CSE/STAT 416

Other Clustering Methods

Pre-Class Videos

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July 31, 2024

Pre-Class Video 1

Clustering Recap

Clustering

SPORTS

WORLD NEWS

Define Clusters

In their simplest form, a **cluster** is defined by

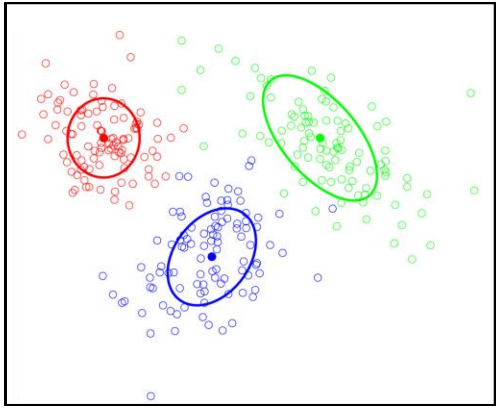
- The location of its center (**centroid**)
- Shape and size of its **spread**

Clustering is the process of finding these clusters and **assigning** each example to a particular cluster.

- x_i gets assigned $z_i \in [1, 2, \dots, k]$
- Usually based on closest centroid

Will define some kind of score for a clustering that determines how good the assignments are

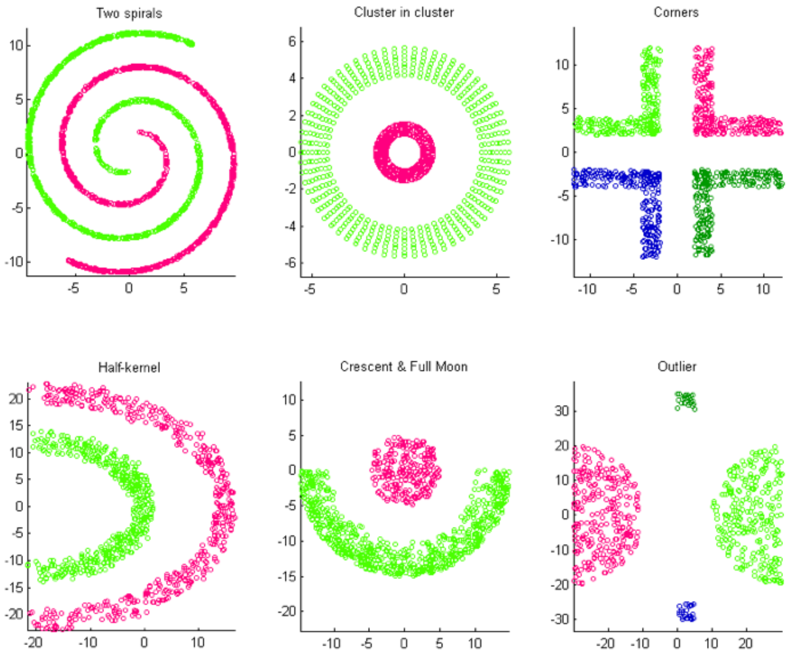
- Based on distance of assigned examples to each cluster



Not Always Easy

There are many clusters that are harder to learn with this setup

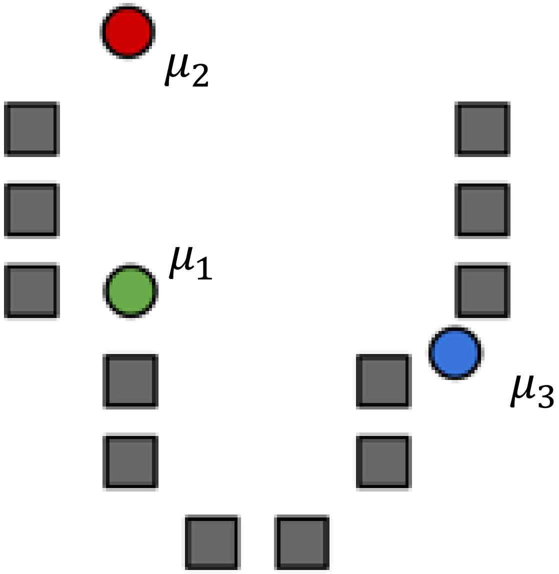
- Distance does not determine clusters



Step 0

Start by choosing the initial cluster centroids

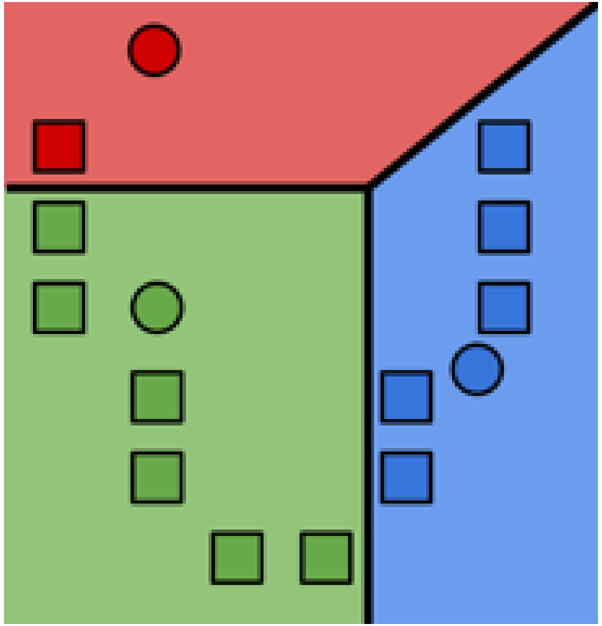
- A common default choice is to choose centroids at random
- Will see later that there are smarter ways of initializing



Step 1

Assign each example to its closest cluster centroid

$$z_i \leftarrow \underset{j \in [k]}{\operatorname{argmin}} \left|\left|\mu_j - x_i\right|\right|^2$$

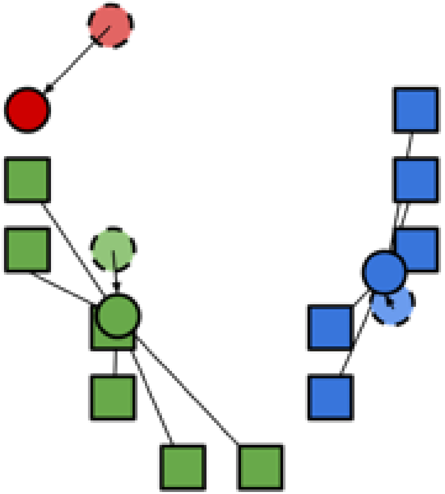


Step 2

Update the centroids to be the mean of all the points assigned to that cluster.

$$\mu_j \leftarrow \frac{1}{n_j} \sum_{i:z_i=j} x_i$$

Computes center of mass for cluster!



Smart Initializing w/ k-means++

Making sure the initialized centroids are "good" is critical to finding quality local optima. Our purely random approach was wasteful since it's very possible that initial centroids start close together.

Idea: Try to select a set of points farther away from each other.

k-means++ does a slightly smarter random initialization

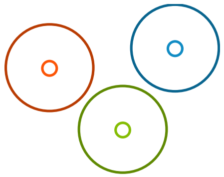
1. Choose first cluster μ_1 from the data uniformly at random
2. For the current set of centroids (starting with just μ_1), compute the distance between each datapoint and its closest centroid
3. Choose a new centroid from the remaining data points with probability of x_i being chosen proportional to $d(x_i)^2$
4. Repeat 2 and 3 until we have selected k centroids

Problems with k-means

In real life, cluster assignments are not always clear cut

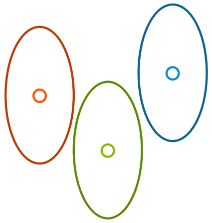
- E.g. The moon landing: Science? World News? Conspiracy?

Because we minimize Euclidean distance, k-means assumes all the clusters are spherical



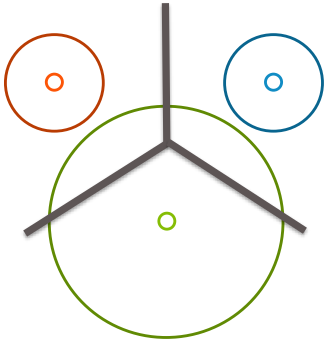
We can change this with weighted Euclidean distance

- Still assumes every cluster is the same shape/orientation

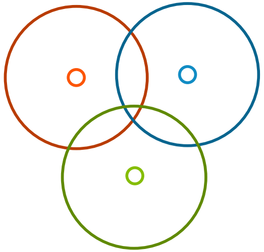


Failure Modes of k-means

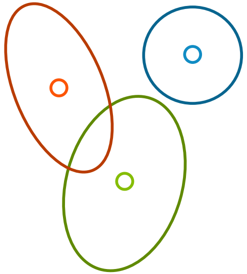
If we don’t meet the assumption of spherical clusters, we will get unexpected results



disparate cluster sizes



overlapping clusters



different shaped/oriented clusters

Mixture Models

A much more flexible approach is modeling with a **mixture model**

Model each cluster as a different probability distribution and learn their parameters

- E.g. Mixture of Gaussians
- Allows for different cluster shapes and sizes
- Typically learned using Expectation Maximization (EM) algorithm

Allows **soft assignments** to clusters

- 54% chance document is about world news, 45% science, 1% conspiracy theory, 0% other

