

STAT 215A Fall 2023

Week 5

Chengzhong Ye

Announcements

- Lab 1 and Homework 1 due **tonight at 11:59pm**
- Lab 2 and Homework 2 will be released today
 - Due in two weeks: **Oct 6 11:59pm**
- Peer reviews will be sent out this weekend
 - Due in 1 week: **Sep 29 11:59pm**

Lab 1 peer review

- Each of you will review the reports of 2 other students (pushed to your repo)
- Will send out a Google form with grading entries and rubrics
- Your grades for lab 1 will be 50% me + 25% peer reviewer 1 + 25% peer reviewer 2
- Homework will just be graded by me

Plan for today:

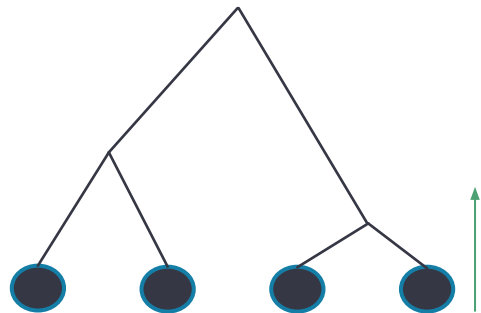
- K-means
- Hierarchical Clustering
- NMF
- Centering and Scaling?
- Introduce Lab 2

Clustering



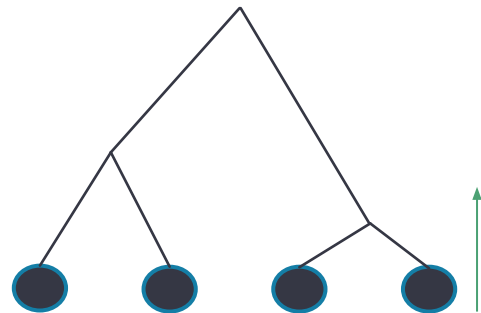
Hierarchical clustering

- Gives family of nested clusterings, presented as a tree



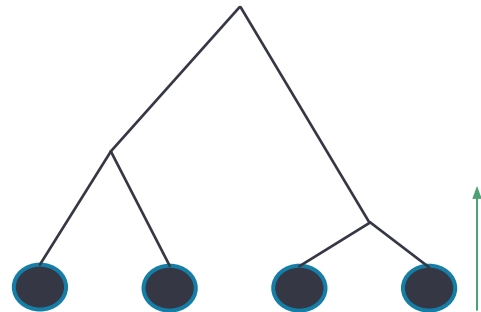
Hierarchical clustering

- Gives family of nested clusterings, presented as a tree
- A **greedy**, agglomerative algorithm, not based upon an optimization problem



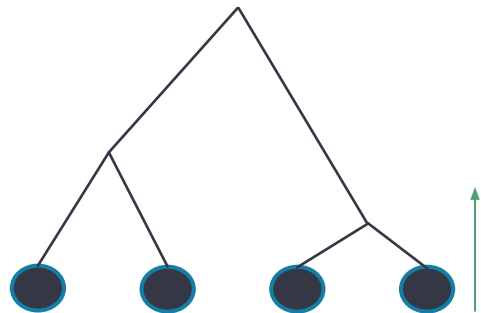
Hierarchical clustering

- Gives family of nested clusterings, presented as a tree
- A **greedy**, agglomerative algorithm, not based upon an optimization problem
- At the **lowest level**, each cluster contains a **single observation**



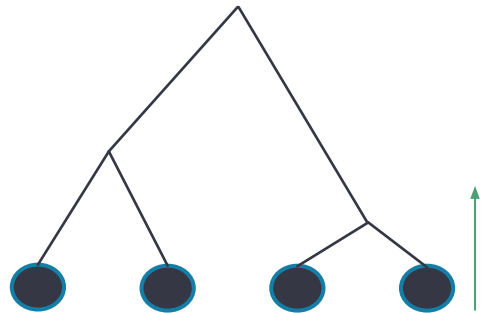
Hierarchical clustering

- Gives family of nested clusterings, presented as a tree
- A **greedy**, agglomerative algorithm, not based upon an optimization problem
- At the **lowest level**, each cluster contains a **single observation**
- As we move up the tree, some leaves begin to fuse into branches – these are observations that are similar to each other.
 - The lower in the tree the fusion occurs, the more similar the groups of observations are to each other

