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Fork of Unsupervised Learning by Kris Sankaran

# Unsupervised Learning

IFT6758, Fall 2020

Reading: ISLR sections 10.1, 10.2 and PDS pg. 462 - 476

## What is unsupervised learning?

- Supervised learning: Learn some mapping $x_i \to y_i$
- Unsupervised learning
  - Usual definition: "Exploring the data $x_i$"
- Less orthodox interpretations
  - Learning with hidden labels (clusters: missing classes)
  - Data compression for human consumption
  - Generation of derived data for human consumption

## Common Themes

- Much harder to evaluate

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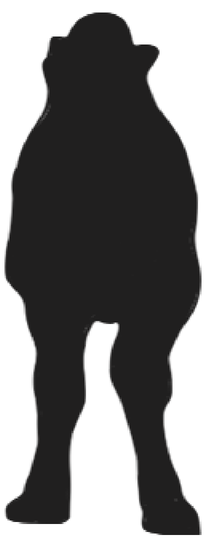
- Most methods can be categorized as either,
    - Dimensionality reduction: Few features that summarize many
    - Clustering: Few "prototypes" that are representative of whole dataset
- We'll review canonical examples,
    - PCA (dimensionality reduction)
    - K-means and Hierarchical Clustering (clustering)

### PCA

What is this?



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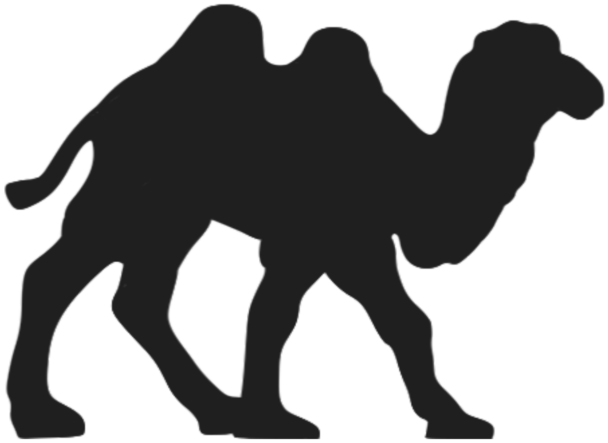


Credit for the idea: Prof. Julie Josse

## PCA

Idea: Certain views of high-dimensional data are more informative than others.

Can you find a low-dimensional representation with as much variation as possible?

## PCA

Can you find a low-dimensional representation with as much variation as possible?

To implement the idea,

- What will be the candidate family of low-dimensional representations?
- How will we choose one of the many candidates?

## Candidates: Linear Mixings

Can you find a **low-dimensional representation** with as much variation as possible?

- For a representation, consider linear combinations of high-dimensional vectors,

$$\begin{aligned} z_i &= \sum_{j=1}^{p} \varphi_{1j} x_{ij} \\ &= \varphi_1^T x_i \end{aligned}$$

- $\varphi_1$ is a free parameter. E.g., if $\varphi_1 = \left(\frac{1}{p}, \dots, \frac{1}{p}\right)$, then we summarize $x_i$ by averaging over its coordinates

## Selection Criteria: Maximal Variance

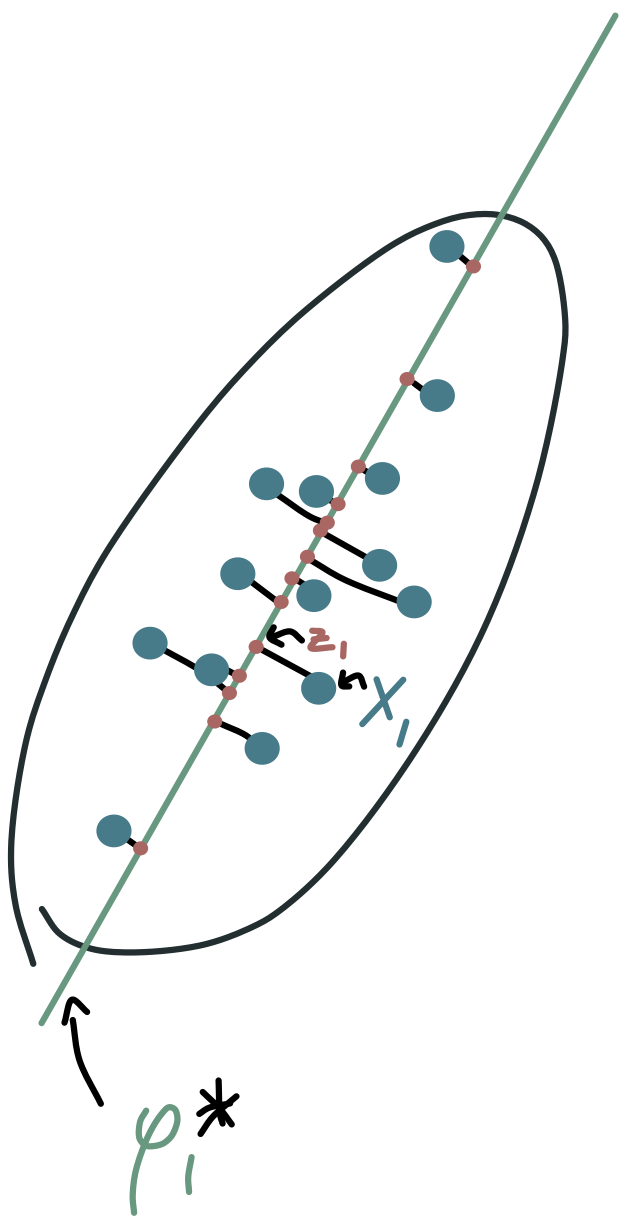
Can you find a low-dimensional representation with **as much variation** as possible?

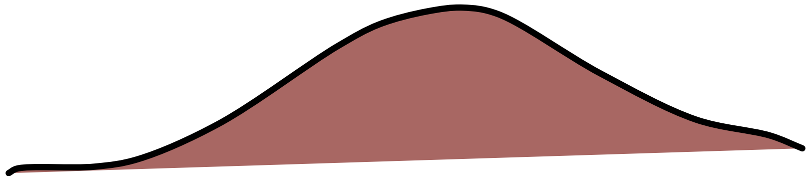
- The $z_i$'s should be as spread out as possible:

$$\text{maximize}_{\varphi_1} \frac{1}{n} \sum_{i=1}^{n} z_i^2$$

  - Subject to constraint $\|\varphi_1\|^2 = 1$.

See the example here. The red arrow is $\varphi_1$ and the points along the 1D axes are the associated $z_i$'s.