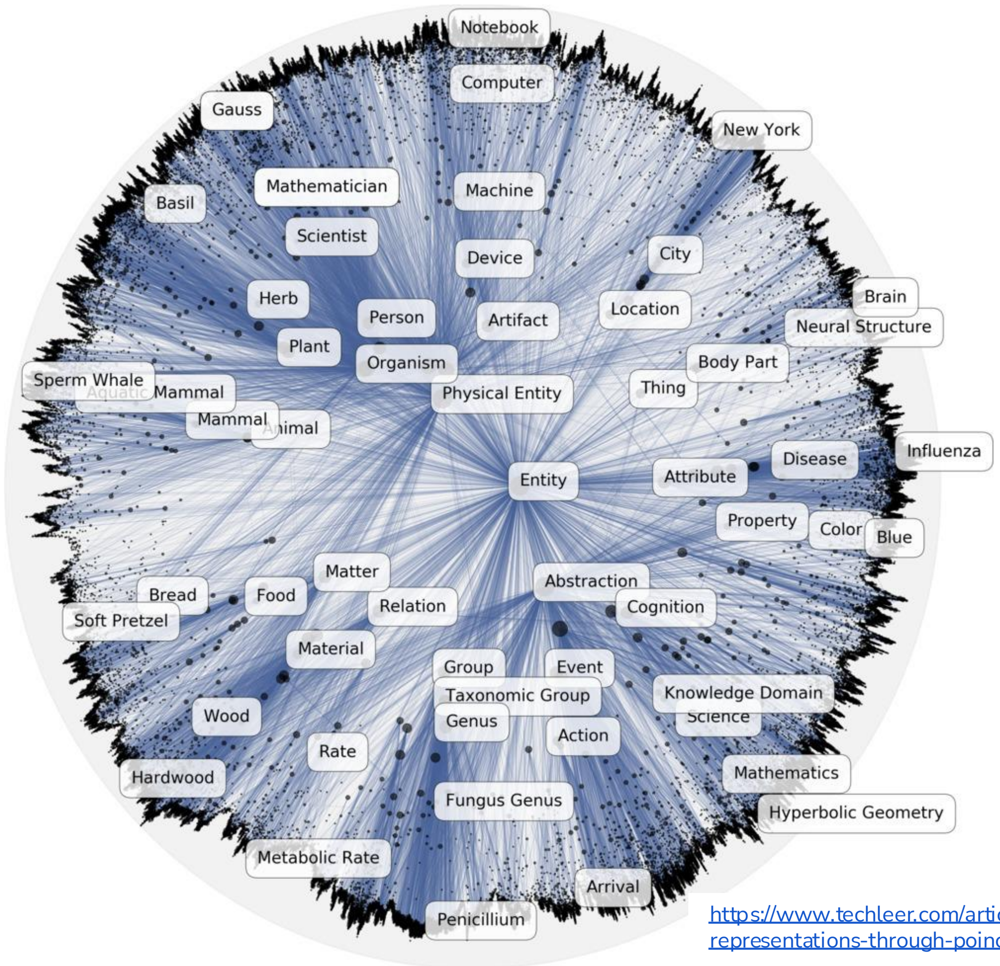
Pre-Class Video 2

Divisive Clustering

Hierarchical Clustering

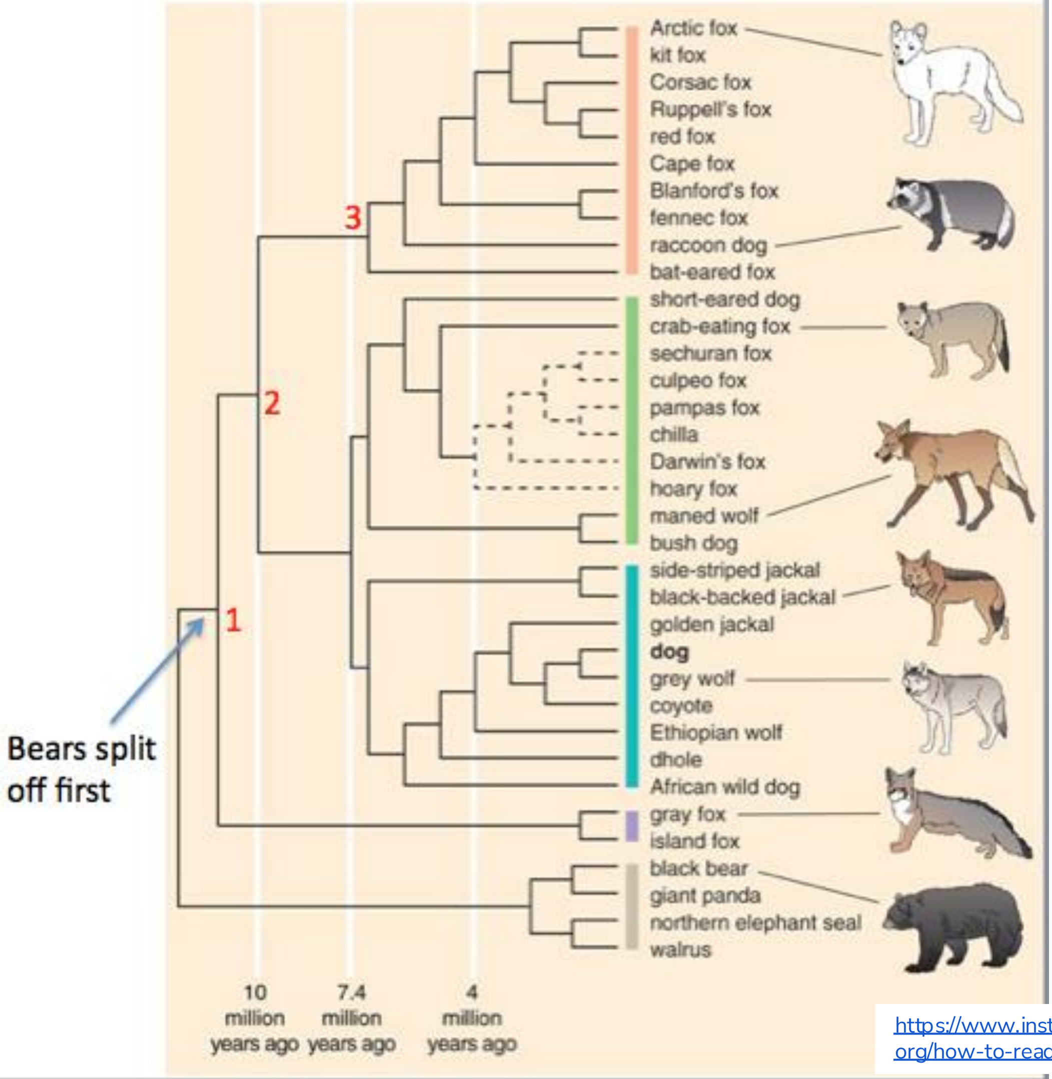
Nouns

Lots of data is hierarchical by nature



https://www.techleer.com/articles/478-insight-into-hierarchical-representations-through-poincare-embedding/

Species

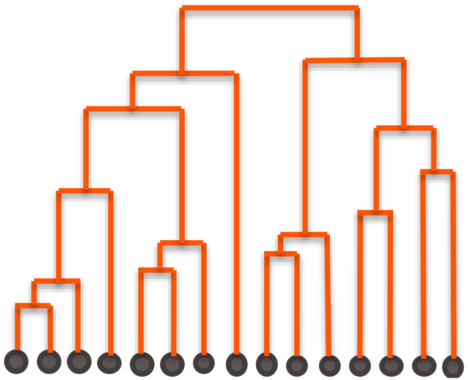


https://www.instituteofcaninebiology.org/how-to-read-a-dendrogram.html

Motivation

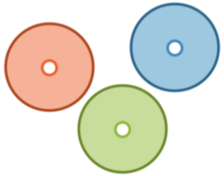
If we try to learn clusters in hierarchies, we can

- Avoid choosing the # of clusters beforehand
- Use **dendrograms** to help visualize different granularities of clusters
- Allow us to use any distance metric
  - K-means requires Euclidean distance
- Can often find more complex shapes than k-means

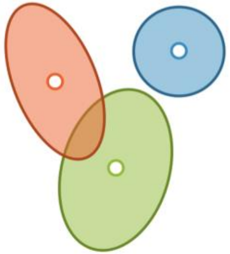


Finding Shapes

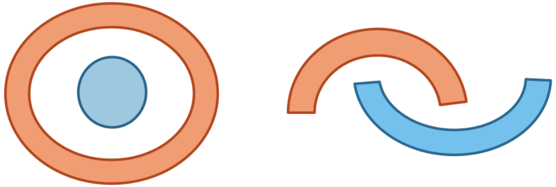
k-means



Mixture Models



Hierarchical Clustering



Types of Algorithms

Divisive, a.k.a. *top-down*

- Start with all the data in one big cluster and then recursively split the data into smaller clusters
  - Example: **recursive k-means**

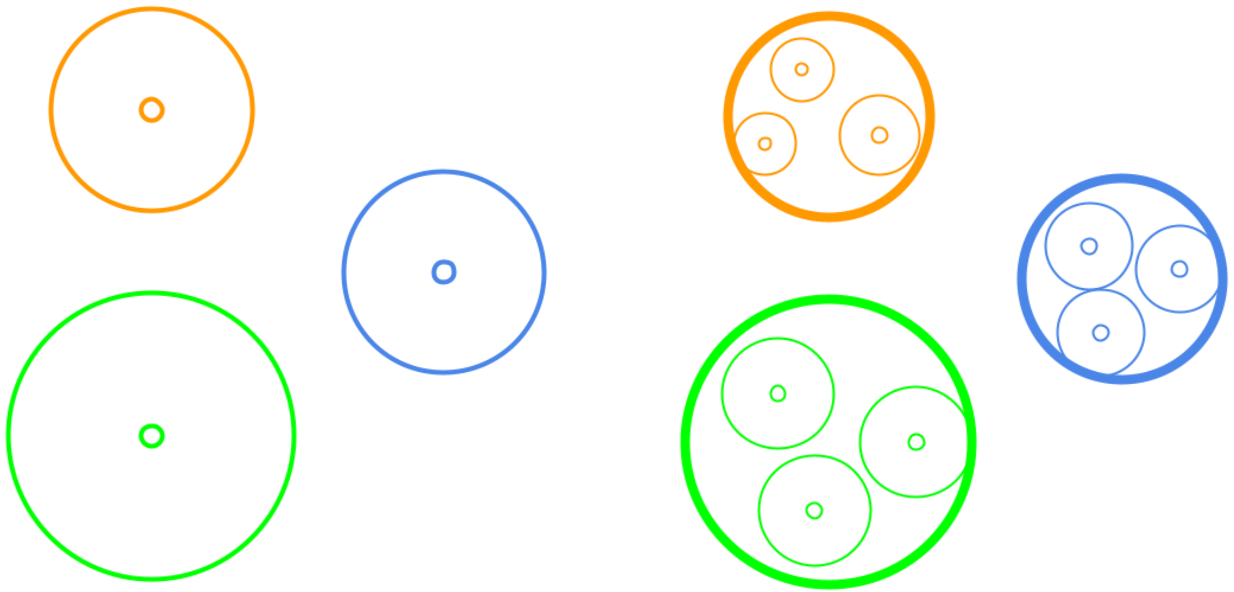
Agglomerative, a.k.a. *bottom-up*:

- Start with each data point in its own cluster. Merge clusters until all points are in one big cluster.
  - Example: **single linkage clustering**

how we measure distance between clusters

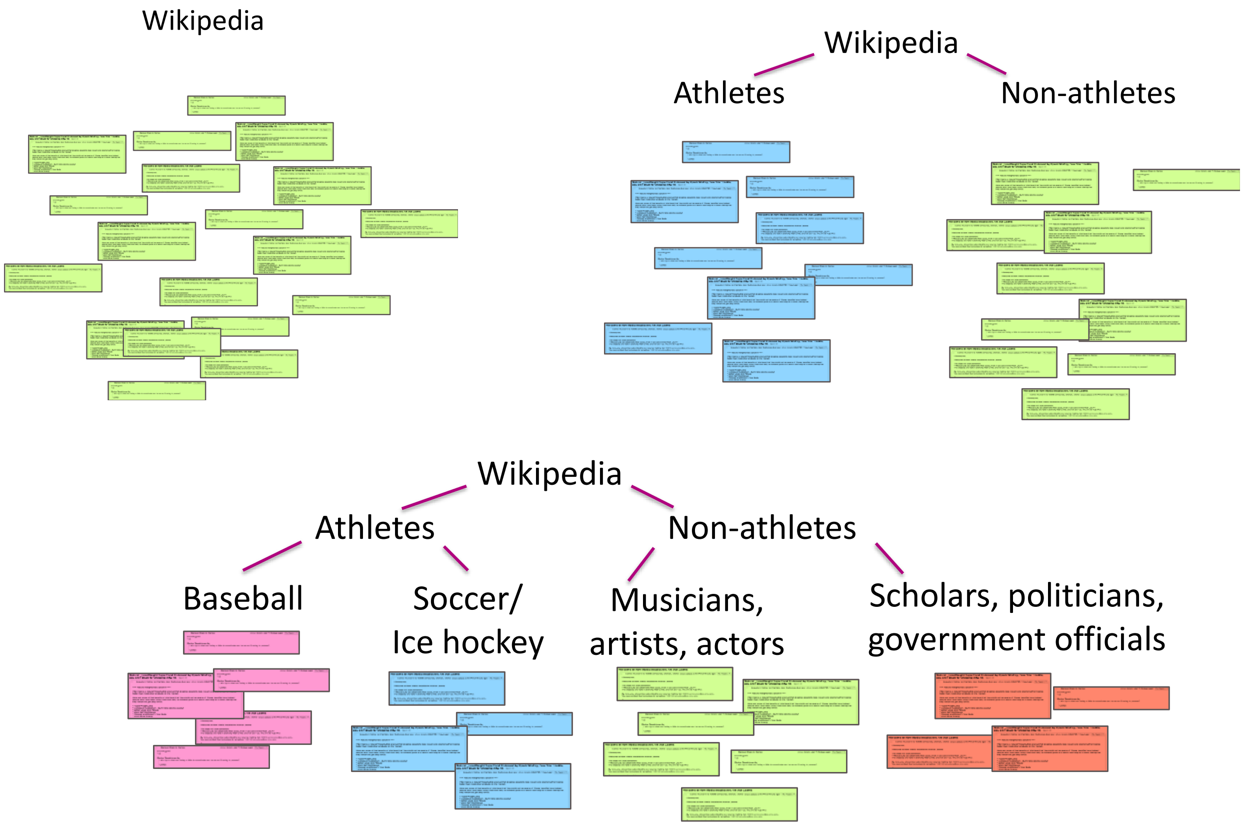
Divisive Clustering

Start with all the data in one cluster, and then repeatedly run k-means to divide the data into smaller clusters. Repeatedly run k-means on each cluster to make sub-clusters.



Example

Using Wikipedia



Choices to Make

For divisive clustering, you need to make the following choices:

- Which algorithm to use (e.g., k-means)
- How many clusters per split
- When to split vs when to stop
  - **Max cluster size**
    Number of points in cluster falls below threshold
  - **Max cluster radius**
    distance to furthest point falls below threshold
  - **Specified # of clusters**
    split until pre-specified # of clusters is reached

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Other Clustering Methods

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❓ **Questions?** Raise hand or **sli.do #cs416**
🎵 **Listening to:** Still Woozy

Define Clusters

In their simplest form, a **cluster** is defined by

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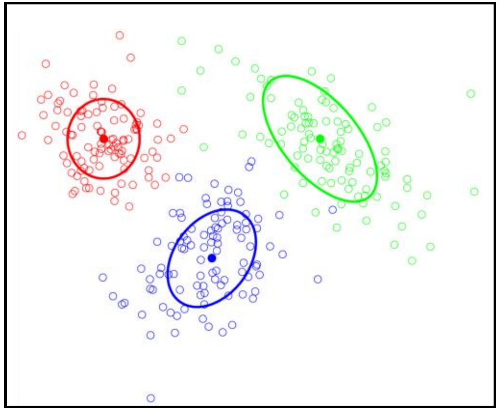
- Shape and size of its **spread**

Clustering is the process of finding these clusters and **assigning** each example to a particular cluster.

- x_i gets assigned $z_i \in [1, 2, \ldots, k]$
- Usually based on closest centroid



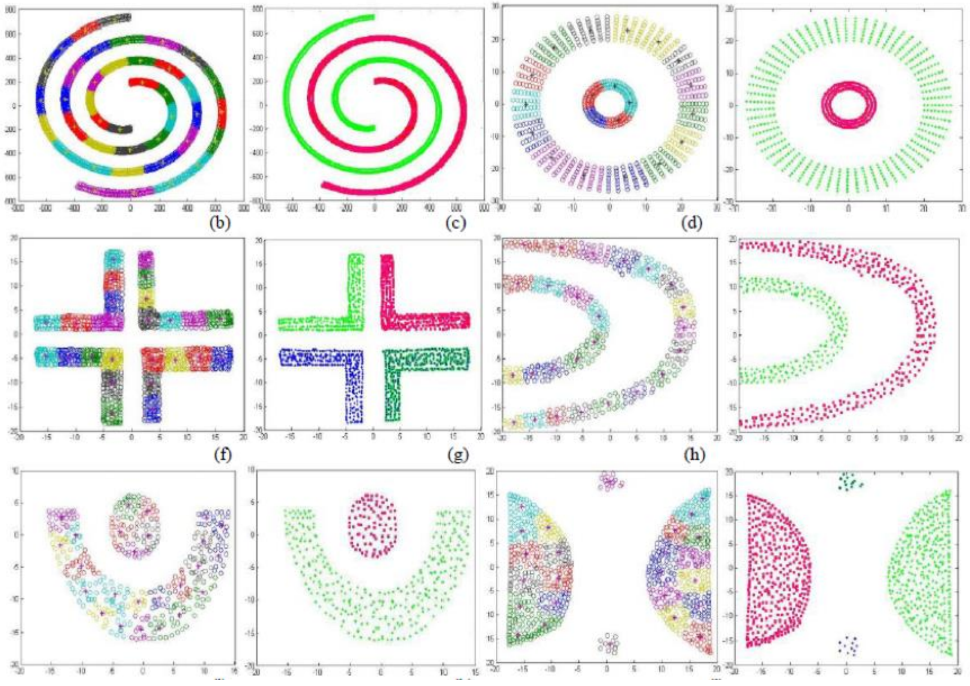
Will define some kind of objective function for a clustering that determines how good the assignments are

- Based on distance of assigned examples to each cluster.
- Close distance reflects strong similarity between datapoints.

Not Always Easy

There are many clusters that are harder to learn with this setup

- Distance does not determine clusters



Visualizing k-means

https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

Poll Everywhere

Think

1.5 min

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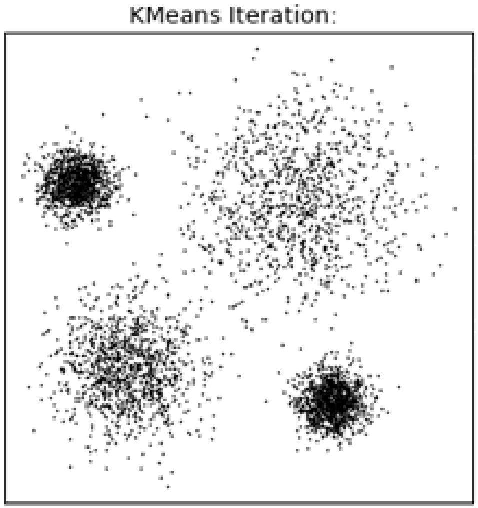
What convergence guarantees do you think we will have with k-means, given a sufficiently large number of iterations?

- Converges to the global optimum
- Converges to a local optima
- None



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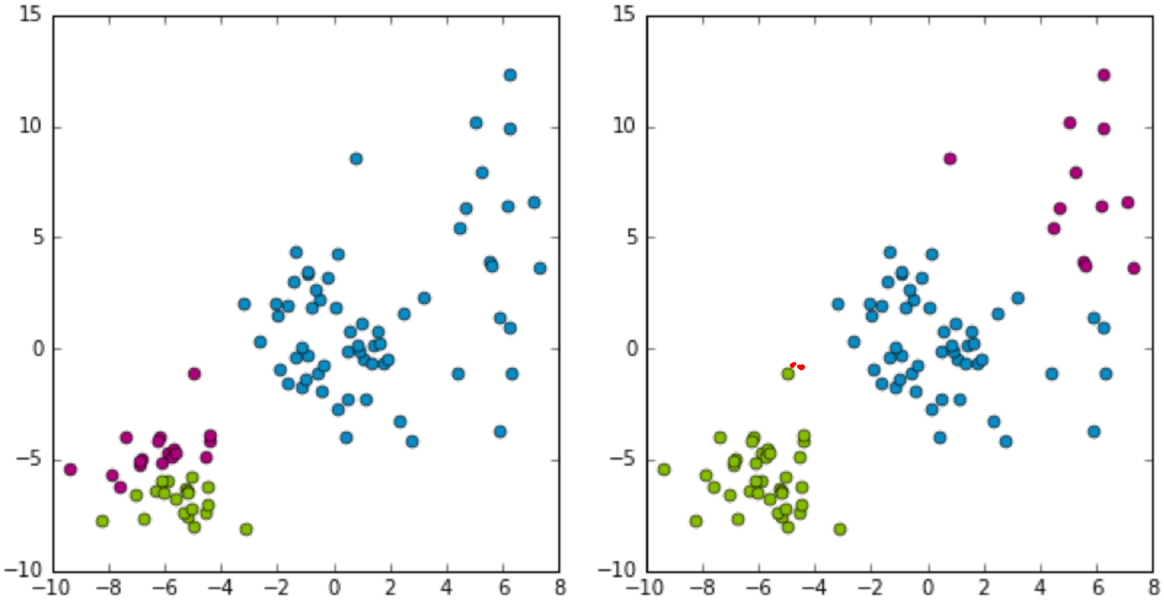
3. Choose a new centroid from the remaining data points, where the probability of x_i being chosen is proportional to $d(x_i)^2$.
4. Repeat 2 and 3 until we have selected k centroids.

Assessing Performance

Which Cluster?

Which clustering would I prefer?

