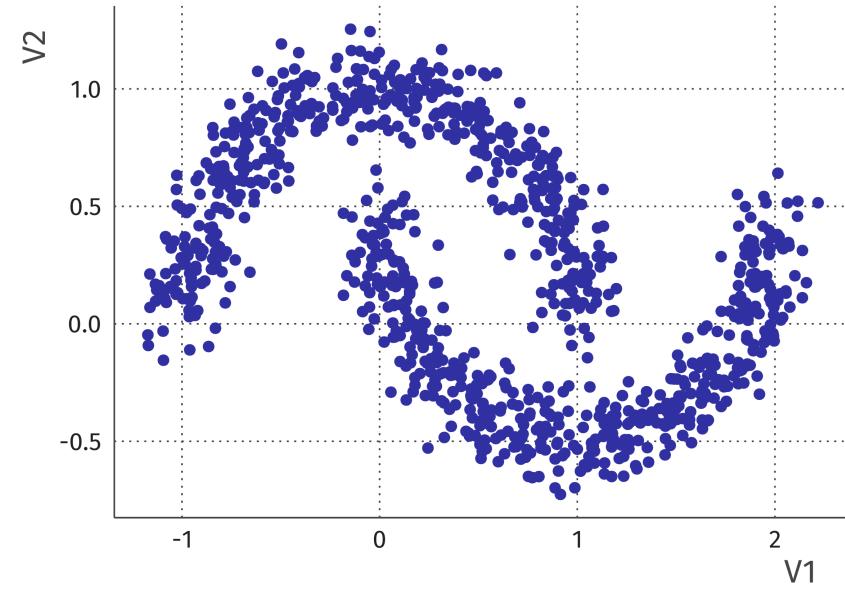
`kmeans` [K = 2]



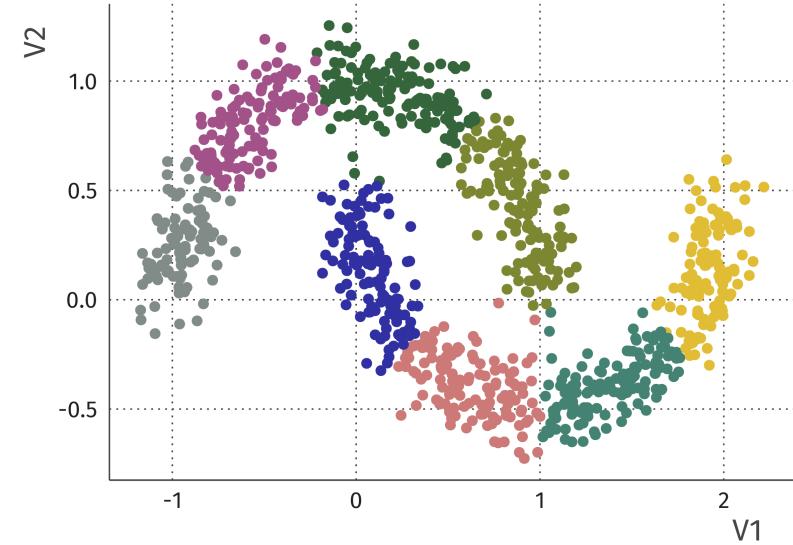
`hclust` [single linkage, 4 cluster cutoff]



`dbSCAN` [noise set to 0.15]



`kmeans` [K = 8]



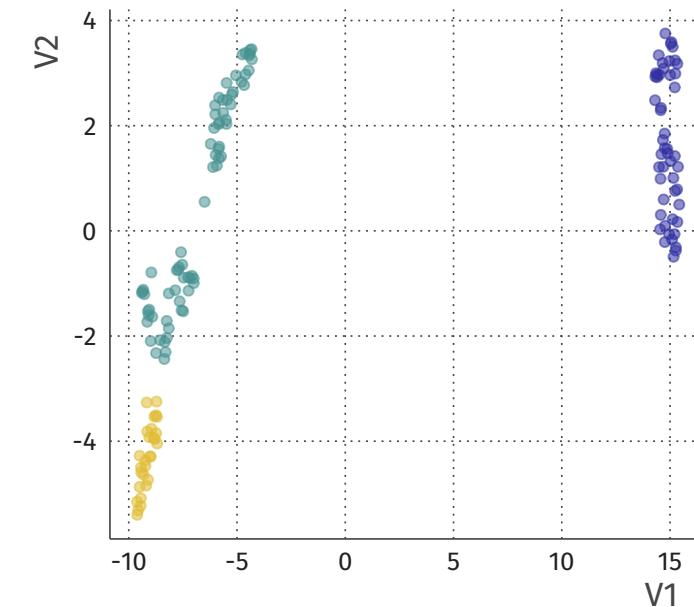
3. Cluster “stability”