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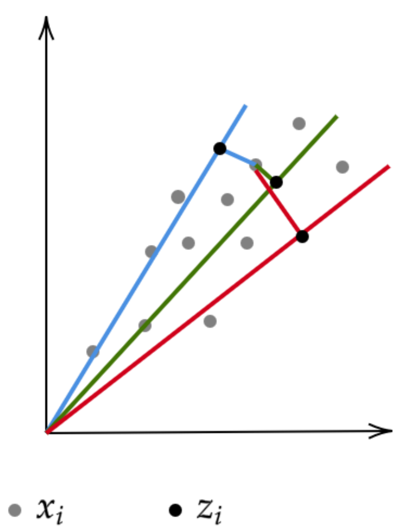
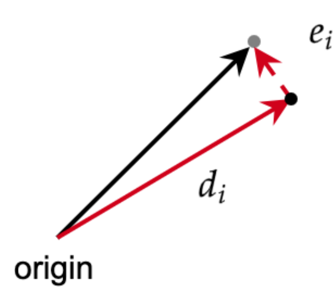
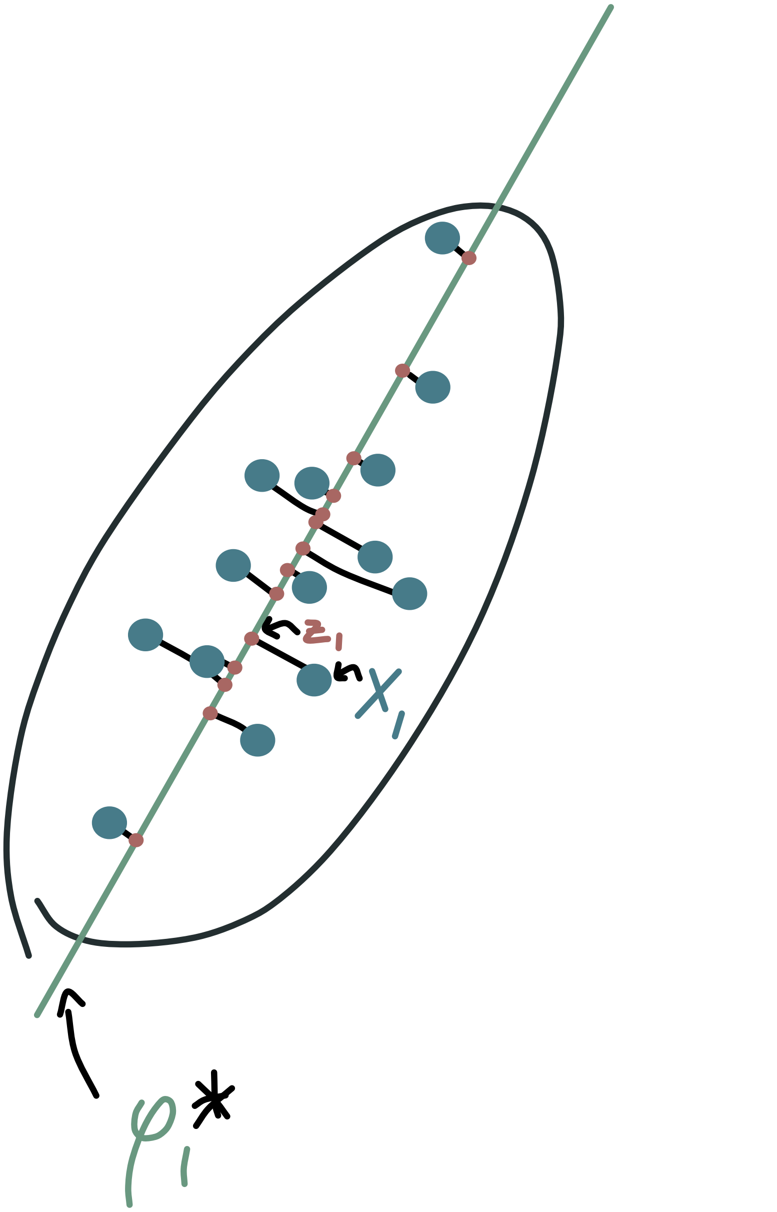
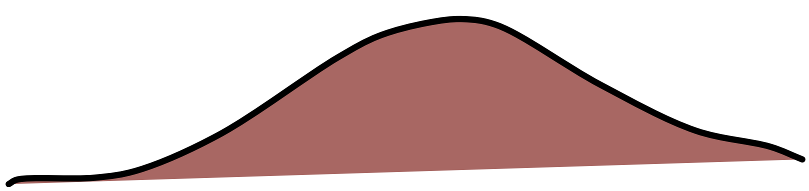




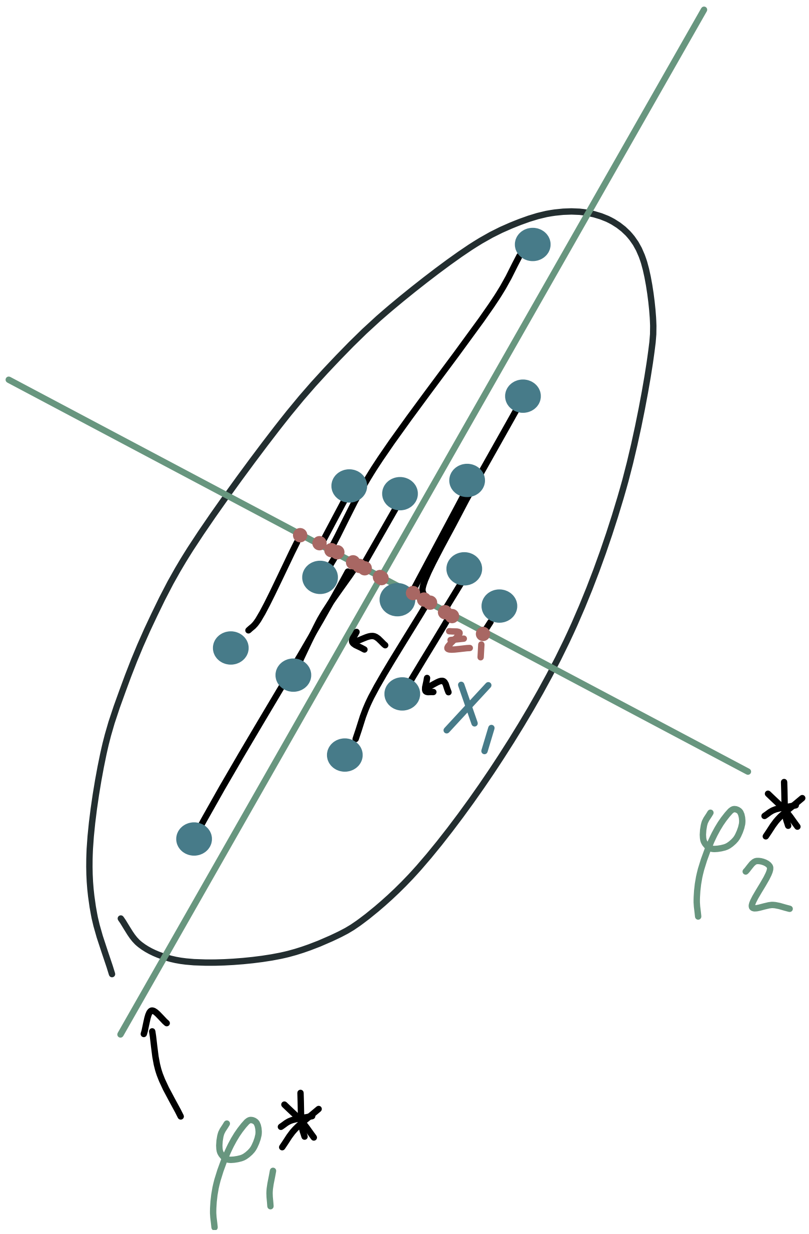



## Second, third, ... PCA directions

- Once you find $\varphi_1$, you can find a "second" direction $\varphi_2$
- Found by solving the exact same optimization, but with a

new constraint that it's at 90 degrees to the previous directions

- Interpretation: PCA is finding a new, better coordinate system for your data




## Semantics

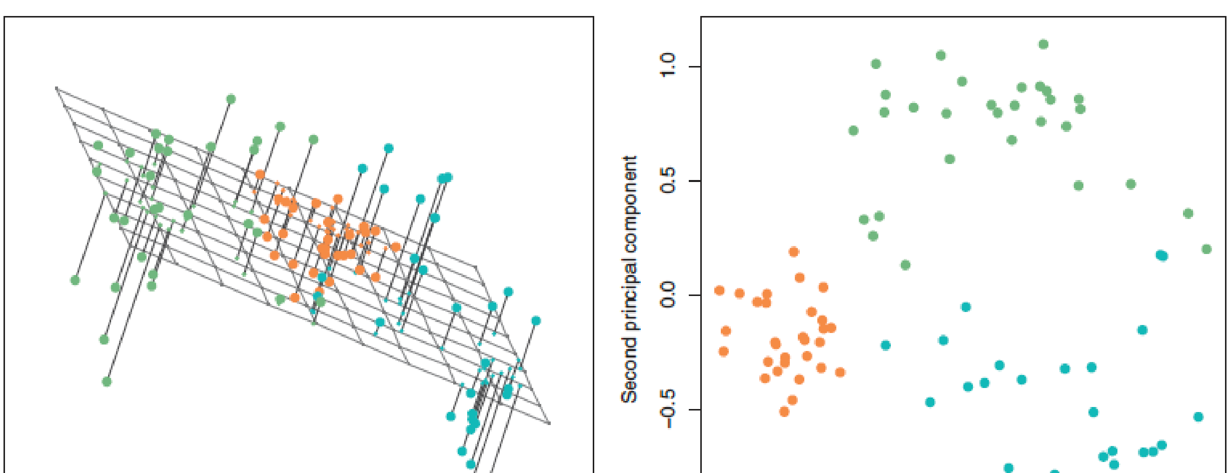
- The $\varphi_k$ are the PCA "directions" or "components."
- The $z_i$ are called "scores."
    - Interpreted as coordinates with respect to the directions $\varphi_k$.