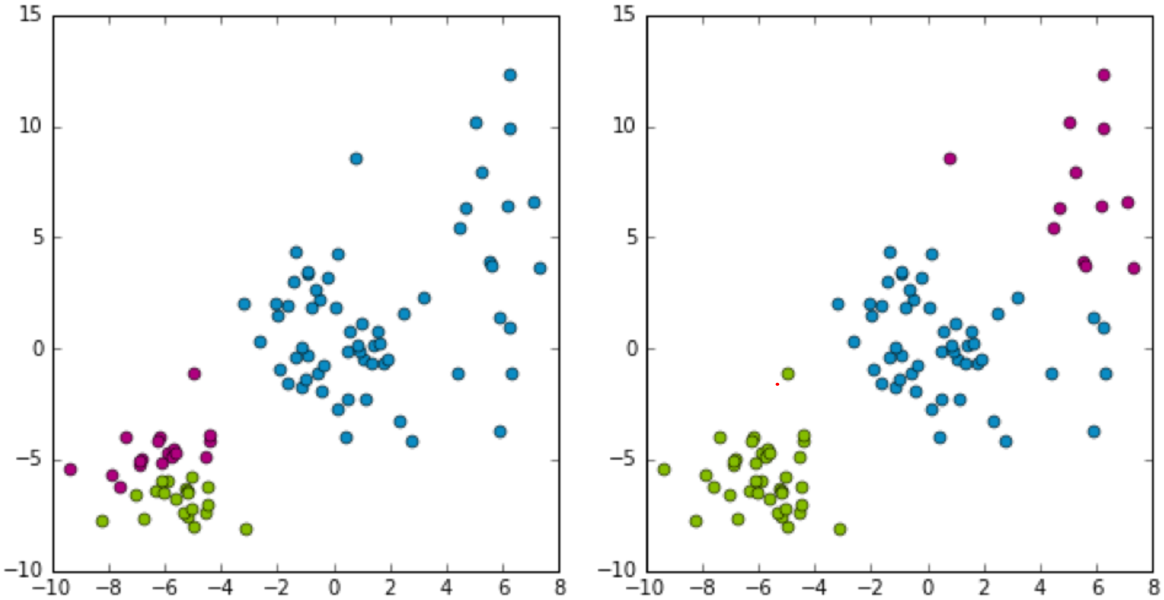


Don't know, there is no "right answer" in clustering 🤷🏾 .

Depends on the practitioner's domain-specific knowledge and interpretation of results!

Which Cluster?

Which clustering does k-means prefer?



k-means is trying to optimize the **heterogeneity** objective

$$\underset{z,\mu}{\operatorname{argmin}} \sum_{j=1}^{k} \sum_{i=1}^{n} \mathbf{1}\{z_i = j\} \left|\left|\mu_j - x_i\right|\right|_2^2$$

Coordinate Descent

k-means is trying to minimize the heterogeneity objective

$$\underset{z,\mu}{\operatorname{argmin}} \sum_{j=1}^{k} \sum_{i=1}^{n} \mathbf{1}\{z_i = j\} \left\| \mu_j - x_i \right\|_2^2$$

Step 0: Initialize cluster centers

Repeat until convergence:

Step 1: Assign each example to its closest cluster centroid

Step 2: Update the centroids to be the mean of all the points assigned to that cluster

Coordinate Descent alternates how it updates parameters to find minima. On each of iteration of Step 1 and Step 2, heterogeneity decreases or stays the same.

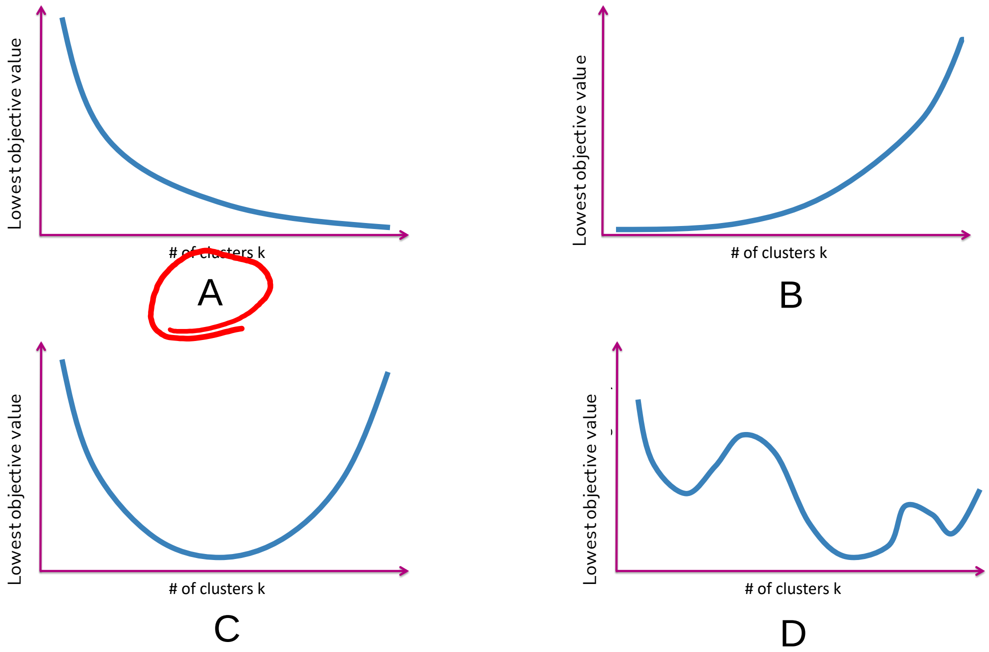
=> Will converge in finite time

Poll Everywhere

Think

1 min

Consider training k-means to convergence for different values of k. Which of the following graphs shows how the heterogeneity objective will change based on the value of k?



k = n

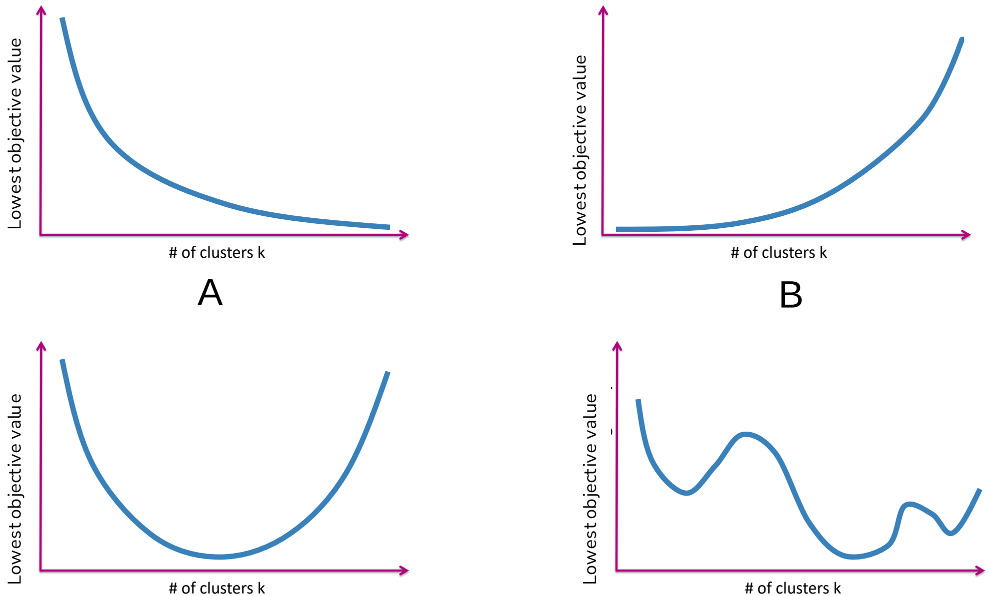
k = 1

Poll Everywhere

Think

2 mins

Consider training k-means to convergence for different values of k. Which of the following graphs shows how the heterogeneity objective will change based on the value of k?

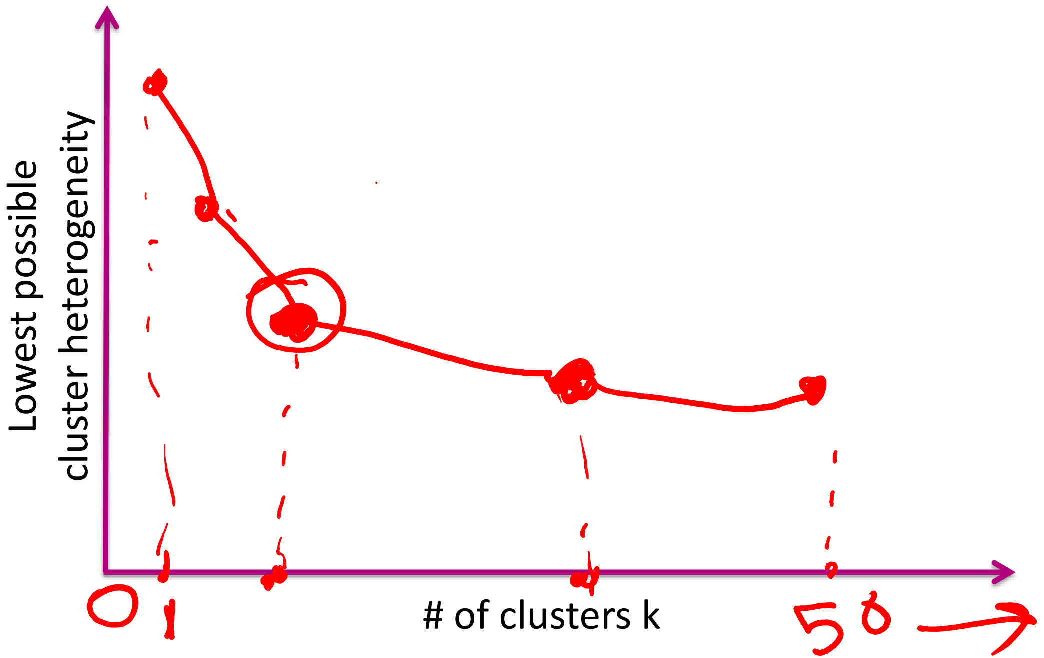


A B C D

How to Choose k?

No right answer! Depends on your application.