Three “stabilities”. How much does clustering change when:

1. Changing some **hyperparameters** (distance metric, linkage, K, ...)
2. Changing some **observations** (bootstrapping, [Hennig, 2007](#))
3. Changing some **features**

Check if observations are classified into same cluster across choices
e.g. using Jaccard index, Rand index





3. Clusterwise stability in R

```
library(fpc)
data(iris)
clusterboot(iris[, 1:4],
            clustermethod = hclustCBI,
            method = "complete", k = 3)
```

Clusterwise Jaccard bootstrap (omitting multiple points) mean:

```
[1] 0.891 0.459 0.719
```

4. Internal validation indices

- Only look at “unsupervised” bit: data and clustering
- Quantify how “successful” the clustering is in some sense
- Popular **measures**:
 - Average sihouette width (**ASW**) *(how close are points to other clusters)*
 - “Gap statistic” *(Tibshirani et al. 2001)*
 - (measures from model-based clustering → tomorrow)

Disadvantage: don't take account of the clustering **aim!**



Silhouette analysis in R

```
distmat_faithful <- dist(faithful)
hclust_faithful <- hclust(distmat_faithful)

clustering_faithful <- cutree(hclust_faithful, 2)
silhouette_scores <- silhouette(clustering_faithful, distmat_faithful)

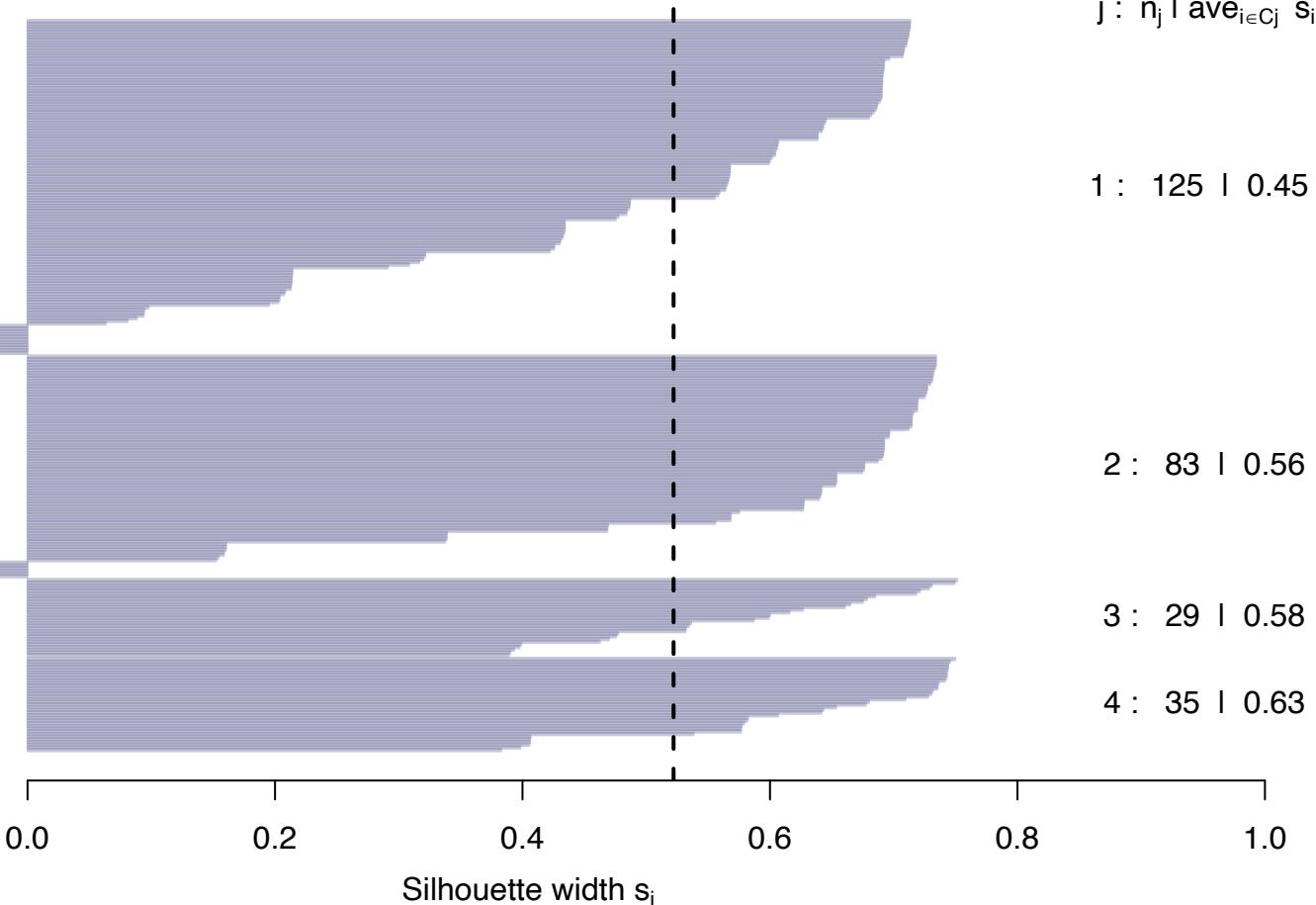
plot(silhouette_scores)
```