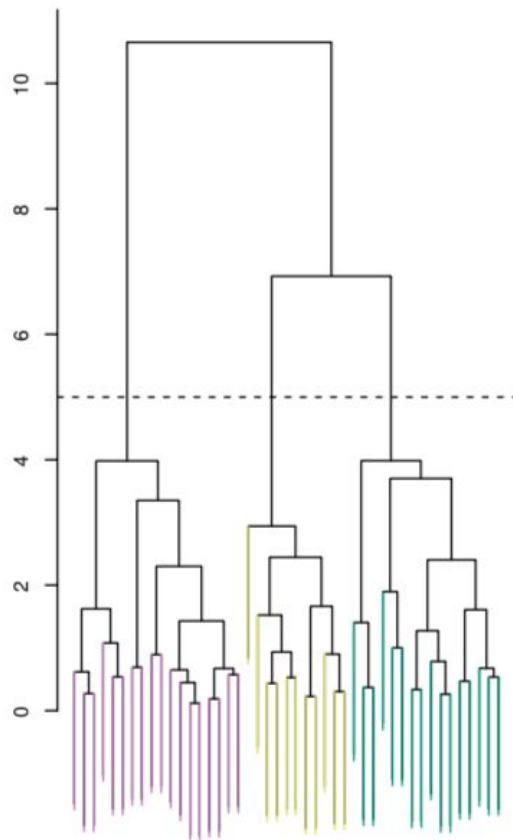
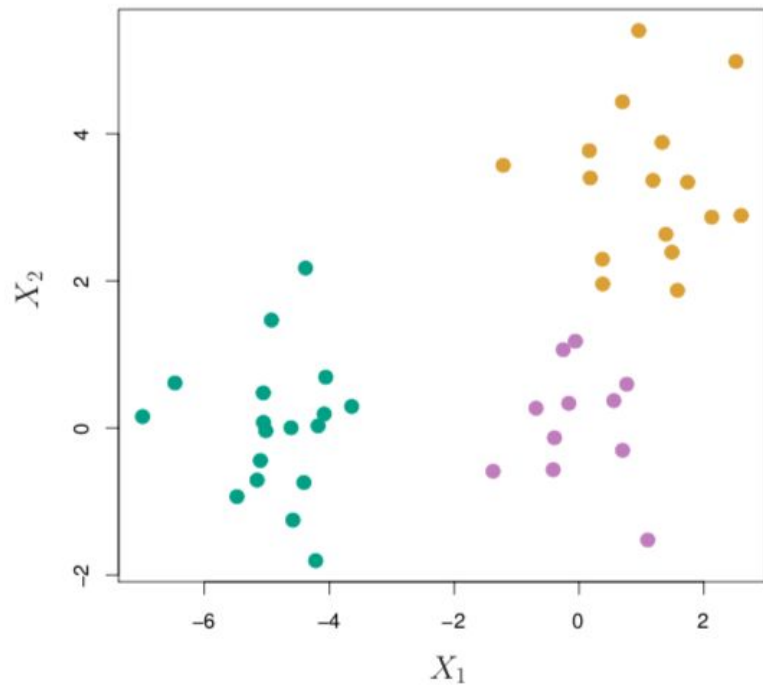


Hierarchical clustering

- Gives family of nested clusterings, presented as a tree
- A **greedy**, agglomerative algorithm, not based upon an optimization problem
- At the **lowest level**, each cluster contains a **single observation**
- As we move up the tree, some leaves begin to fuse into branches – these are observations that are similar to each other.
 - The lower in the tree the fusion occurs, the more similar the groups of observations are to each other
- At the **highest level**, there is **only one cluster** containing all observations



Interpreting dendrograms



How to join clusters/observations

1. **Distance metric:** a measure of dissimilarity between two observations

$$d(x, y)$$

- Examples: L^2 , L^1 , your favorite norm, $1 - \text{cor}(x, y)$

How to join clusters/observations

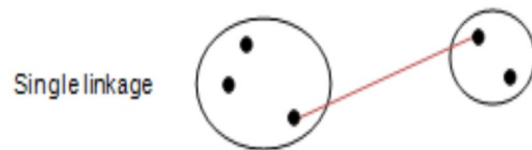
1. **Distance metric:** a measure of dissimilarity between two observations

$$d(x, y)$$

- Examples: L^2 , L^1 , your favorite norm, $1 - \text{cor}(x, y)$

2. **Linkage metric:** rule for joining two clusters

- Single linkage



How to join clusters/observations

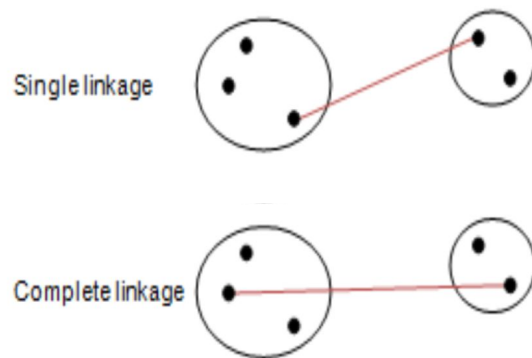
1. **Distance metric:** a measure of dissimilarity between two observations