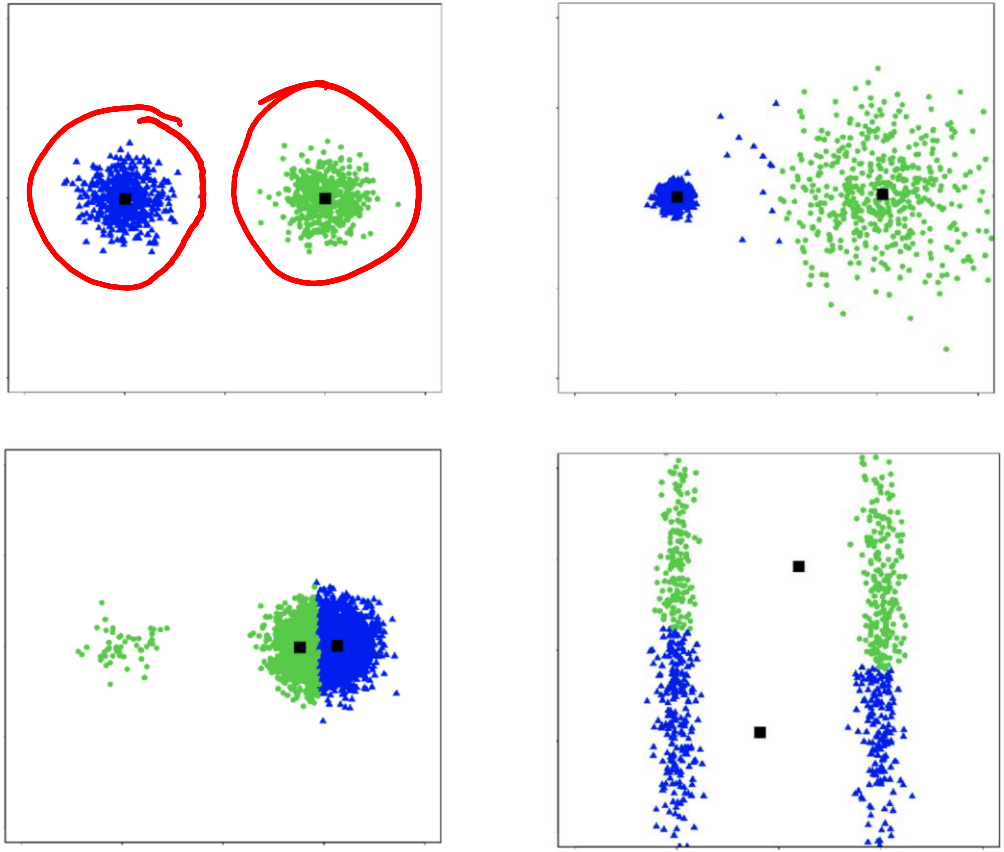
- General, look for the "elbow" in the graph



Note: You will usually have to run k-means multiple times for each k

Cluster shape

- k-means works well for well-separated **hyper-spherical** clusters of the same size



Clustering vs Classification

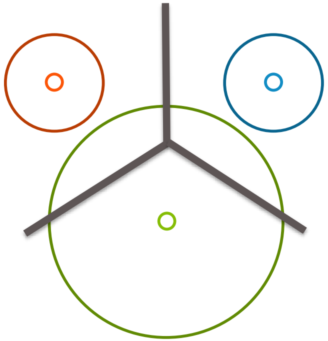
- Clustering looks like we assigned labels (by coloring or numbering different groups) but we didn't use any **labeled** data.
- In clustering, the "labels" don't have meaning. To give meaning to the labels, human inputs is required
- Classification learns from minimizing the error between a prediction and an actual **label**.
- Clustering learns by minimizing the distance between points in a cluster.
- Classification quality metrics (accuracy / loss) do not apply to clustering (since there is no label).
- You can't use validation set / cross-validation to choose the best choice of k for clustering.

Recap

- Differences between classification and clustering
- What types of clusters can be formed by k-means
- K-means algorithm
- Convergence of k-means
- How to choose k
- Better initialization using k-means++

Failure Modes of k-means

If we don't meet the assumption of spherical clusters, we will get unexpected results



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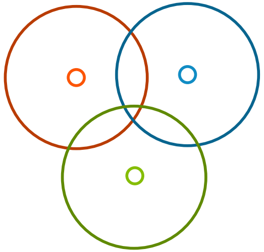

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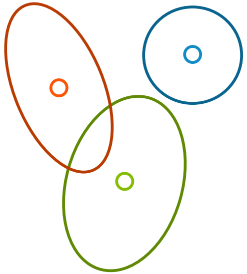
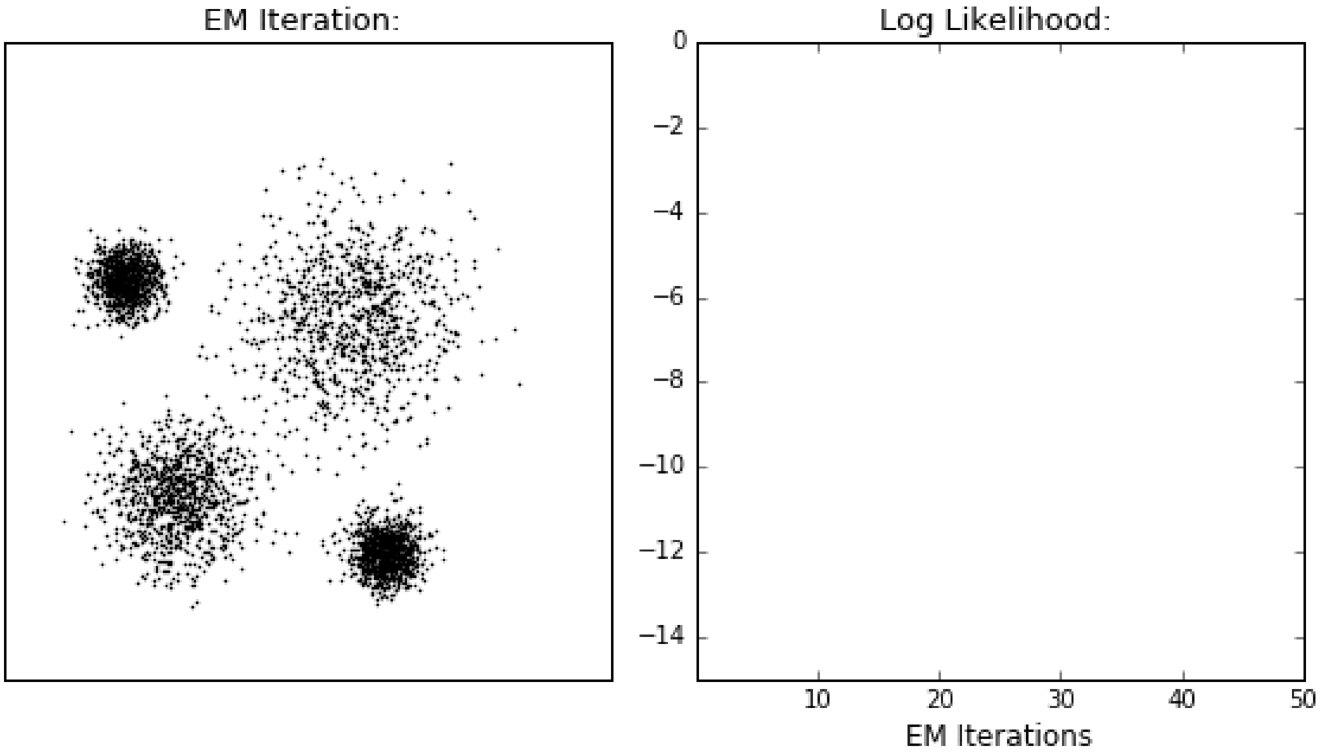


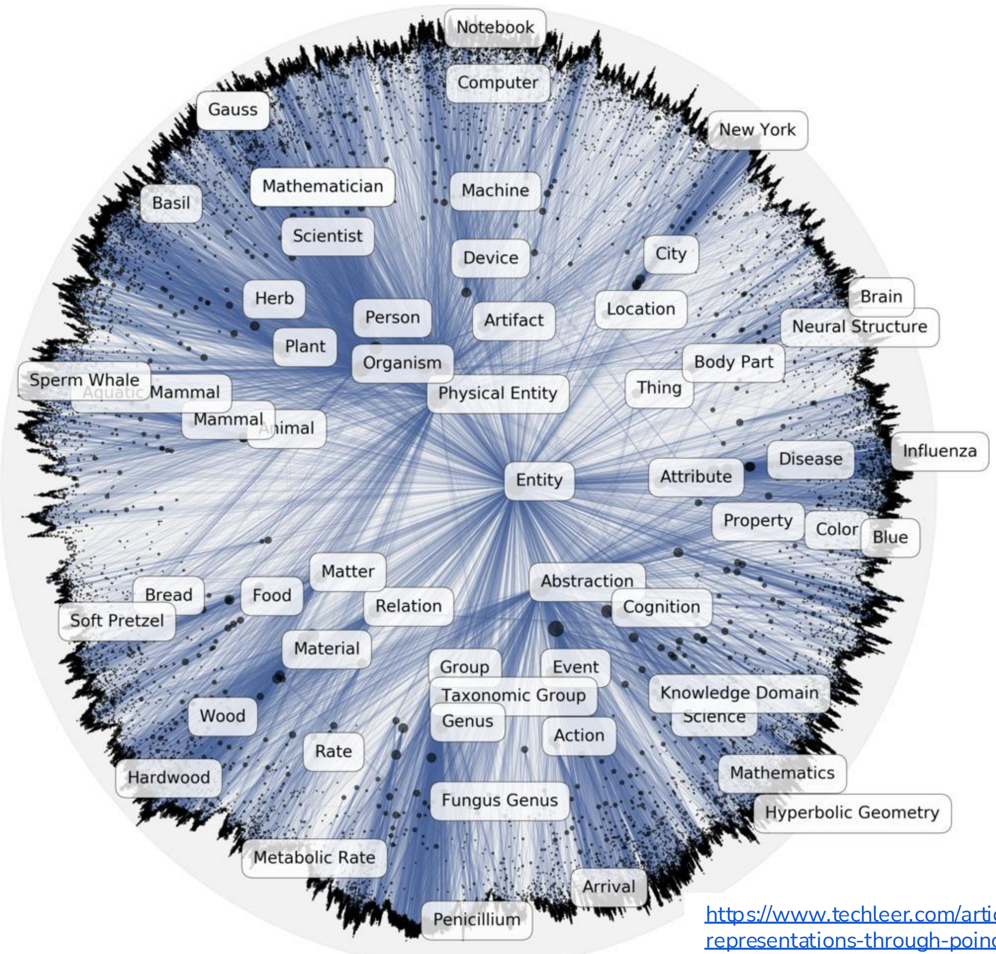
different shaped/oriented clusters

Visualizing Gaussian Mixture Models



Nouns

Lots of data is hierarchical by nature



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Agglomerative, a.k.a. *bottom-up*:

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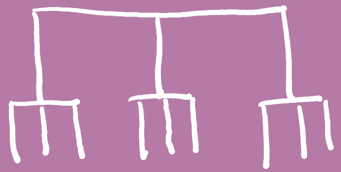
  - Example: **single linkage clustering**