Note that this works for any type of clustering!

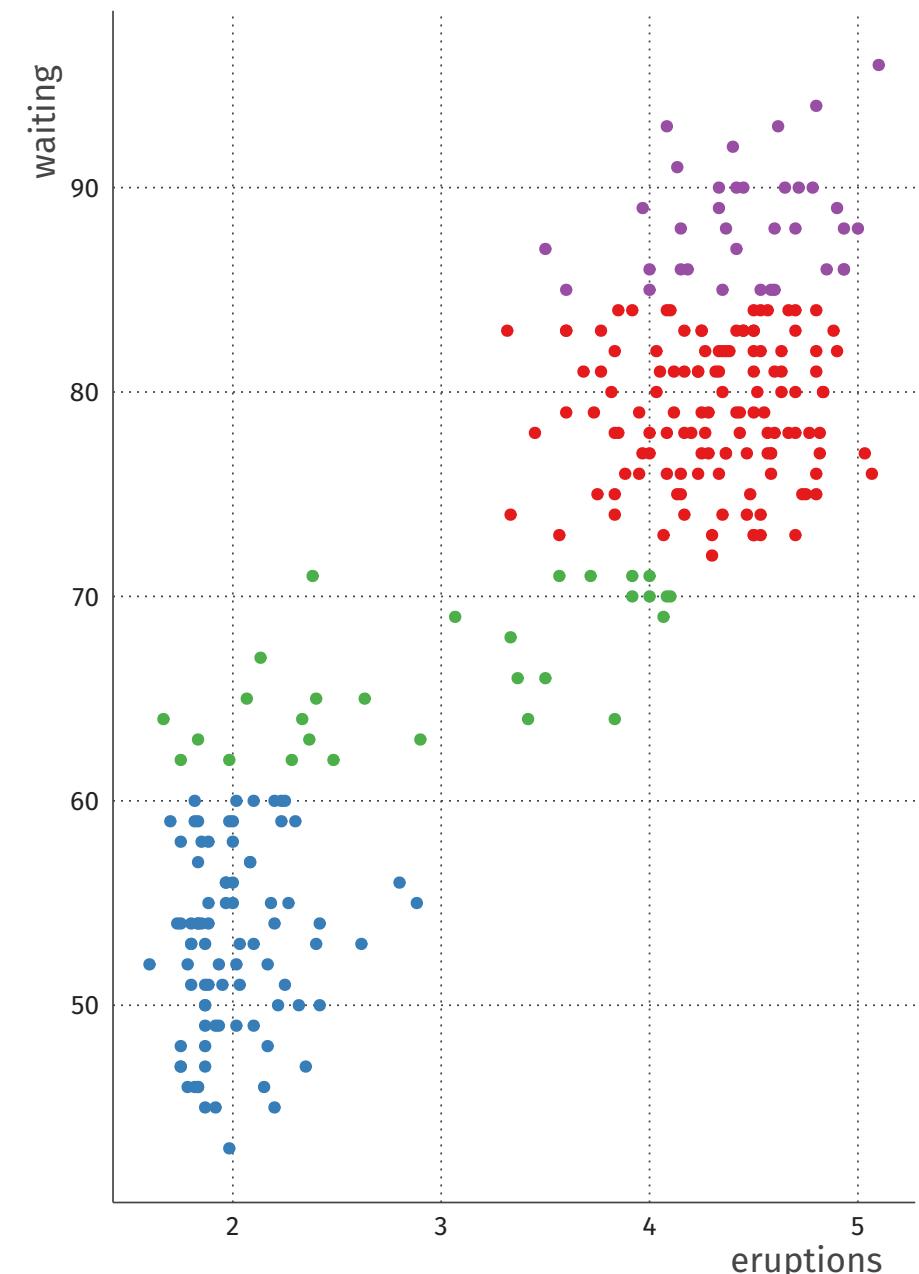


Silhouette plot of (x = clustering_faithful, dist = distmat_faithful)