$$d(x, y)$$

- Examples: L^2 , L^1 , your favorite norm, $1 - \text{cor}(x, y)$

2. **Linkage metric:** rule for joining two clusters

- Single linkage
- Complete linkage



How to join clusters/observations

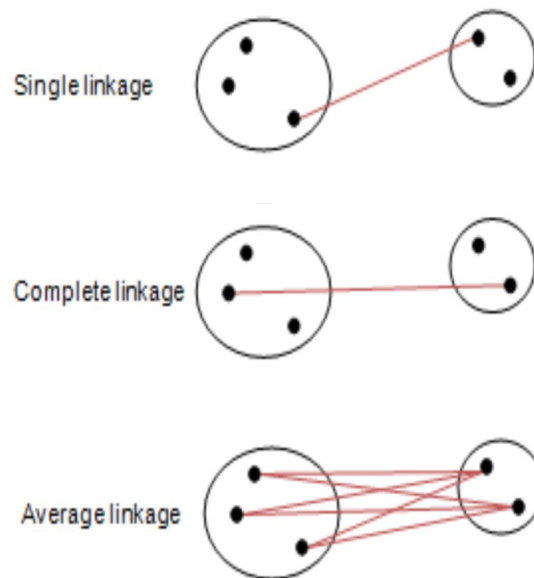
1. **Distance metric:** a measure of dissimilarity between two observations

$$d(x, y)$$

- Examples: L^2 , L^1 , your favorite norm, $1 - \text{cor}(x, y)$

2. **Linkage metric:** rule for joining two clusters

- Single linkage
- Complete linkage
- Average linkage



How to join clusters/observations

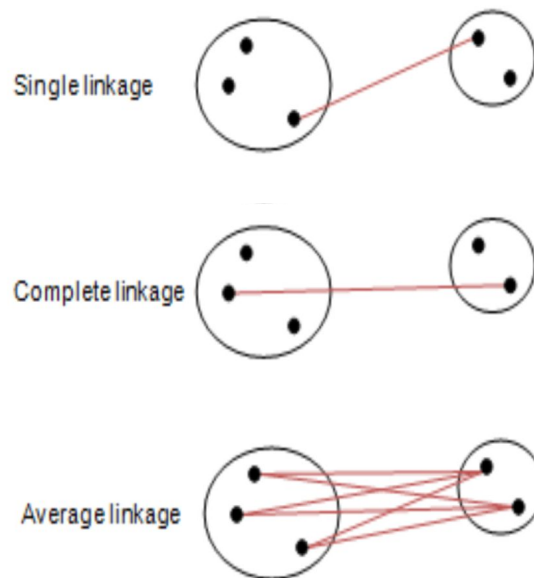
1. **Distance metric:** a measure of dissimilarity between two observations

$$d(x, y)$$

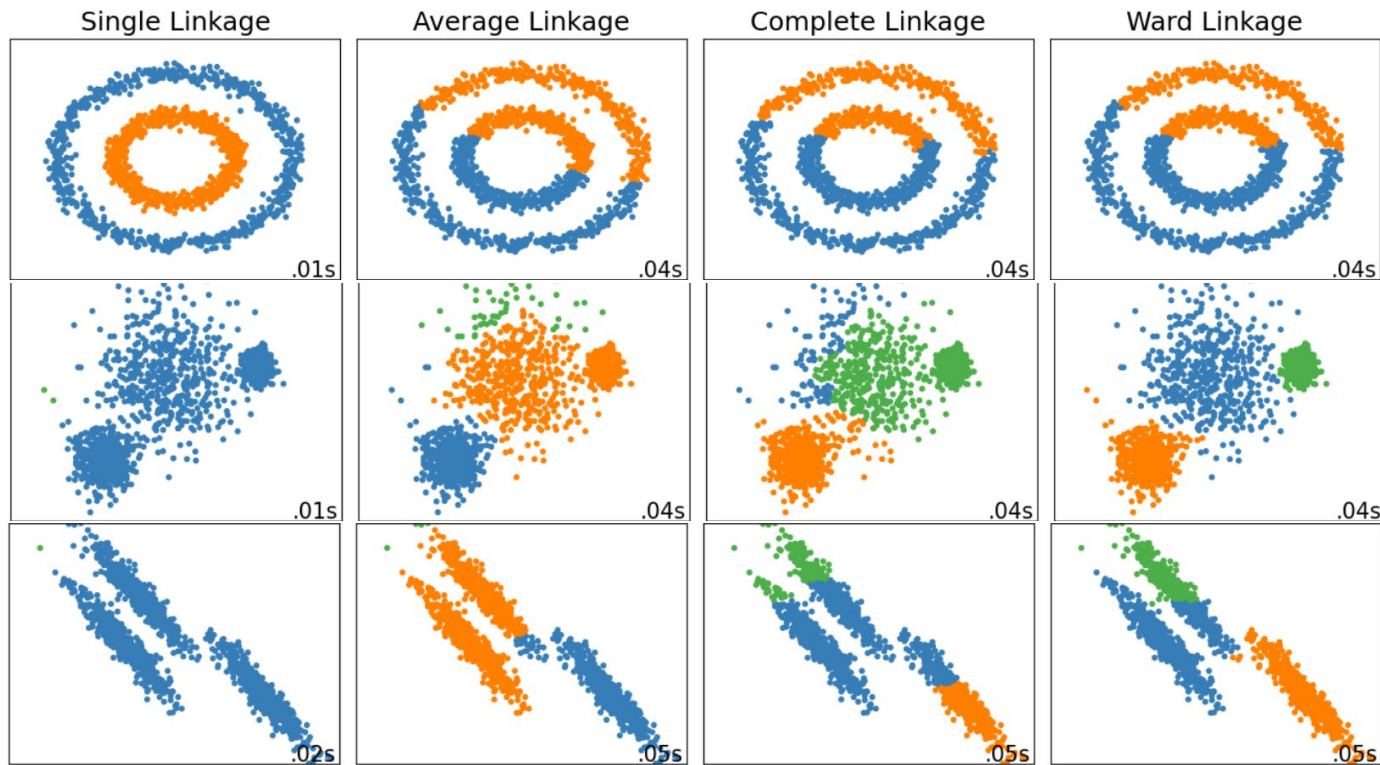
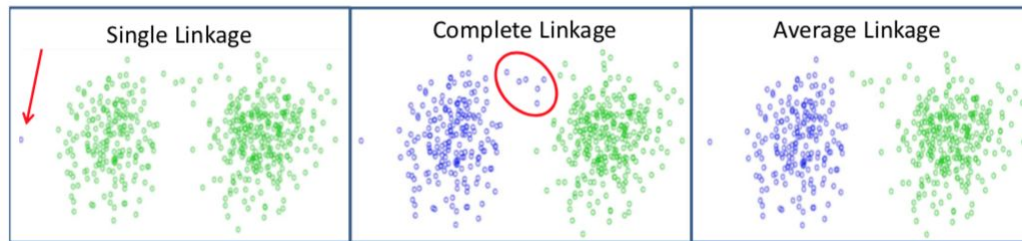
- Examples: L^2 , L^1 , your favorite norm, $1 - \text{cor}(x, y)$