→ how we measure distance between clusters

Divisive Clustering

k=3



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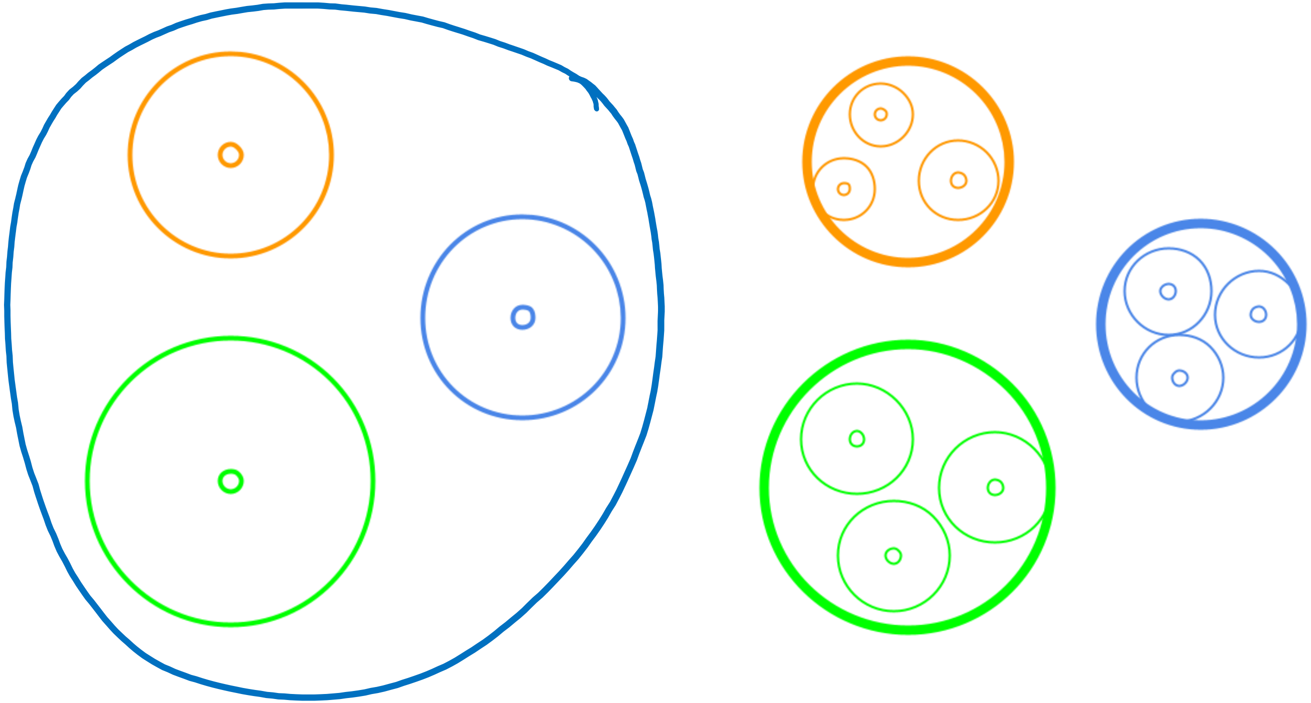
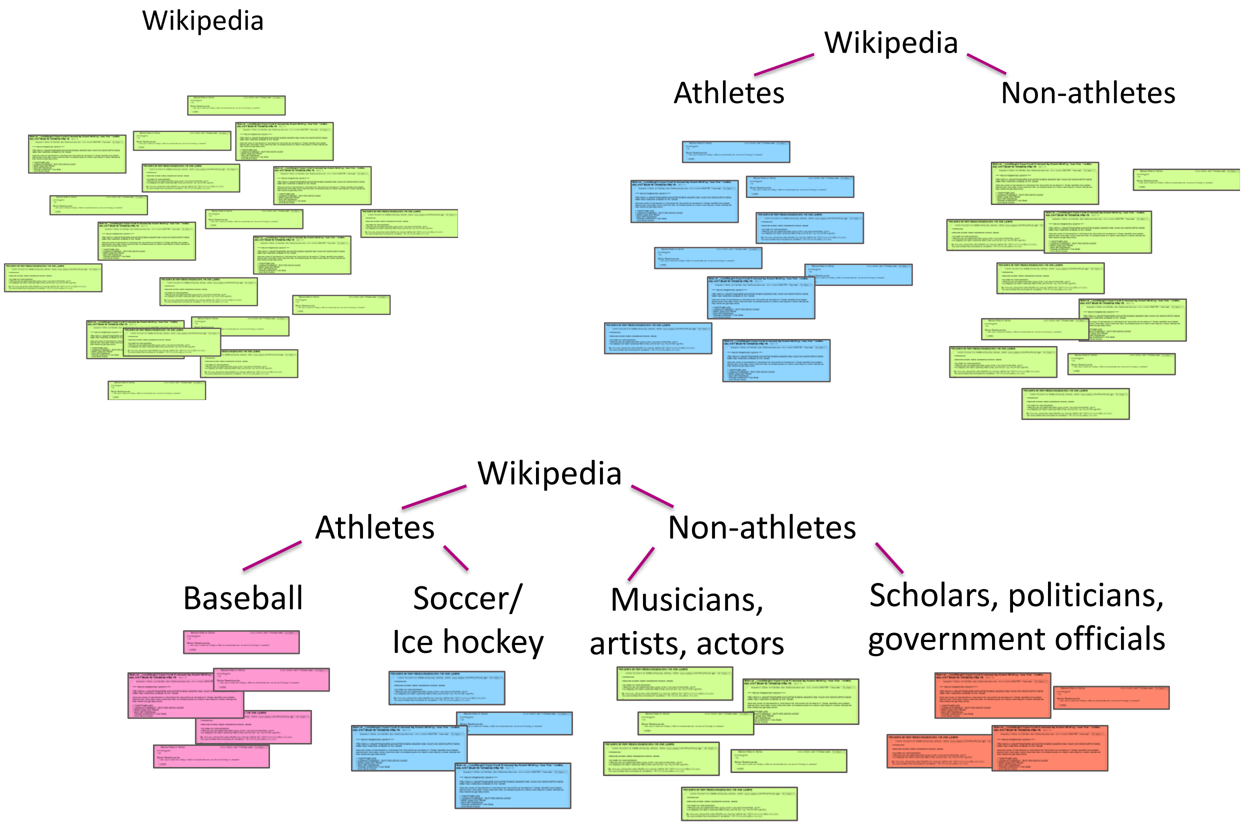


Example

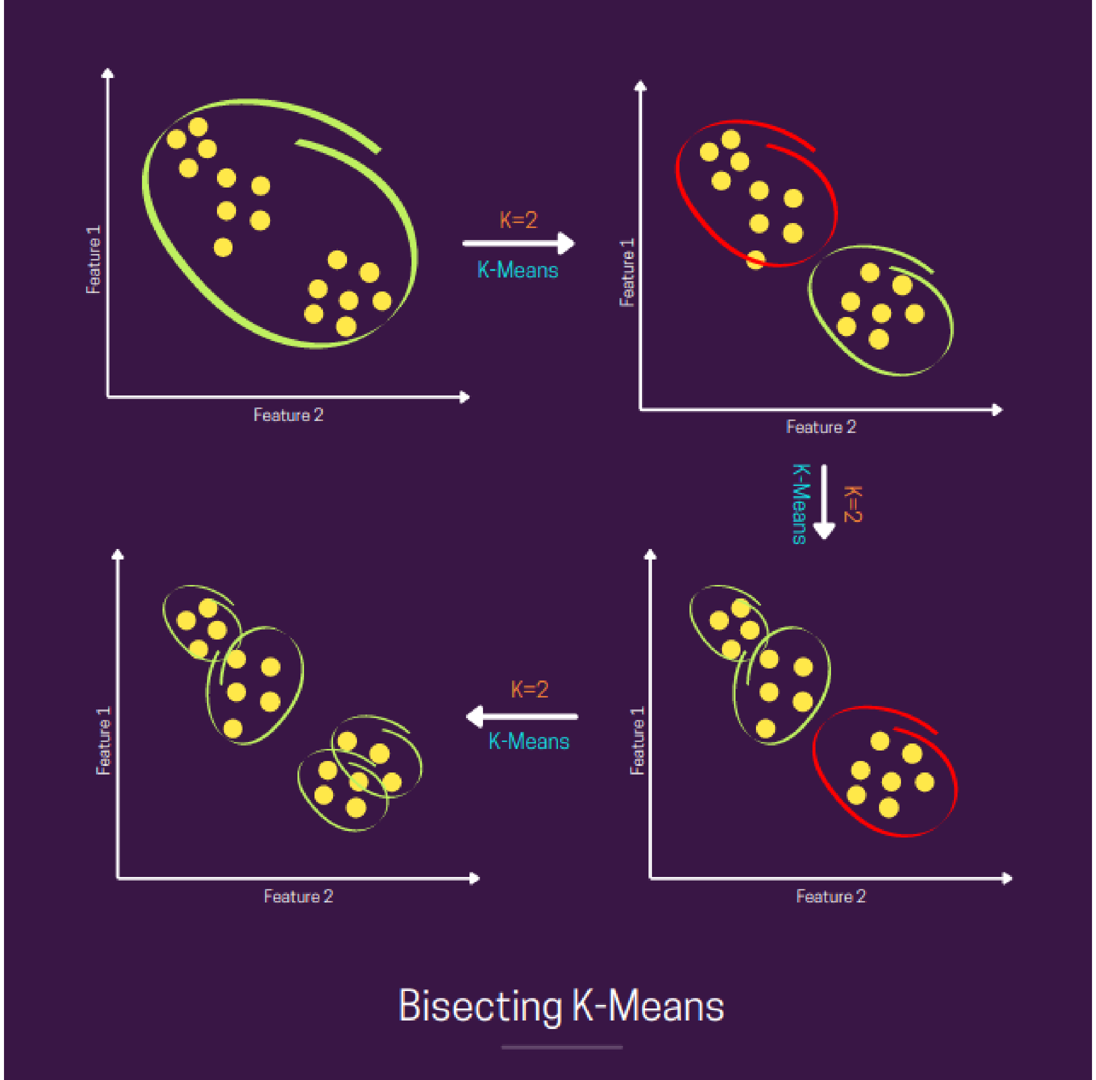
K=2

Bisecting k-means

Using Wikipedia



Bisecting K-Means

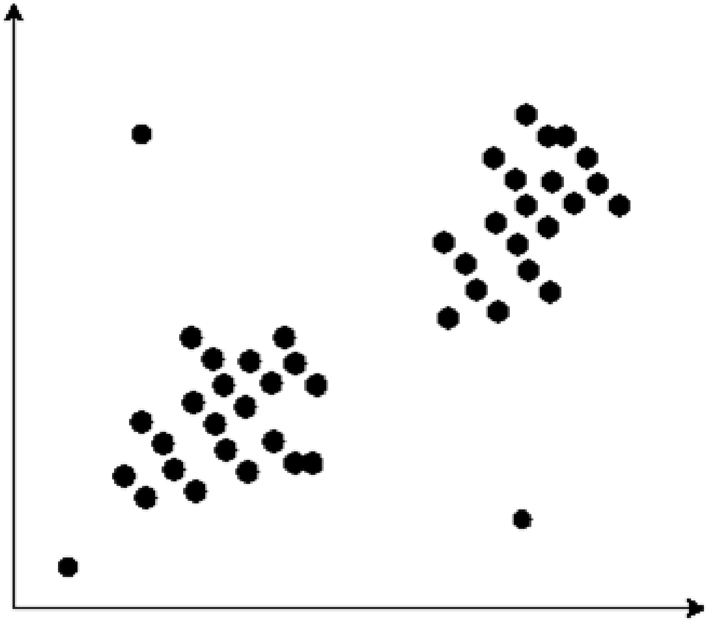


Poll Everywhere

Think

1 min

- You want to detect outliers in a dataset (shown below).
  - How would you use k-means clustering to detect outliers?
  - How would you use divisive clustering to detect outliers?