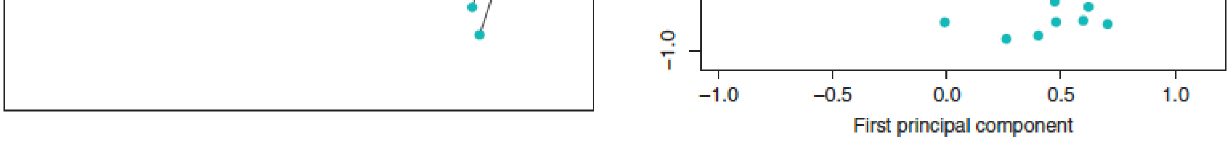
## Alternative Interpretation: Linear Approximation

- The first $K$ directions in PCA find the best $K$-dimensional linear approximation (using sum of squared error to measure approximation quality).
- This means it's fair to say

$$x_{ij} \approx \sum_{k=1}^{K} z_{ik} \varphi_{kj}$$

- Or, in matrix notation, $x_i \approx \Phi z_i$, where $\Phi$ concatenates the $\varphi_k$'s vertically
    - $x_i$ is a mixture of the components $\varphi_k$ with weights $z_{ik}$.

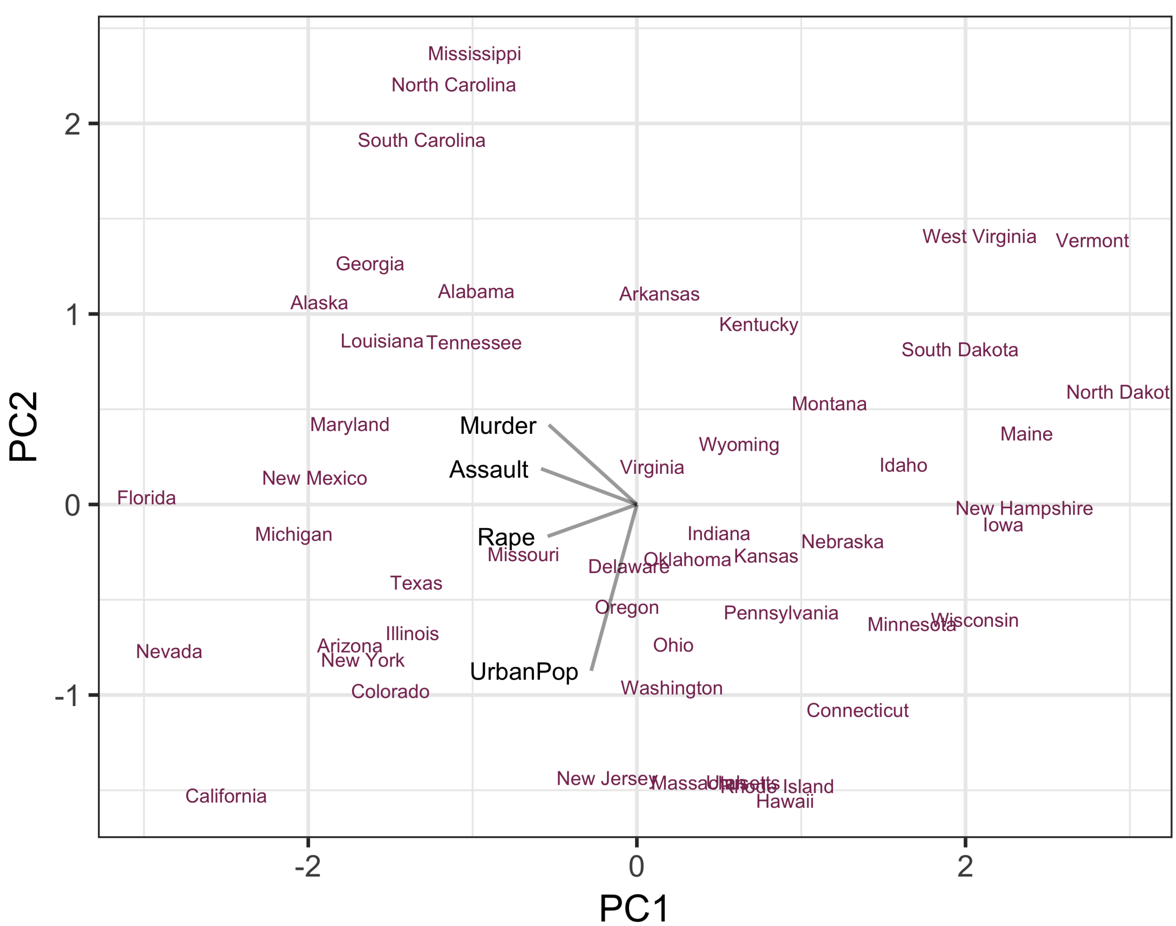





## Example with two principal components

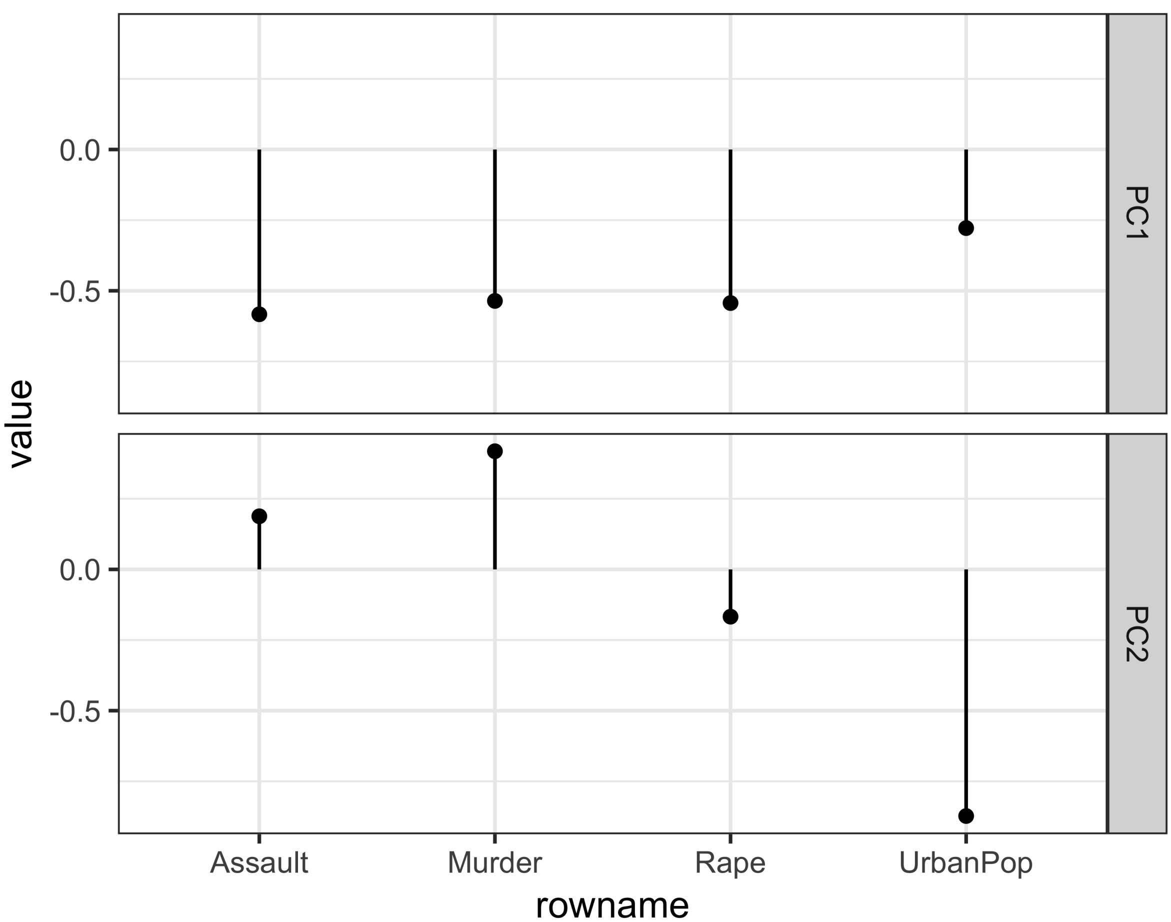
We'll practice reading PCA plots using `USArrests` --- a little dark but you will see more of such *breaking bad* themed examples in ISLR

- $z_i$'s give the states' coordinates
- Can interpret components by looking at how variables contribute. Variable $j$ is plotted at $(\varphi_{1j}, \varphi_{2j})$.
  - E.g., the second PC mostly captures variation related to urban population



## Biplots

Arrows come from the $\varphi_1$ and $\varphi_2$. The $(x, y)$-coordinate of the arrows comes from viewing these PCs in 2D.