2. **Linkage metric:** rule for joining two clusters

- Single linkage
- Complete linkage
- Average linkage
- Ward's linkage



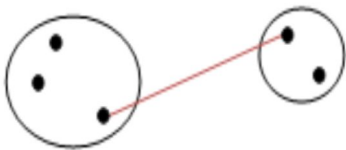
Linkage examples



Linkages

Single Linkage (min)

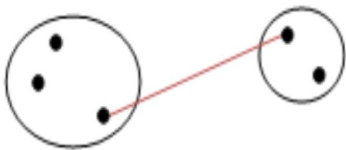
- $O(n^2)$
- Can handle diverse shapes
- Very sensitive to outliers or noise
- Often results in unbalanced clusters
- Extended, trailing clusters in which observations fused one at a time – chaining



Linkages

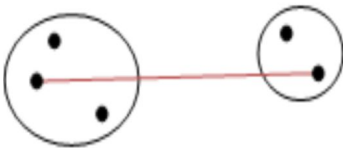
Single Linkage (min)

- $O(n^2)$
- Can handle diverse shapes
- Very sensitive to outliers or noise
- Often results in unbalanced clusters
- Extended, trailing clusters in which observations fused one at a time – chaining



Complete Linkage (max)

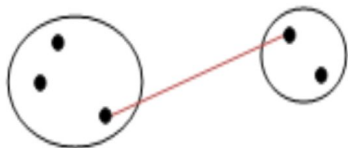
- $O(n^2)$
- Often gives cluster with similar sizes
- Less sensitive to outliers
- Works better with spherical distributions



Linkages

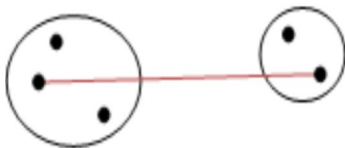
Single Linkage (min)

- $O(n^2)$
- Can handle diverse shapes
- Very sensitive to outliers or noise
- Often results in unbalanced clusters
- Extended, trailing clusters in which observations fused one at a time – chaining



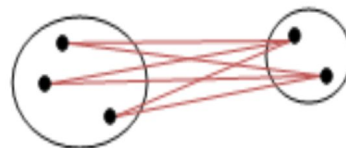
Complete Linkage (max)

- $O(n^2)$
- Often gives cluster with similar sizes
- Less sensitive to outliers
- Works better with spherical distributions



Average Linkage

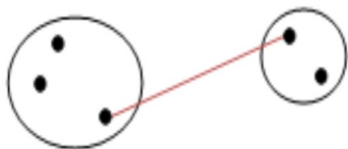
- A compromise between single and complete linkage
- Less sensitive to outliers than complete linkage, but not as robust as single linkage
- Works better with spherical distributions



Linkages

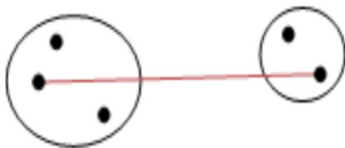
Single Linkage (min)

- Can handle diverse shapes
- Very sensitive to outliers or noise
- Often results in unbalanced clusters
- Extended, trailing clusters in which observations fused one at a time – chaining



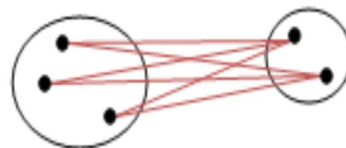
Complete Linkage (max)

- Often gives cluster with similar sizes
- Less sensitive to outliers
- Works better with spherical distributions



Average Linkage

- A compromise between single and complete linkage
- Less sensitive to outliers than complete linkage, but not as robust as single linkage
- Works better with spherical distributions