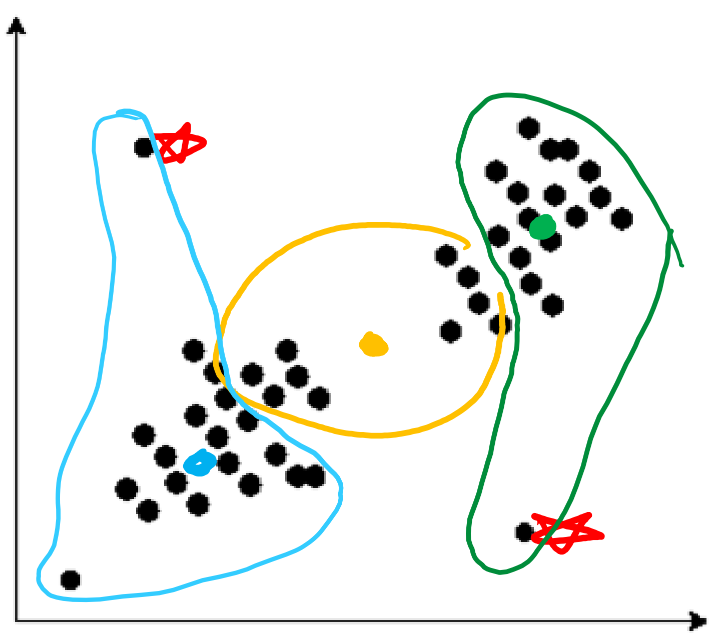


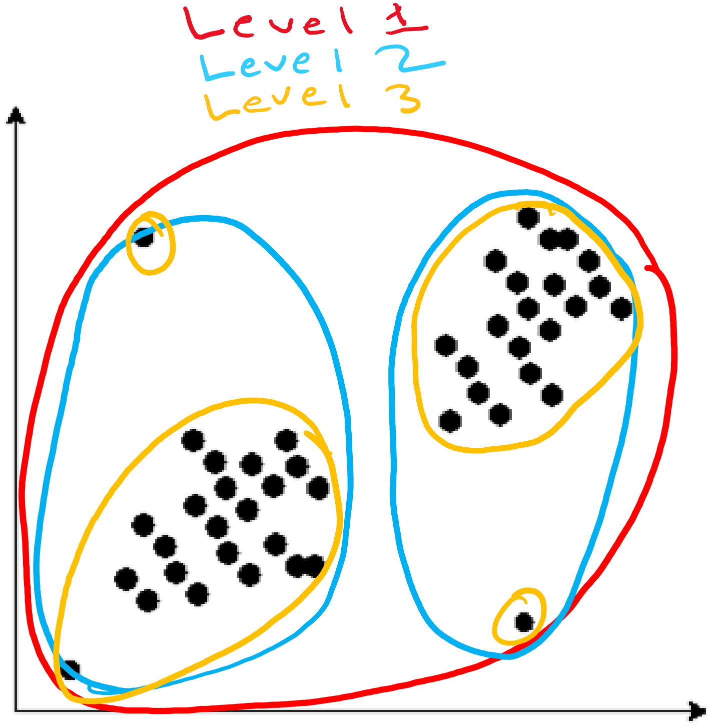
Poll Everywhere

Think

2 min

- You want to detect outliers in a dataset (shown below).
  - How would you use k-means clustering to detect outliers?
  - How would you use divisive clustering to detect outliers?

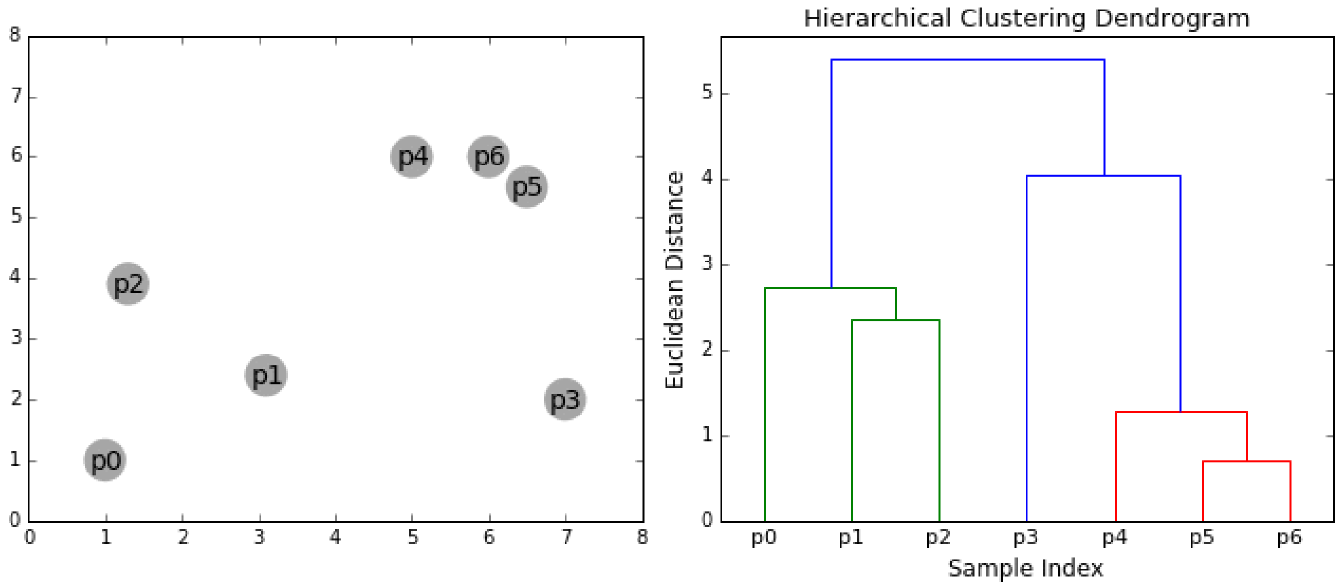




Agglomerative Clustering

Agglomerative Clustering

Merge closest pair of clusters



Agglomerative Clustering

Algorithm at a glance

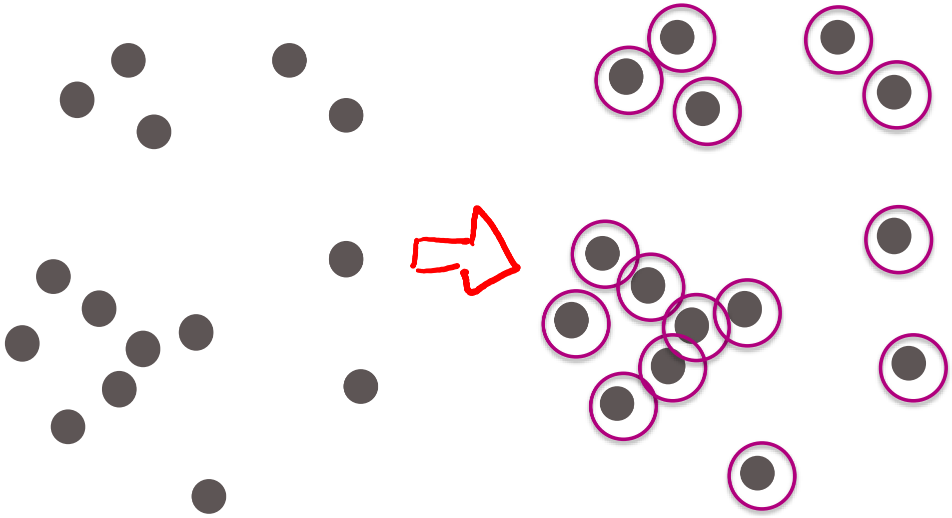
1. Initialize each point in its own cluster
2. Define a distance metric between clusters ← Hyperparameter

While there is more than one cluster

3. Merge the two closest clusters (and add it to dendrogram)

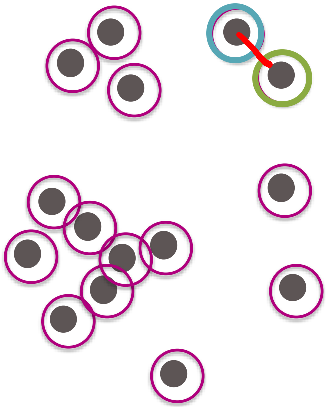
Step 1

1. Initialize each point to be its own cluster



Step 2

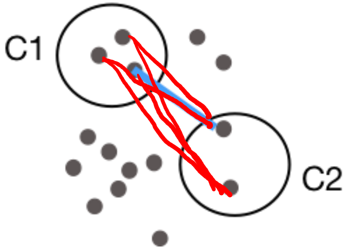
2. Define a distance metric between clusters



Single Linkage

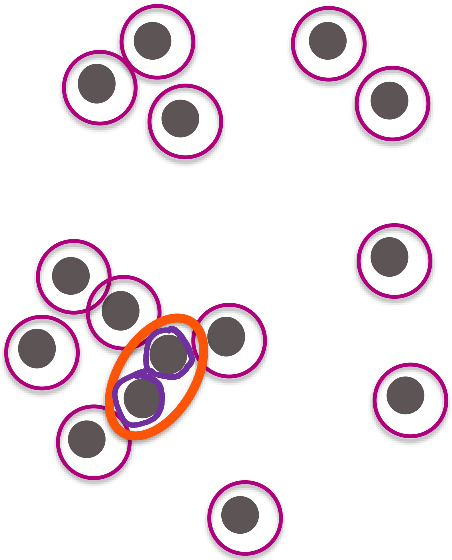
$$distance(C_1, C_2) = \min_{x_i \in C_1, x_j \in C_2} d(x_i, x_j)$$

This formula means we are defining the distance between two clusters as the smallest distance between any pair of points between the clusters.