## Biplots

- The coordinate of $x_i$ on the biplot is $(z_{i1}, z_{i2})$

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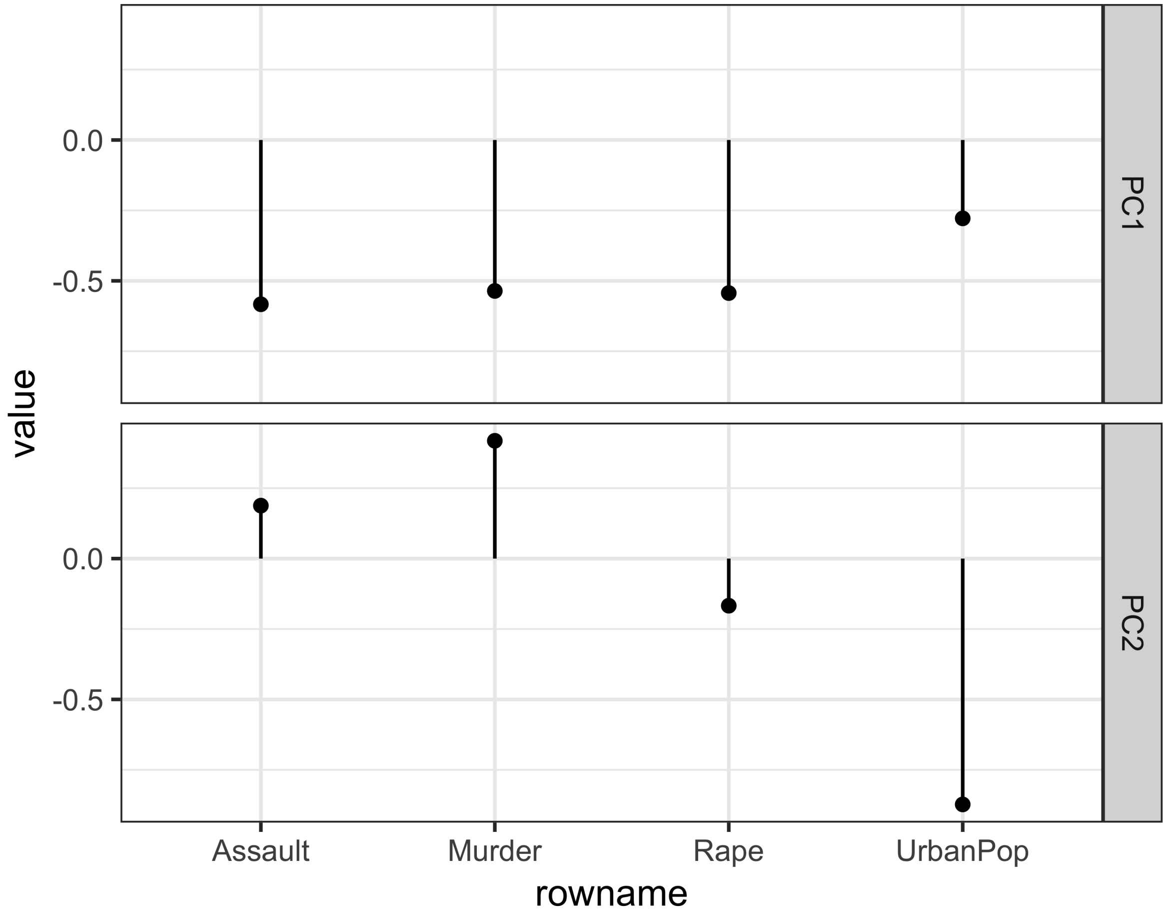
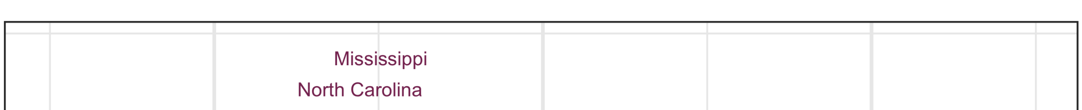
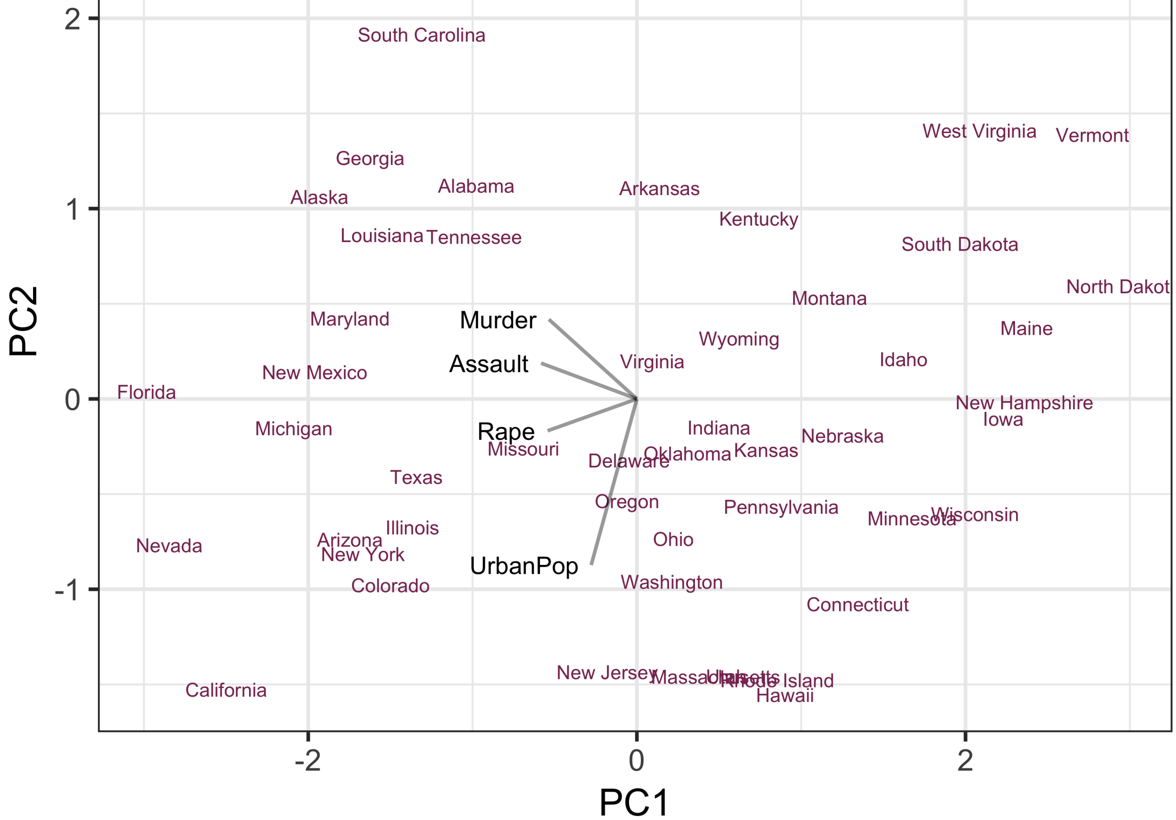
- Since $x_i \approx z_{i1}\varphi_1 + z_{i2}\varphi_2$, they have large values for variables with large loadings in the coordinate directions where $x_i$ is farther along




## Biplots

- For example, California $\approx -2.5\varphi_1 - 1.52\varphi_2$
- Since $\varphi_1$ puts negative weight on the crimes, California has more than the average # of crimes $(- \times - = +)$
- Since $\varphi_2$ puts negative weight on urban population, California has larger than the average population