- **Ward's Linkage:** join sets that minimize the increased variance when merging two clusters
- Average and Ward's linkages are more widely used

Hierarchical clustering

Advantages

- Gives nested family of clusterings
- Convenient visualizations with dendrograms

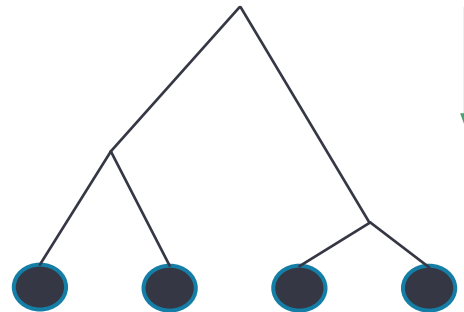
Disadvantages

- Depends heavily on hyperparameter choices (linkage)
- Local solution
- Slow: $O(n^3)$ in the worst case (depends on linkage)
- Uses a lot of memory: $O(n^2)$
- $p \gg n$ (“Curse of Dimensionality”)

Hierarchical clustering: divisive approach

Top-down approach (“divisive”)

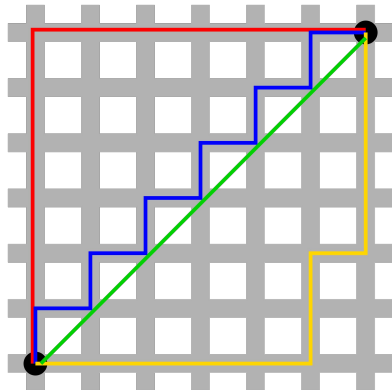
- Start with a single big cluster
- Use a subroutine (like k-means) to separate the data into successively more and more cluster
- **Advantages:**
 - Can be faster than agglomerative version (depends on subroutine)
 - Makes decisions based on global structure
- **Disadvantages:**
 - More complex, have to choose subroutine



k-Means (with L^2 distance)

Idea: find clusters C which minimize the within-cluster sum of squares

$$\operatorname{argmin}_C \sum_{k=1}^K \sum_{\mathbf{x} \in C_k} \|\mathbf{x} - \boldsymbol{\mu}_k\|_2^2, \quad \text{where} \quad \boldsymbol{\mu}_k = \frac{1}{n_k} \sum_{\mathbf{x} \in C_k} \mathbf{x}$$



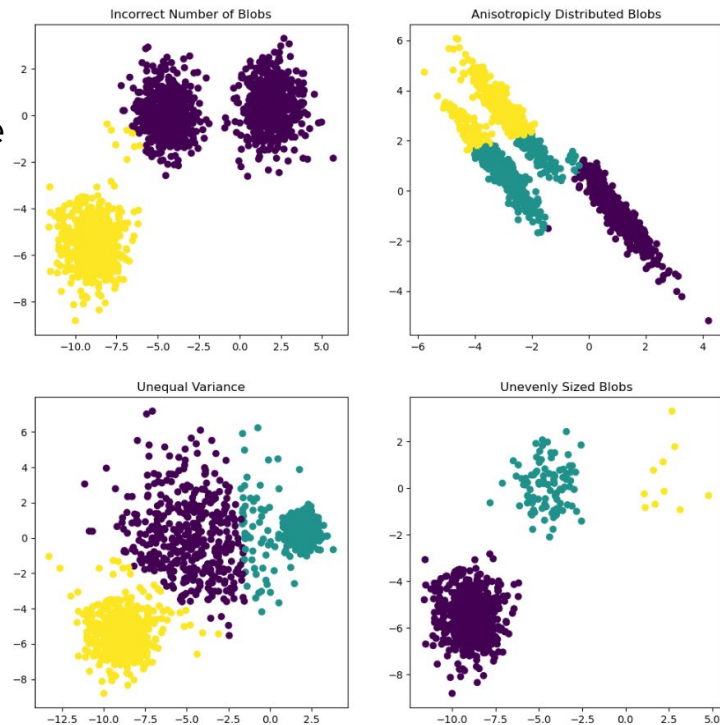
k-Means (with L^2 distance)

Advantages

- Fast
- Good when clusters are spherical balls and linearly separable

Disadvantages

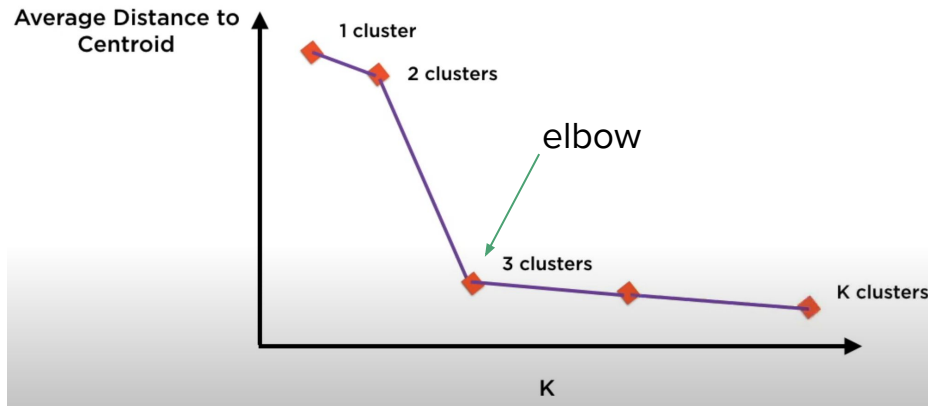
- Bad when clusters not spherical
- Bad when clusters have different variances
- $p \gg n$ (“Curse of Dimensionality”)
- You need to choose k
- Heuristic solution depends on initialization
 - Exact solution is NP-hard



Good discussion here: <https://stats.stackexchange.com/questions/133656/how-to-understand-the-drawbacks-of-k-means>

How to choose K?