n = 272

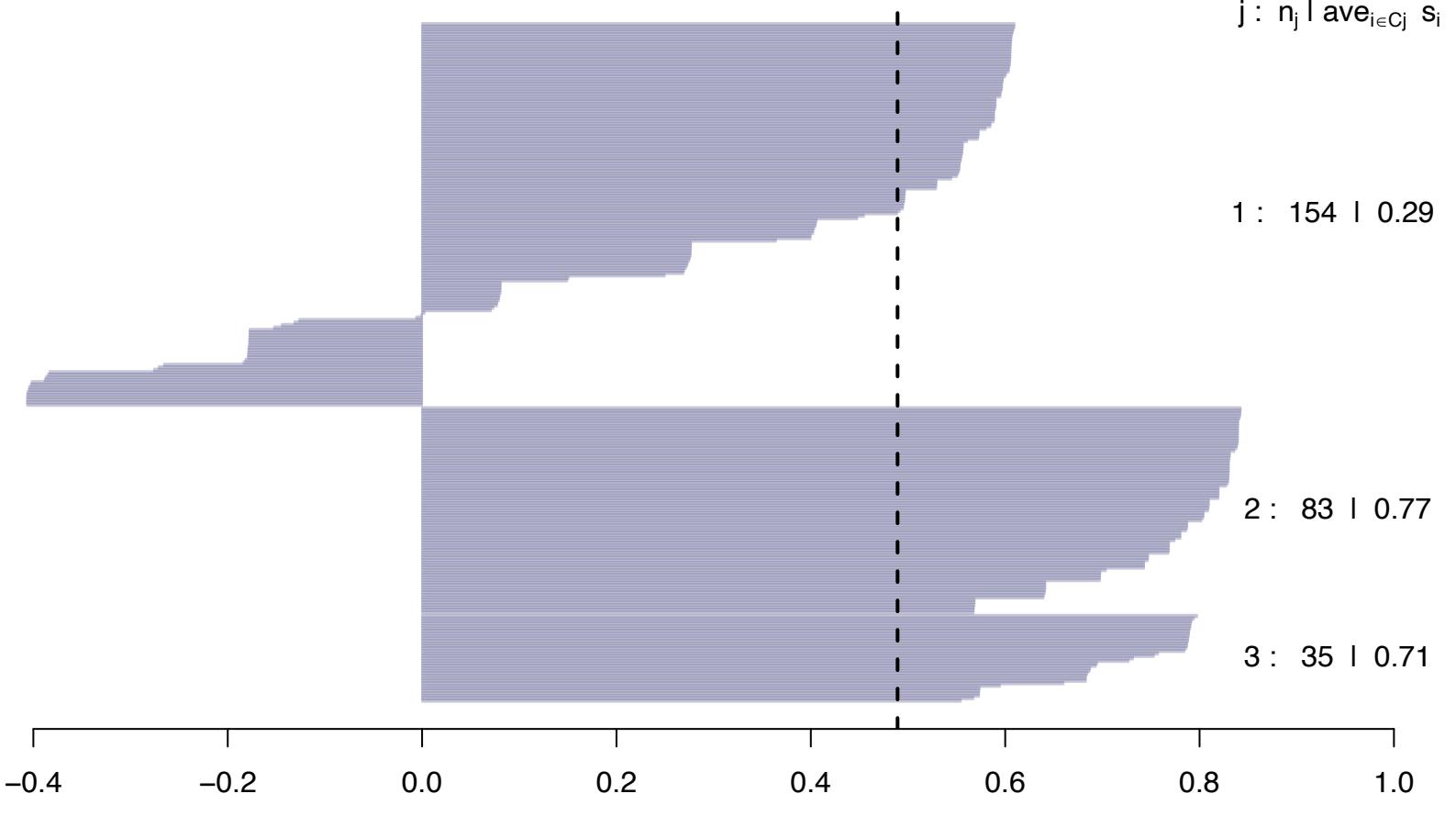


4 clusters C_j
 $j : n_j | \text{ave}_{i \in C_j} s_i$



Silhouette plot of (x = clustering_faithful, dist = distmat_faithful)