## Explained Variation

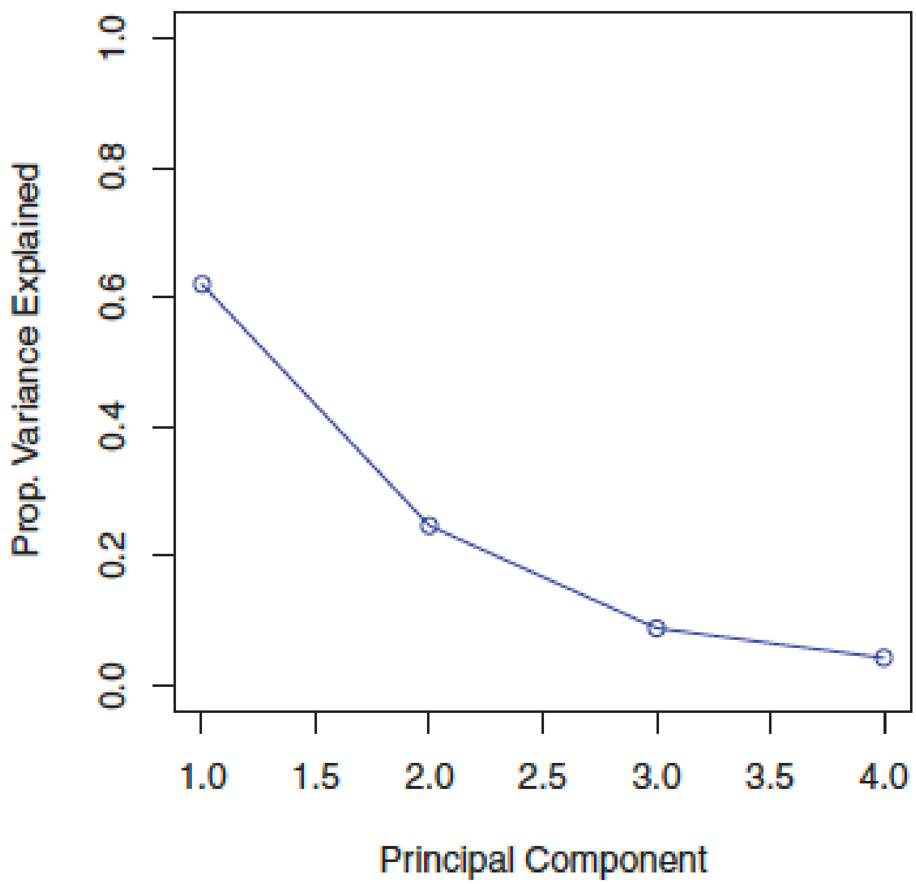
- Amount explained by $k^{th}$ component,

$$\frac{\sum_{i=1}^{n} ||z_{ki}||^2}{\sum_{i=1}^{n} ||x_i||^2}$$

- If no directions are preferred, get $\approx \frac{1}{p}\%$ everywhere
- How to compute?
  - Consider the covariance matrix of the data. Check total variance. Now look at the transformed covariance matrix and find the ratio of variances of each component.

- Exercise: What would the plot below look like if the data were shaped like...

  - a pancake (two long directions, one short one)
  - a cigar (one long direction, two short ones).




## Things to watch out for

- Even though the method is easy to run, there are lots of potential issues,
  - Variables might be at different scales, and there might be ambiguity about whether to rescale them
  - The directions are only unique up to sign

- Choosing $K$ is tricky (although might not be crucial)

## Clustering

Idea: Partition the observations, so that those that are similar to each other appear together

Look for homogeneous subgroups in your heterogeneous data.

## Formalization

A partition $C_1, \ldots, C_k$ is a collection of subsets satisfying,

- Each sample is in a subset:

$$\cup_{k=1}^{K} C_k = \{1, \ldots, n\}$$

- Subsets are disjoint: For any pair,

$$C_k \cap C_{k'} = \emptyset$$

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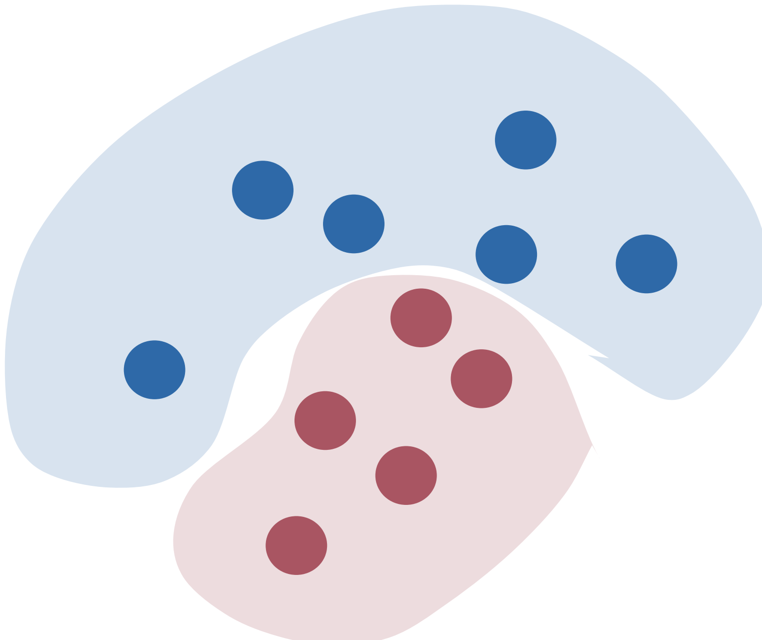

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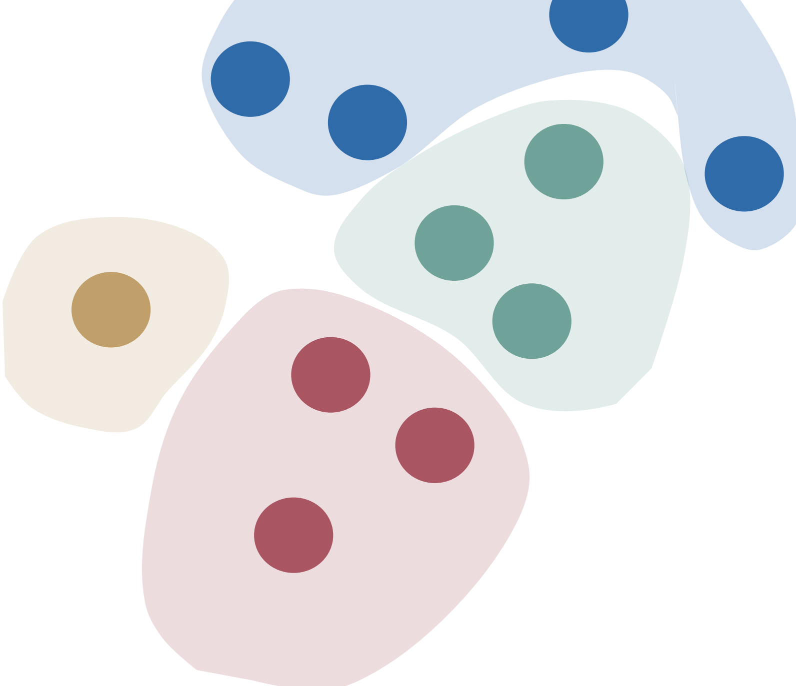

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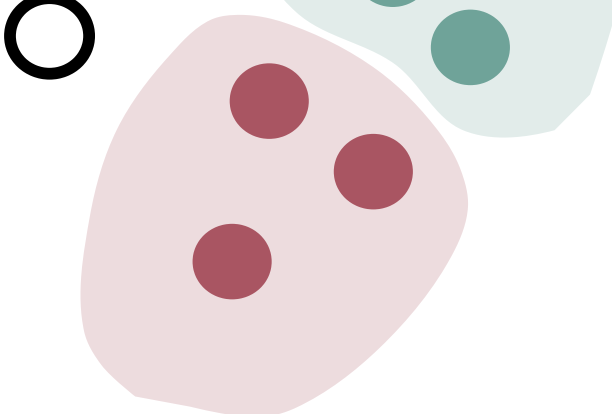