- Elbow plots

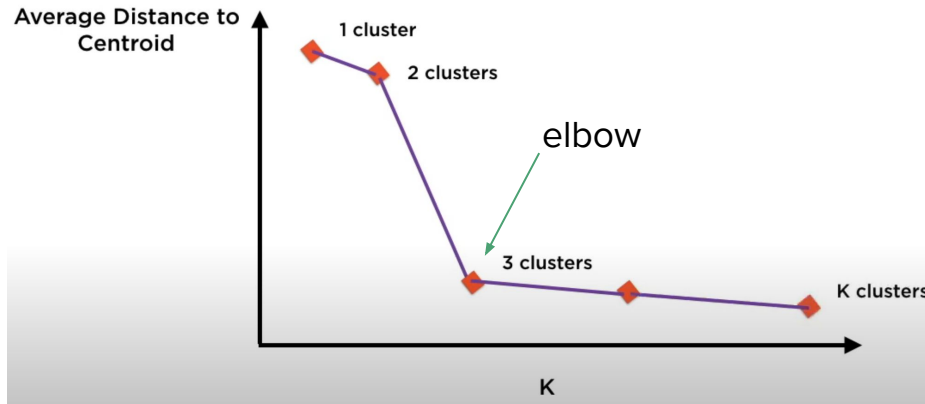


Source: <https://www.youtube.com/watch?v=AtxQ0rvdQIA>

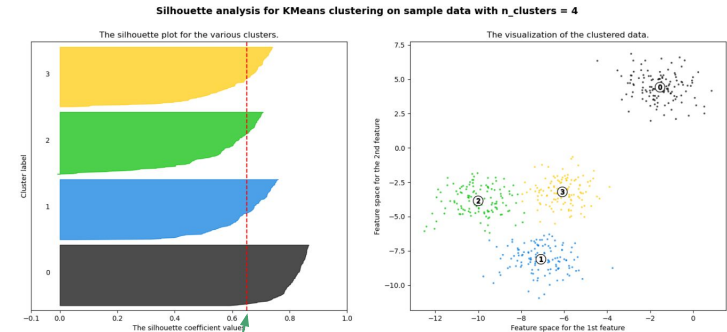
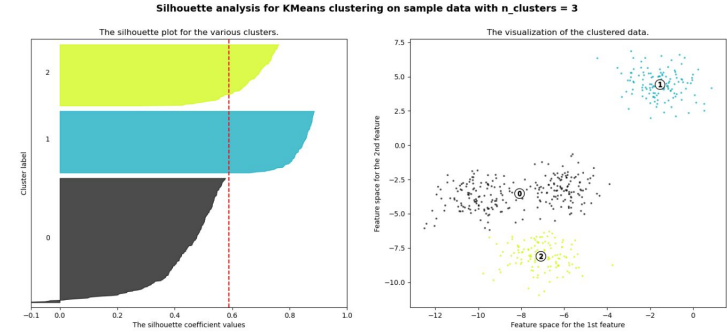
How to choose K?

- Elbow plots
- Silhouette statistic. For each point, calculate:
 - avg. dist. to points in same cluster
 - avg. dist. to points in other clusters

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$



Source: [Selecting the number of clusters with silhouette analysis on KMeans clustering](#)



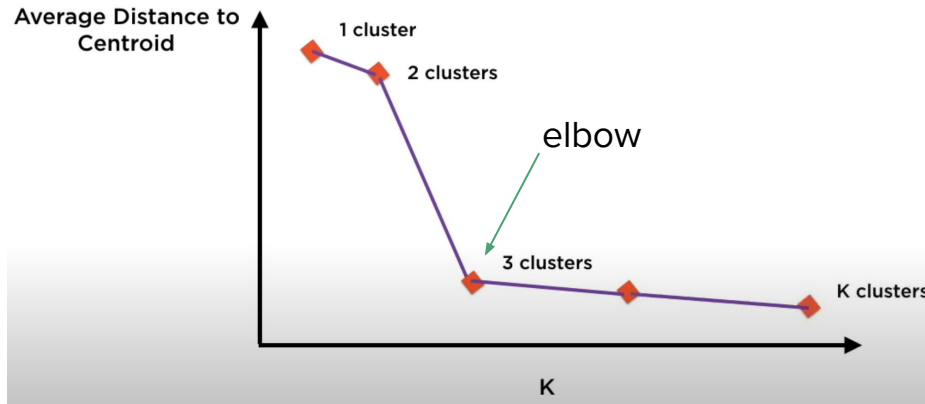
Choose K that leads to highest mean silhouette