n = 272



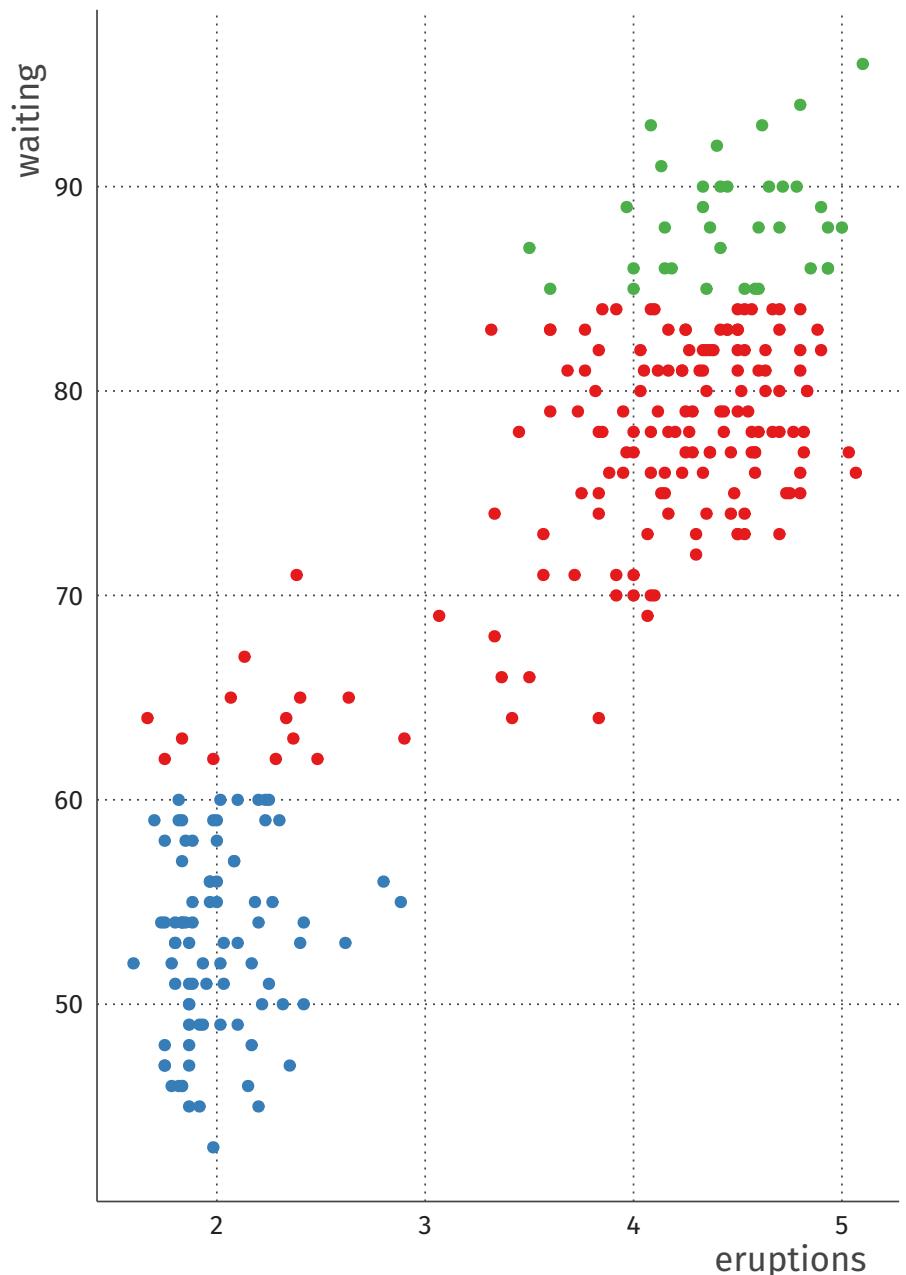
Average silhouette width : 0.49