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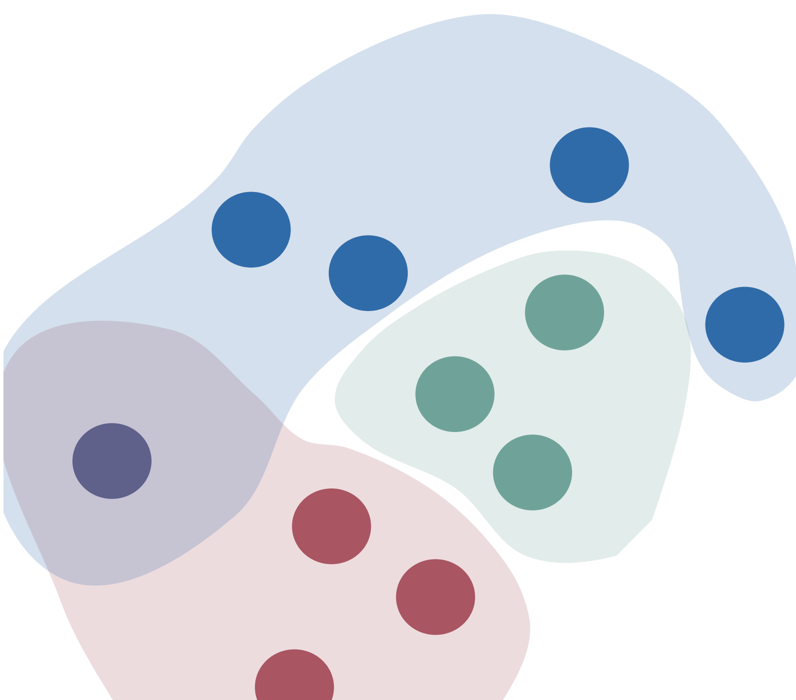
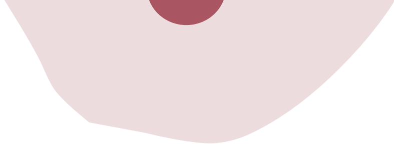


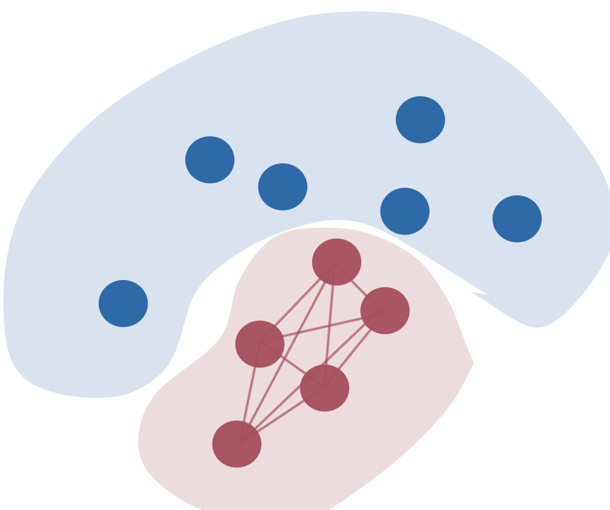


# Formalization

We don't want just any partition, but the one that minimizes within group variation, which we'll call $W$.

$$\underset{C_k}{\text{minimize}} \sum_{k=1}^{K} W\left(C_k\right)$$

Usually, we use $W\left(C_k\right) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \|x_i - x_i'\|^2$.



## Algorithm

This is a combinatorial optimization problem, and finding the global optimum is computationally challenging.

*However* the following algorithm usually finds good local optima,

1. Arbitrarily assign each $x_i$ to one of the clusters, $C_1, \ldots, C_K$.

2. Iterate until convergence,

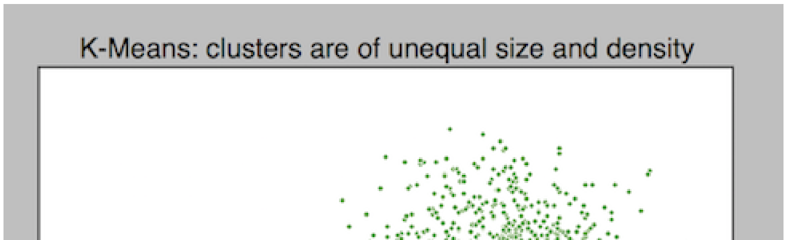
   a. Compute the mean $\bar{x}_k$ of the points in $C_k$.

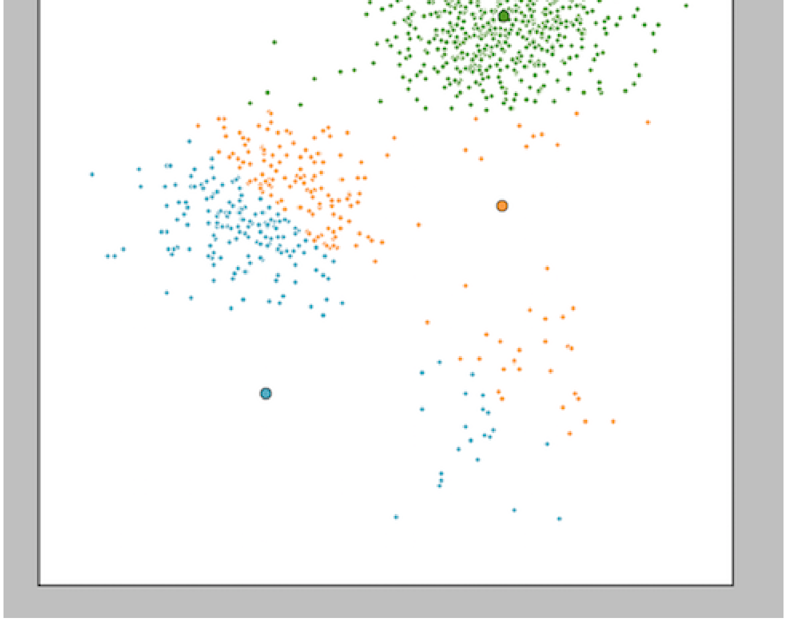
   b. Reassign the points $x_i$, so they are put in the cluster whose centroid they are closest to.

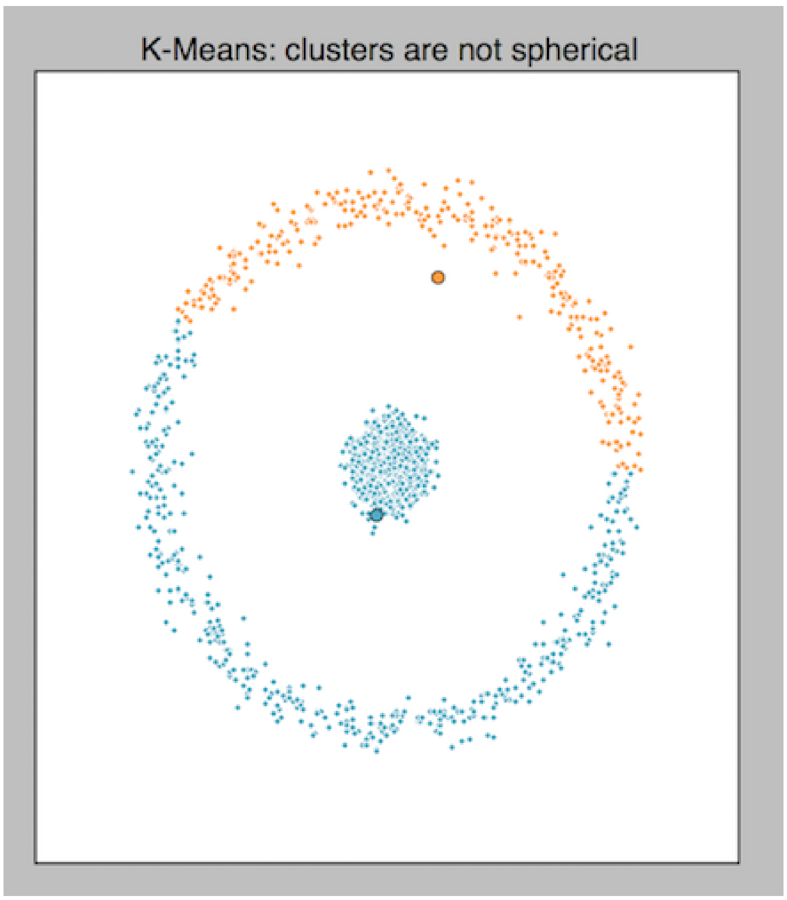
Here is a nice demo. The procedure reduces the criterion under study at each step, which means we will converge to a local optimum.

## Limitations of $K$-means

$K$-means often does not do a good job in clustering when there are variations in density, nonspherical shapes of clusetrs and outliers.