Source: <https://www.youtube.com/watch?v=AtxQ0rvdQIA>

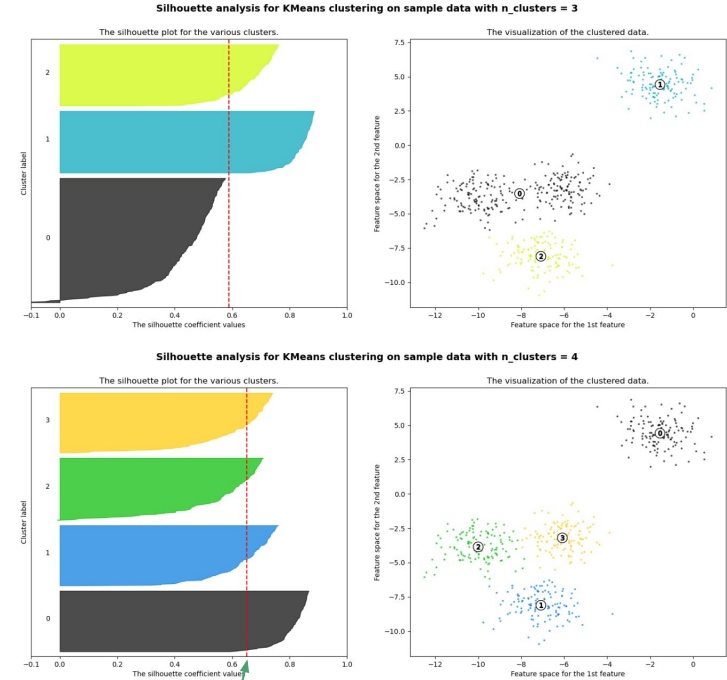
How to choose K?

- Elbow plots
- Silhouette statistic. For each point, calculate:
 - avg. dist. to points in same cluster
 - avg. dist. to points in other clusters
- Stability (will get some practice soon)

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$



Source: [Selecting the number of clusters with silhouette analysis on KMeans clustering](https://www.youtube.com/watch?v=AtxQ0rvdQIA)



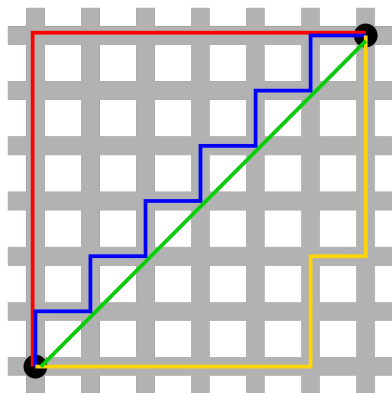
Choose K that leads to highest mean silhouette

Source: <https://www.youtube.com/watch?v=AtxQ0rvdQIA>

k-Medians (with L^1 distance)

Idea: find clusters C which minimize the within-cluster absolute value

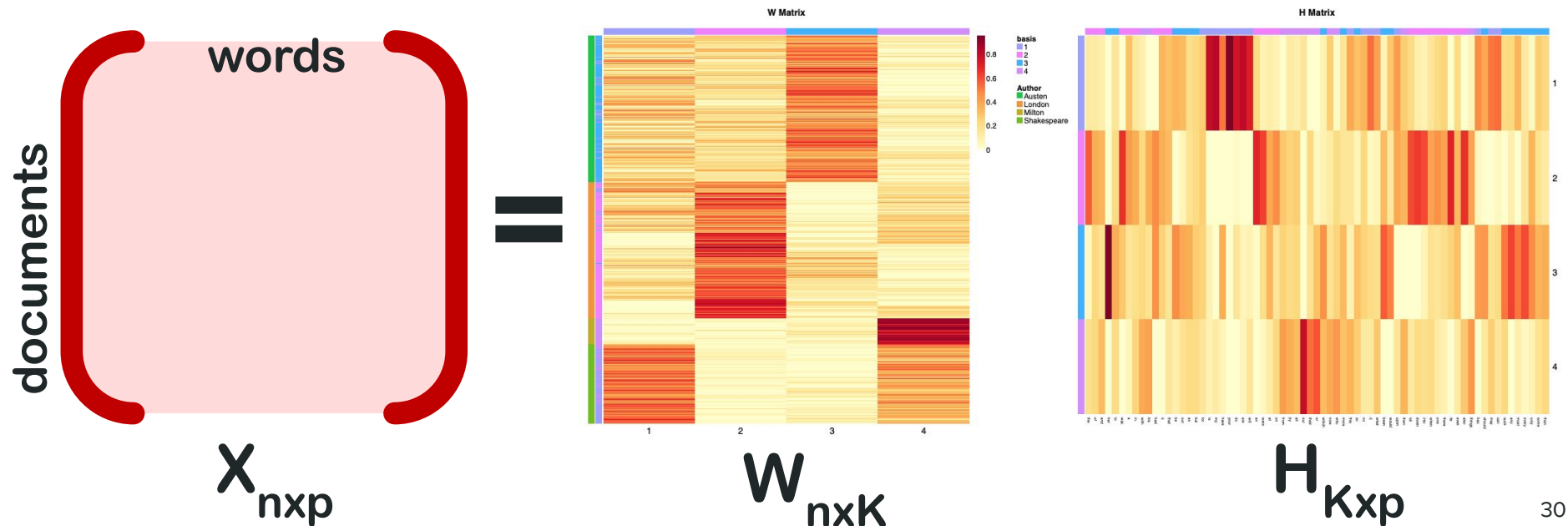
$$\operatorname{argmin}_C \sum_{k=1}^K \sum_{x \in C_k} \|x - m_k\|_1$$