3 clusters C_j
j : n_j | ave $_{i \in C_j}$ s_i

1 : 154 | 0.29

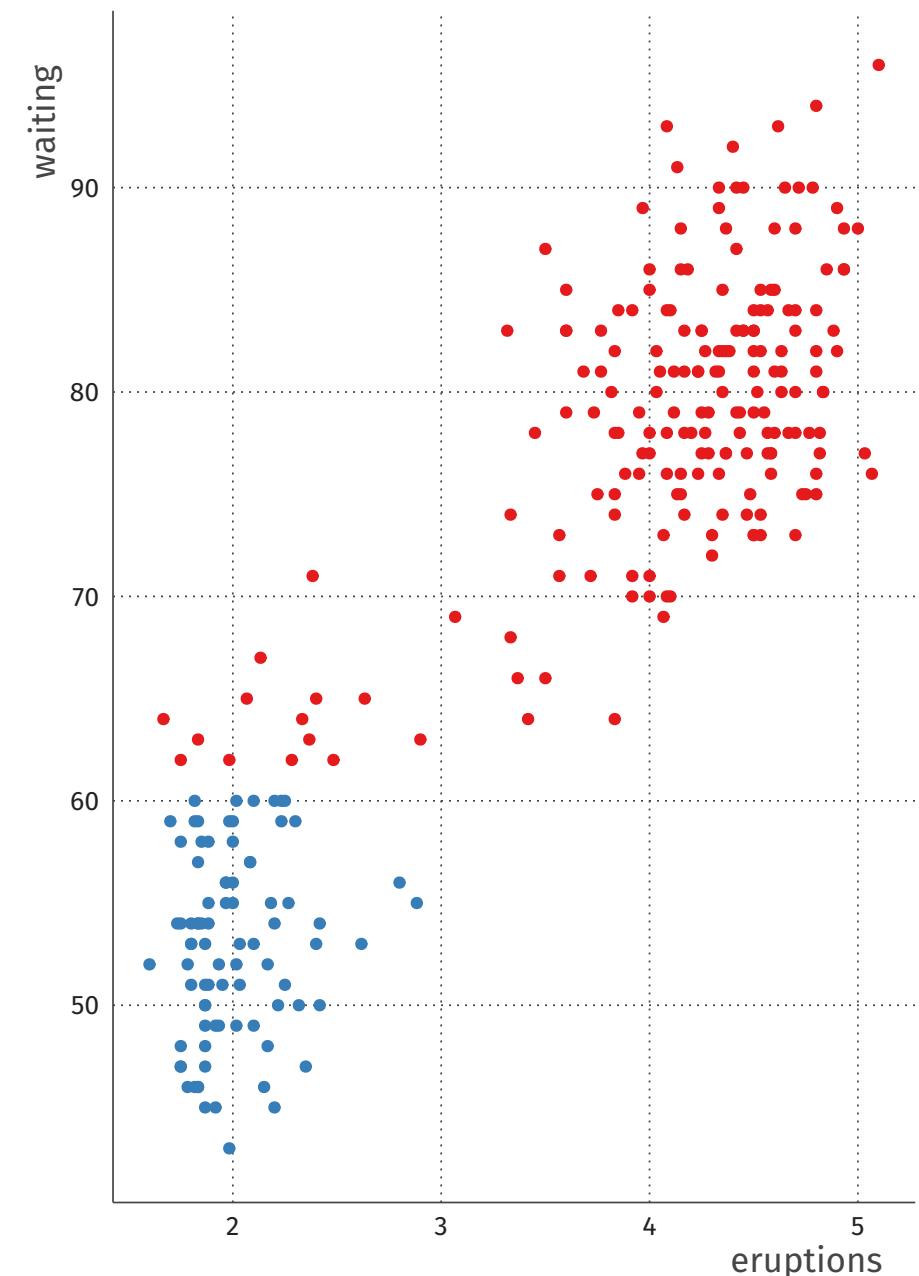
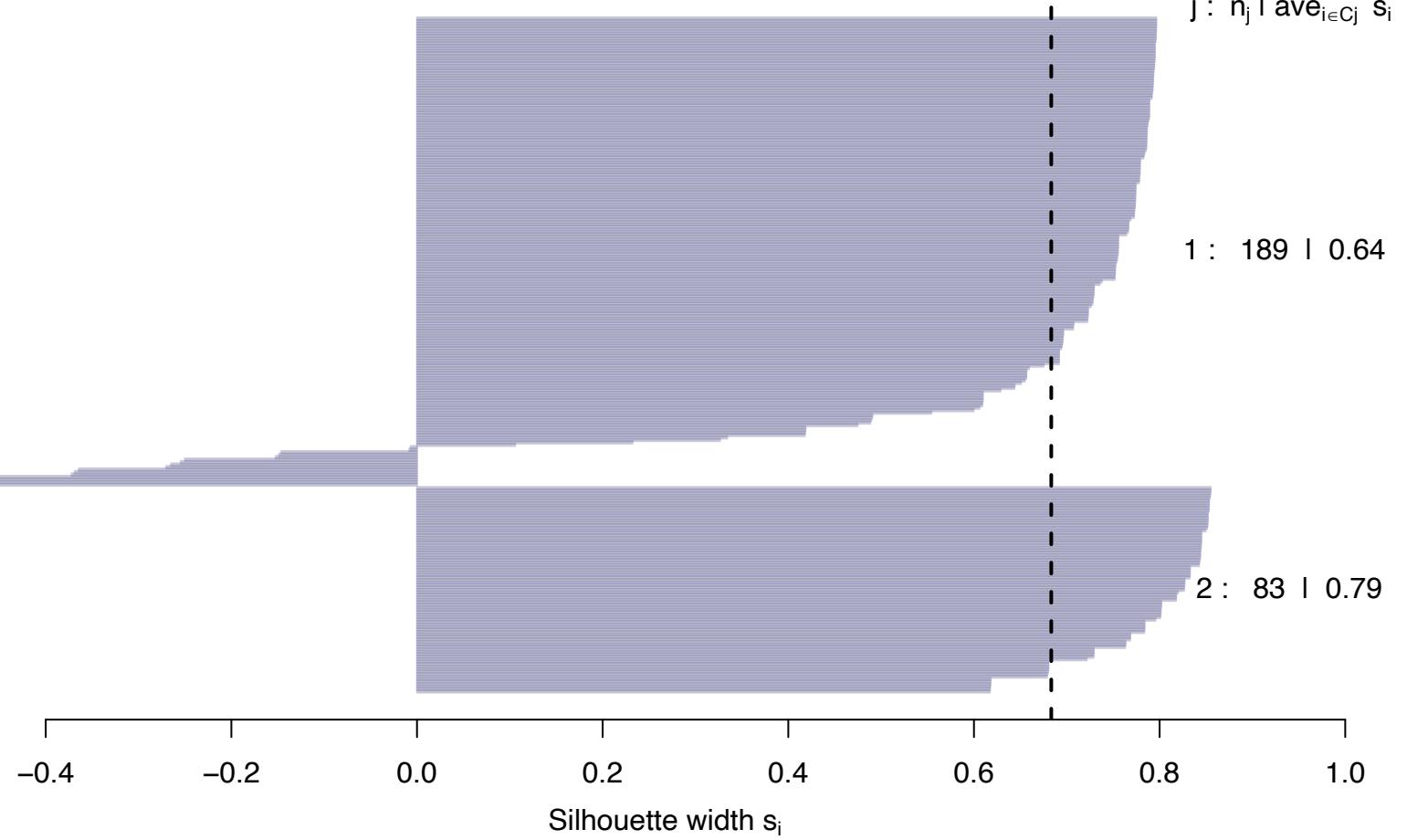
2 : 83 | 0.77