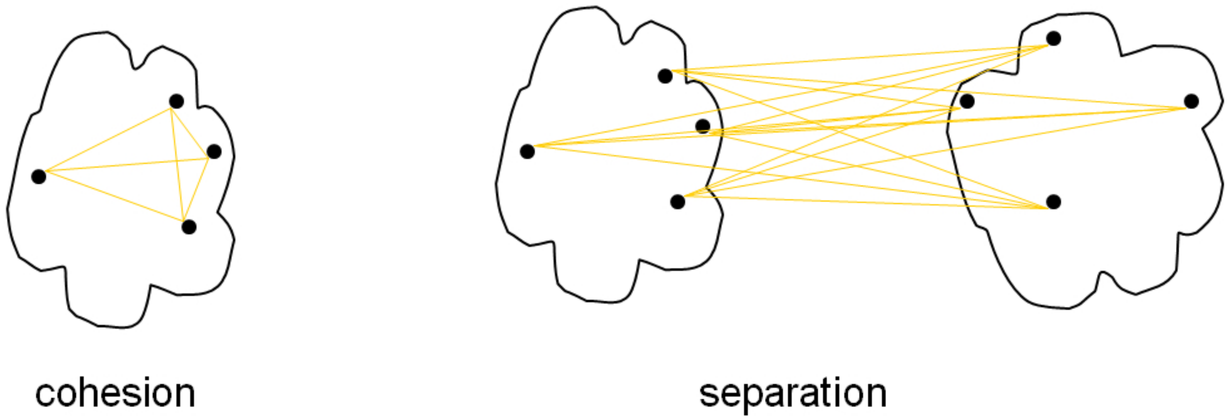



### How to evaluate $K$-means results?

- Supervised evaluation: use a pre-classified dataset as a benchmark
    - Given the knowledge of the ground truth class assignments of the samples, use some metric, e.g., *homogeneity*, *completeness*, *v-score*, to evaluate the goodness of the the clustering (higher score is better)

- Python: from **sklearn** import **metrics**; *metrics.homogeneity_score(labels_true, labels_pred)*

- Unsupervised evaluation: minimize intra-cluser distance (maximize *cohesiveness*) and maximize inter-clusetr distance (*separation*)



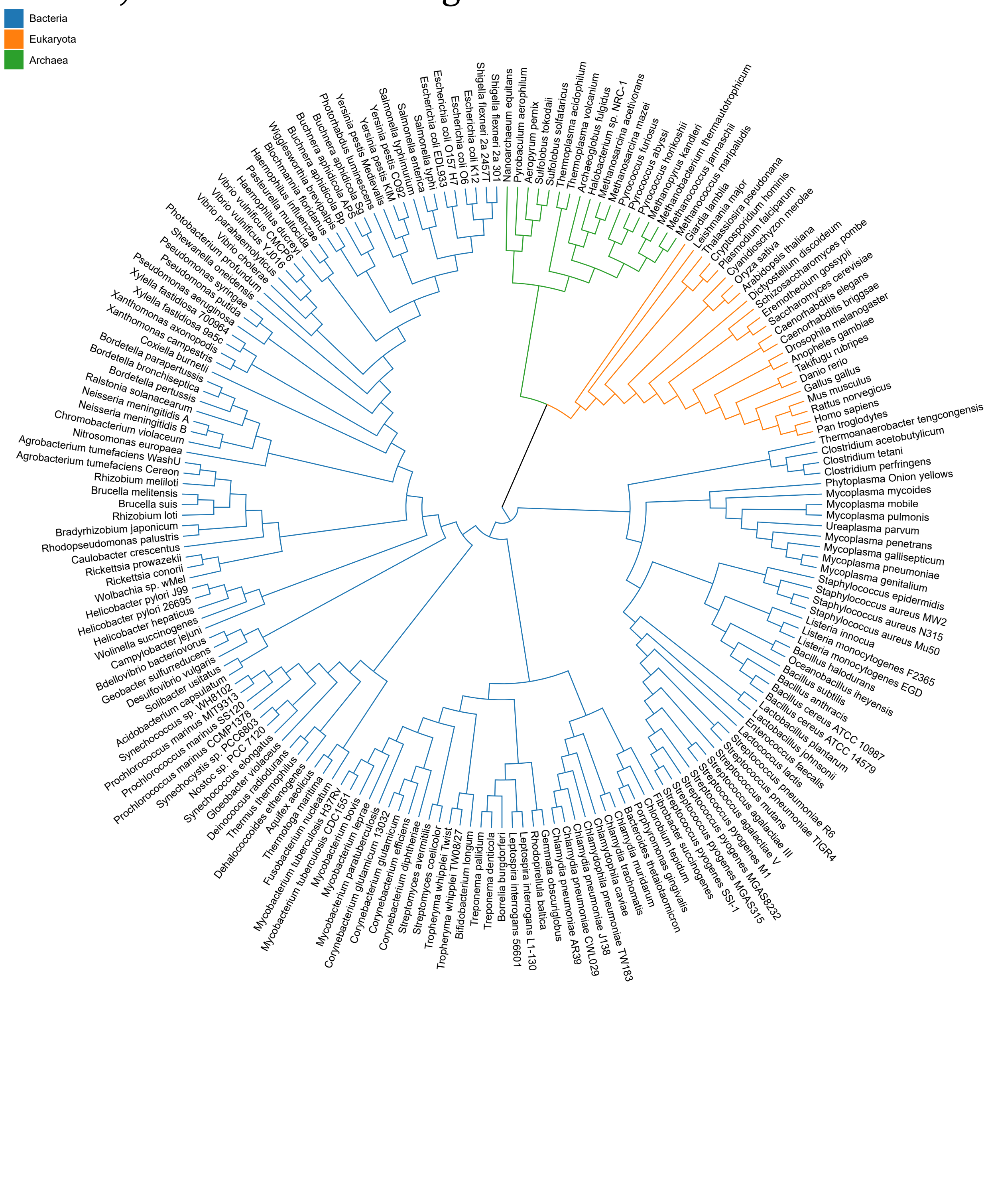

Details: Cluster Analysis Using K-means Explained

## Hierarchical Clustering

- $K$ controls the "magnification" at which we do the clustering.
- What if we could do the clustering at many different scales, all at once?

# Hierarchical Clustering

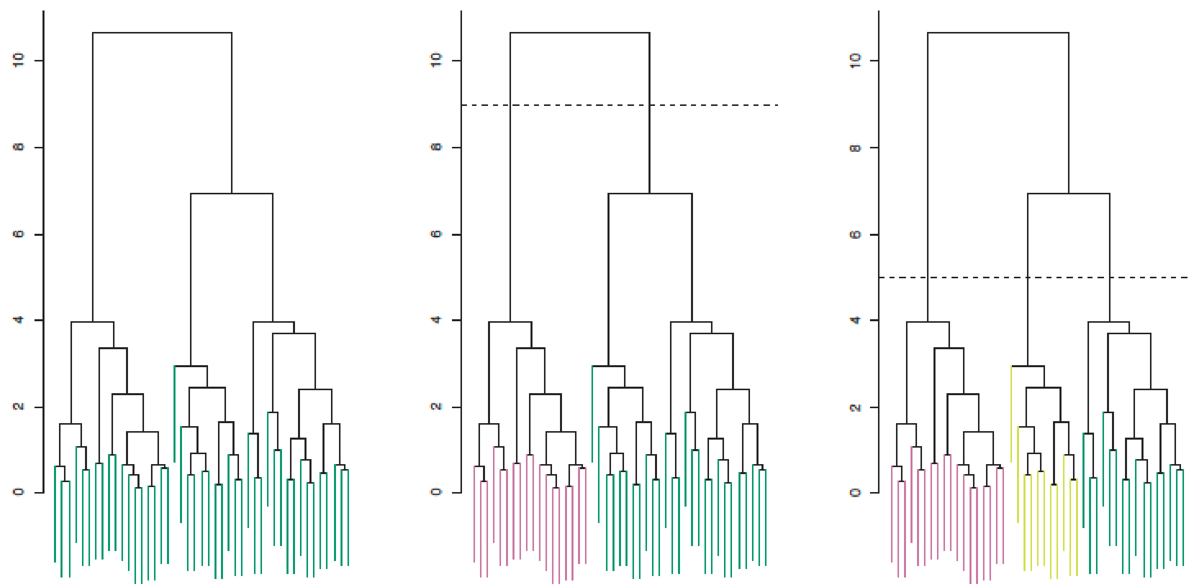
Behold, the cluster dendrogram.