vector of medians along
each dimension

Nonnegative Matrix Factorizations (NMF)

- Given a non-negative matrix \mathbf{X} , NMF solves $\min_{\mathbf{W} \geq 0, \mathbf{H} \geq 0} \|\mathbf{X} - \mathbf{W} \mathbf{H}\|_F^2$
- Tool for dimension reduction, pattern recognition, and soft clustering with positive data



Nonnegative Matrix Factorizations (NMF)

Advantages

- “Soft” clustering
- Inherently gives sparse feature matrix \mathbf{H} (unlike PCA)
- Great for pattern recognition with positive data

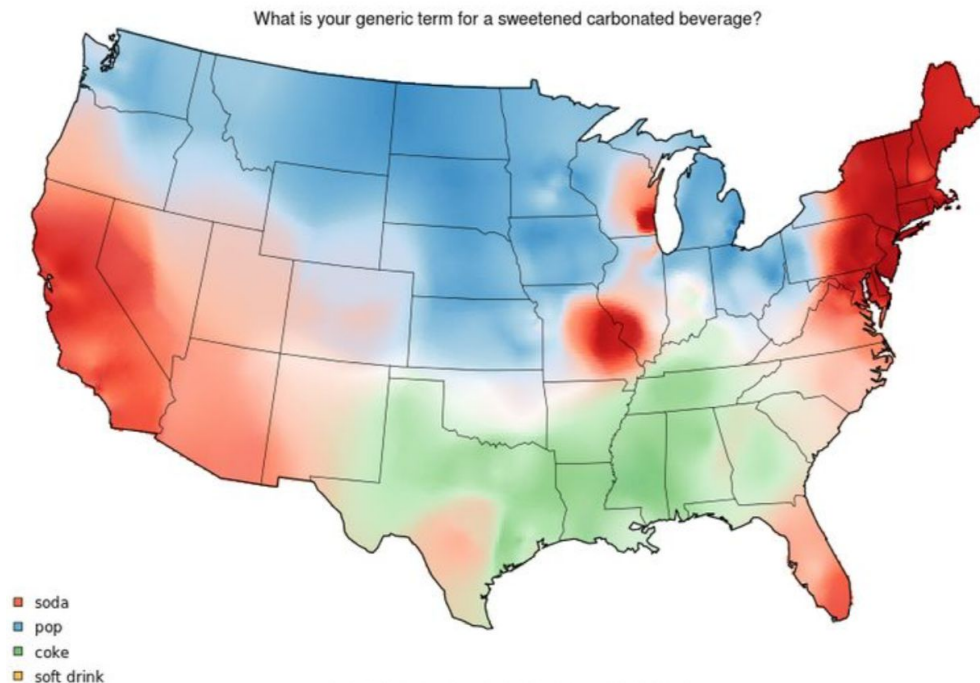
Disadvantages

- Not a convex problem □ depends on initialization of algorithm
- Components are unordered and not nested
 - Change number of components K can give vastly different results
- Can't find *strength* of patterns as in PCA

To center/scale or not to center/scale...

- By **centering**, I mean subtracting the sample mean from each column in your data matrix so that the mean of each column/feature is 0
- By **scaling**, I mean dividing each column by some constant so that the 2-norm of each column/feature is 1
- Very subjective...
- If it is meaningful to compare the variance of different features in your data matrix, don't *need* to scale
 - Gene expression data
- If features are measured on different scales, definitely need to scale (and maybe center?)
 - Income and number of kids
- Centering may result in a loss in interpretability (e.g., with positive data)
- What most people do in practice: try both

Lab 2 – Linguistics Survey (Due October 6 11:59pm)



Joshua Katz, Department of Statistics, NC State University

<https://www.businessinsider.com/22-maps-that-show-the-deepest-linguistic-conflicts-in-america-2013-6#ok-this-one-is-crazy-everyone-pronounces-pecan-pie-differently-10>

Lab 2 – Linguistics Survey

- Your primary goal is to:
 - Perform EDA/dimension reduction and clustering
 - Evaluate stability of clustering
- Other things to keep in mind
 - Readability of narrative and code
 - Clear and effective visualizations
 - Clarity of folder structure
 - Only push files required to reproduce the report (minus data)
- Don't forget about HW



Exercise in
/week5 folder

Also a K-means
animation



**KEEP
CALM
AND
START
EARLY**