3 : 35 | 0.71



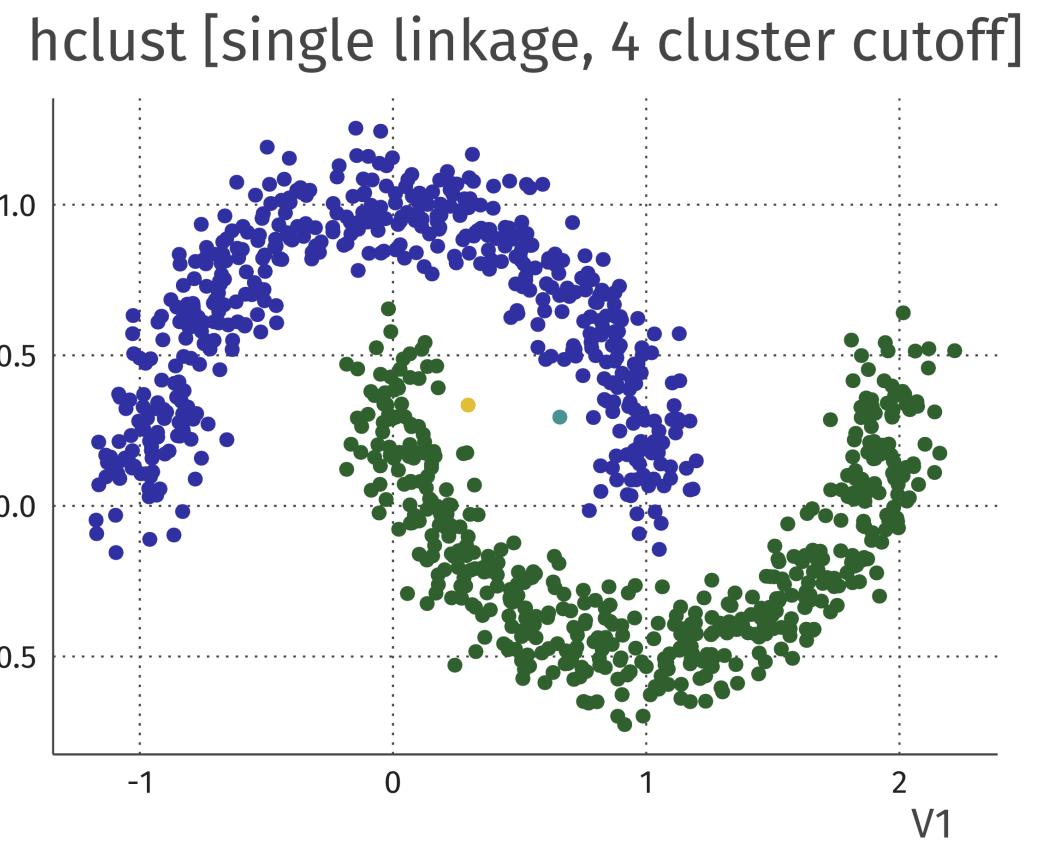
Silhouette plot of (x = clustering_faithful, dist = distmat_faithful)

n = 272



What do you think the average silhouette width (ASW) of this solution will approximately be?

<hidden solution>



Conclusion: clustering

- Clustering looks for “similar” groups of observations
- Two basic clustering methods:
 1. **Hierarchical** clustering (e.g. bottom-up agglomerative, top-down divisive, ...)
 2. **Partitional** clustering (e.g. k-means, DBSCAN, ...).
- Cluster evaluation is an important and subtle topic;
- No way to get rid of critical thought.

- Next lecture: **model-based** clustering / *mixture modeling*
- Before the exam wednesday: **read ISLR § 10.3!**