# Interpretation

- Samples which are similar to each other are put on the

- Samples which are similar to each other are put on the same subtree.
- Pairs of samples that are very similar to one another share very recent common ancestors
  - Beware: Samples can be close by at the leaves without being close in the subtree sense
- You can get a standard clustering by "cutting" tree at some horizontal level

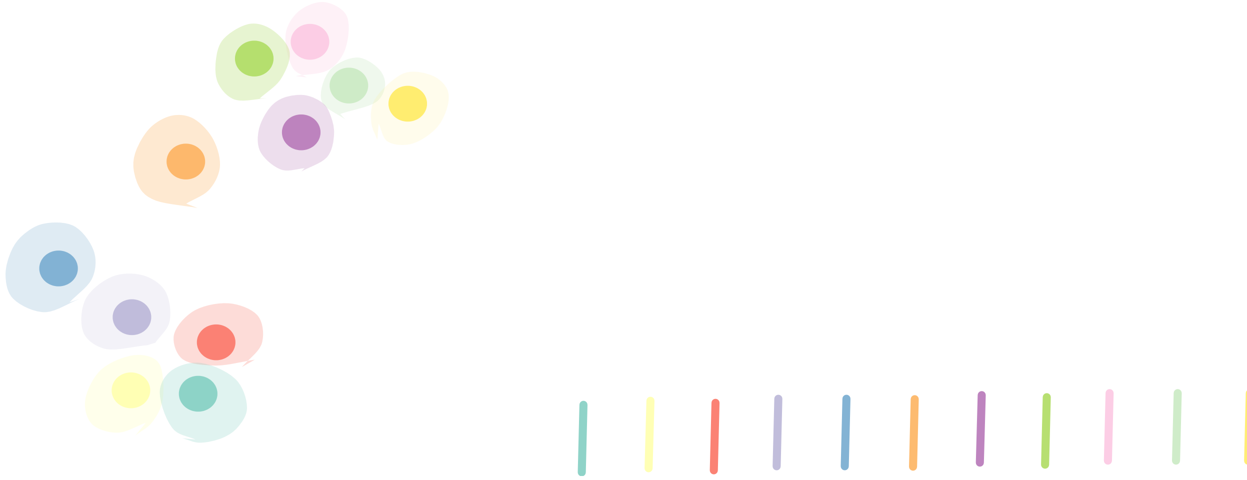


## That's cool, how do I make it?

- These trees are informative. We'd like an automated procedure for creating them.
  - Agglomerative: *bottom-up*
  - Divisive: *top-down*

### Agglomerative

a. Initialize: Associate each point with a cluster $C_i := \{x_i\}$
b. Iterate until only one cluster: Look at all pairs of clusters. Merge the pair $C_k, C_{k'}$ which are the most similar.



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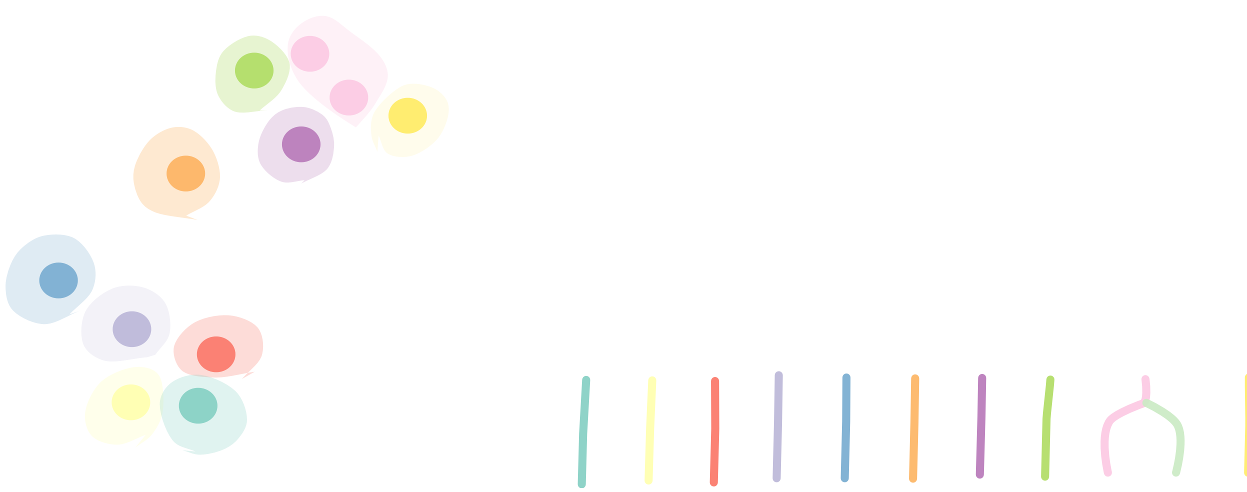

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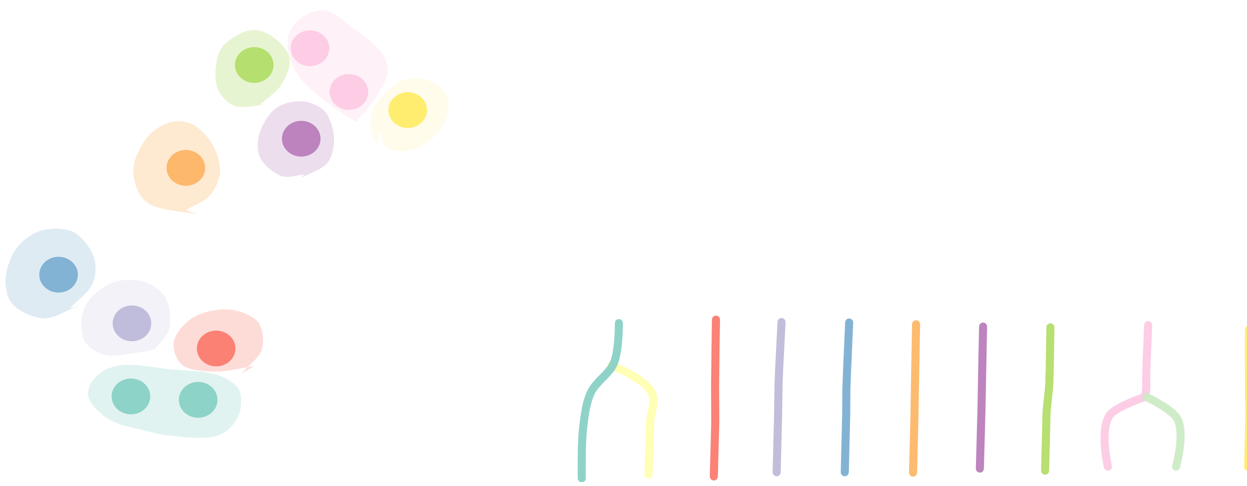

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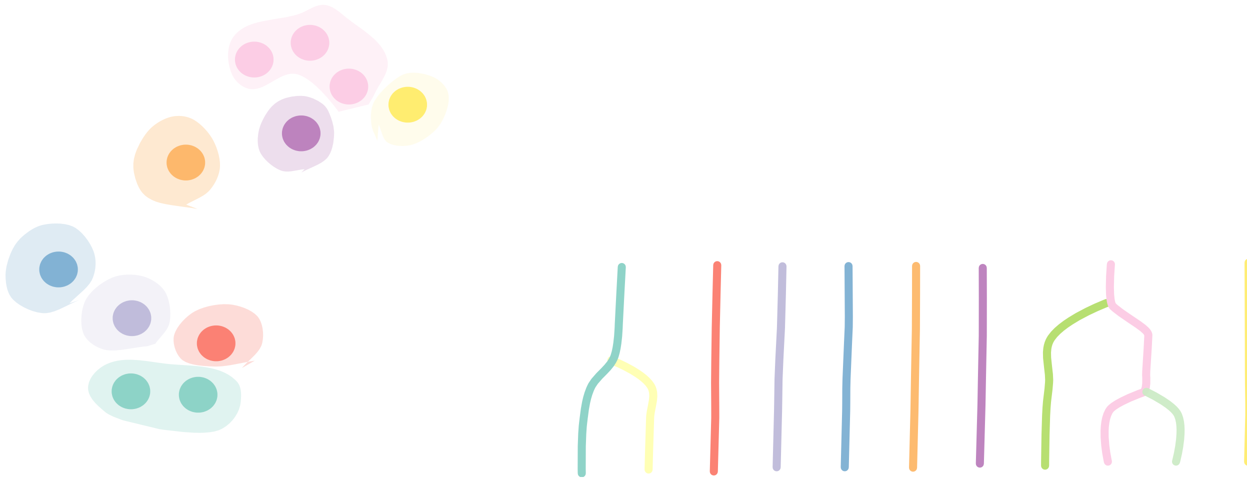

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