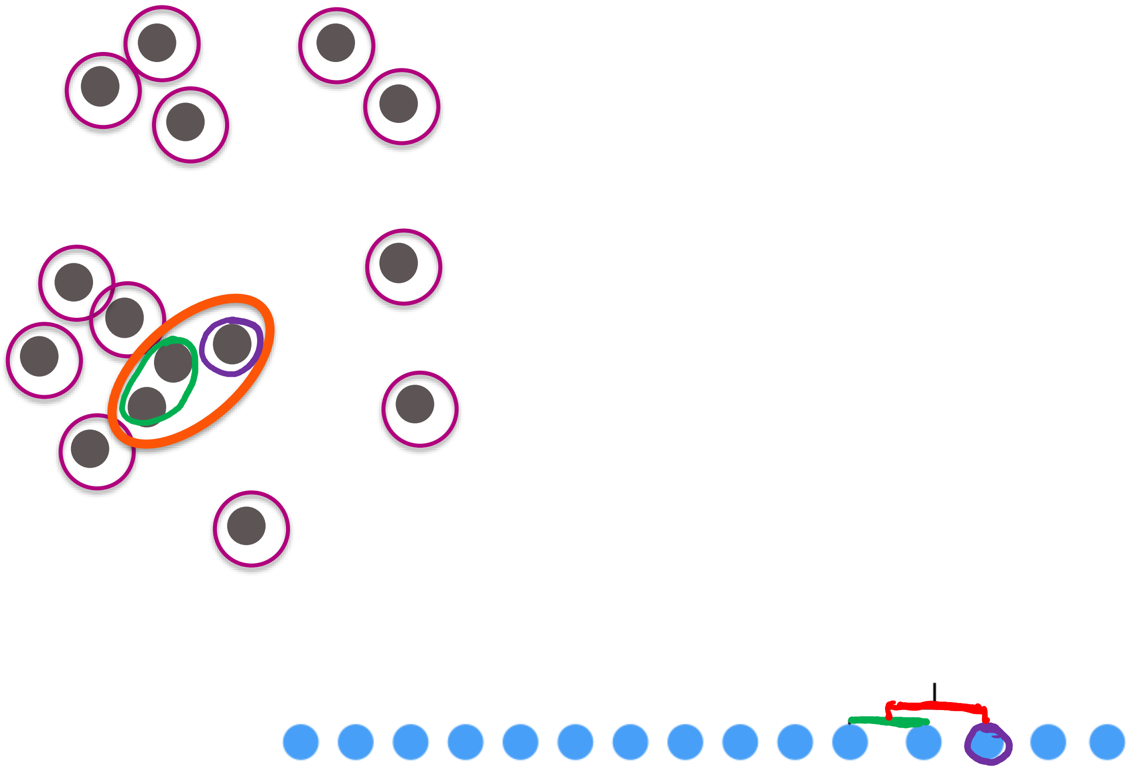


Step 3

Merge closest pair of clusters

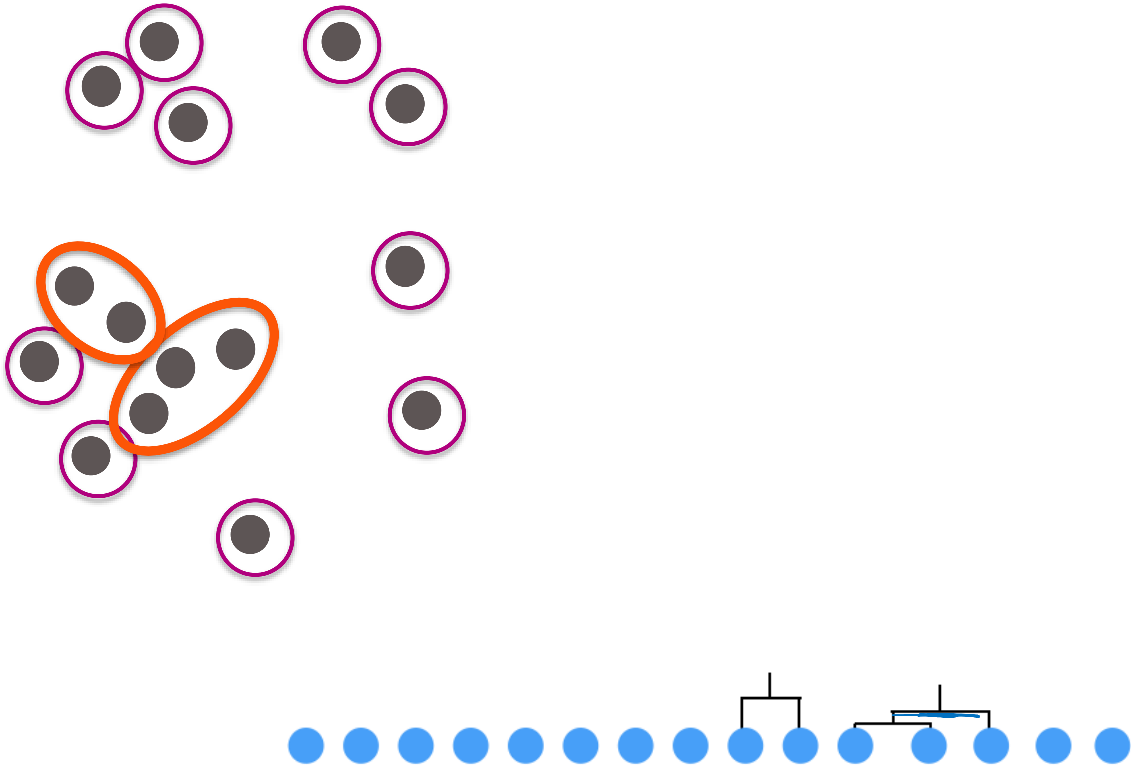


Repeat

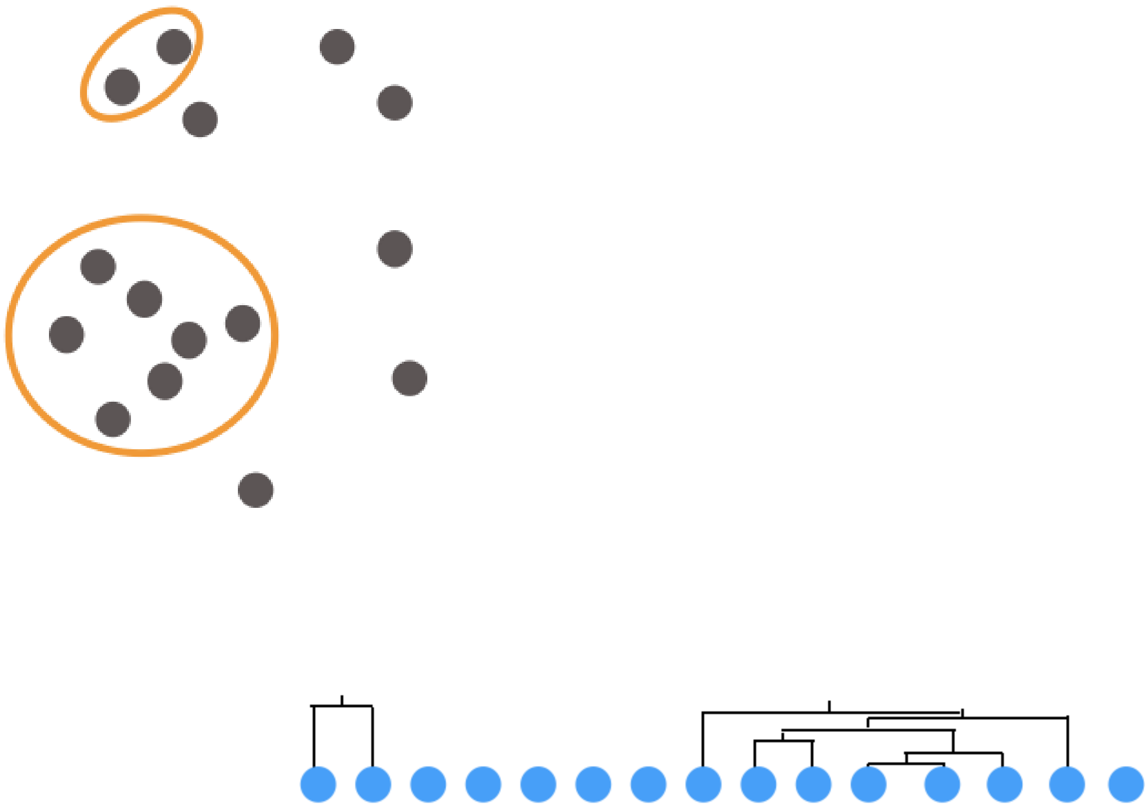


Repeat

Notice that the height of the dendrogram is growing as we group points farther from each other



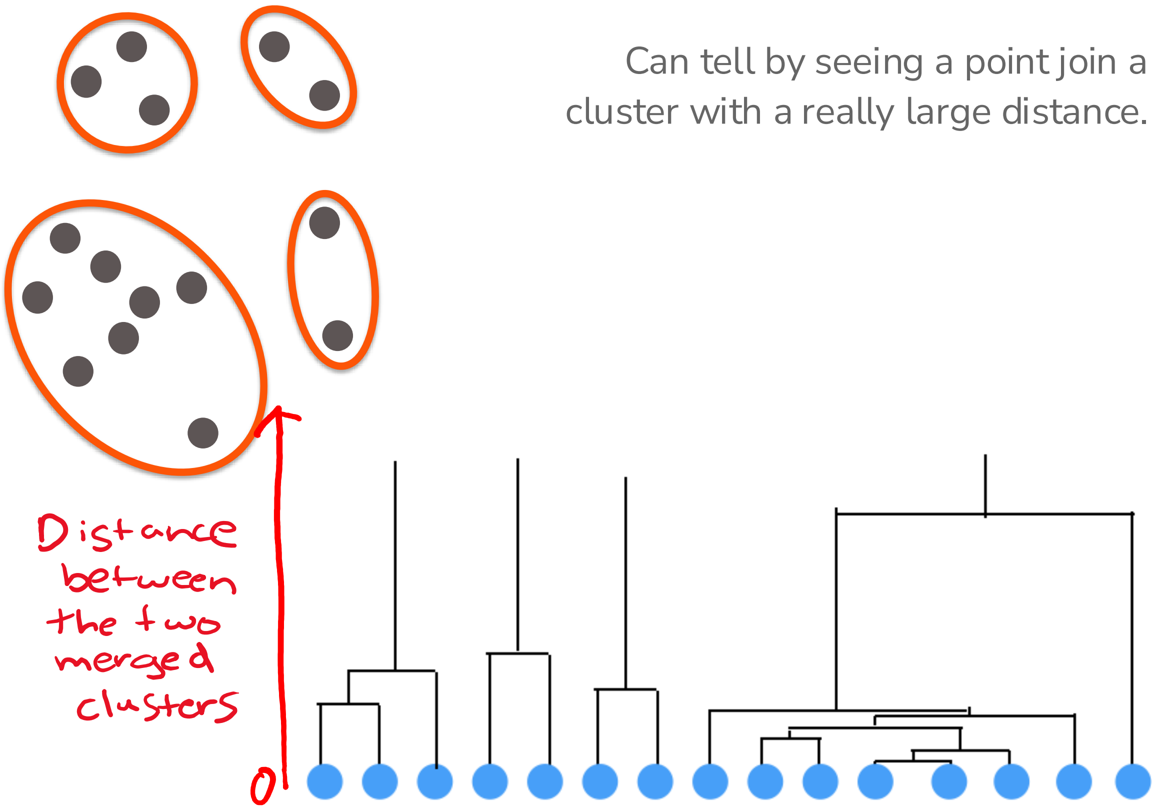
Repeat



Repeat

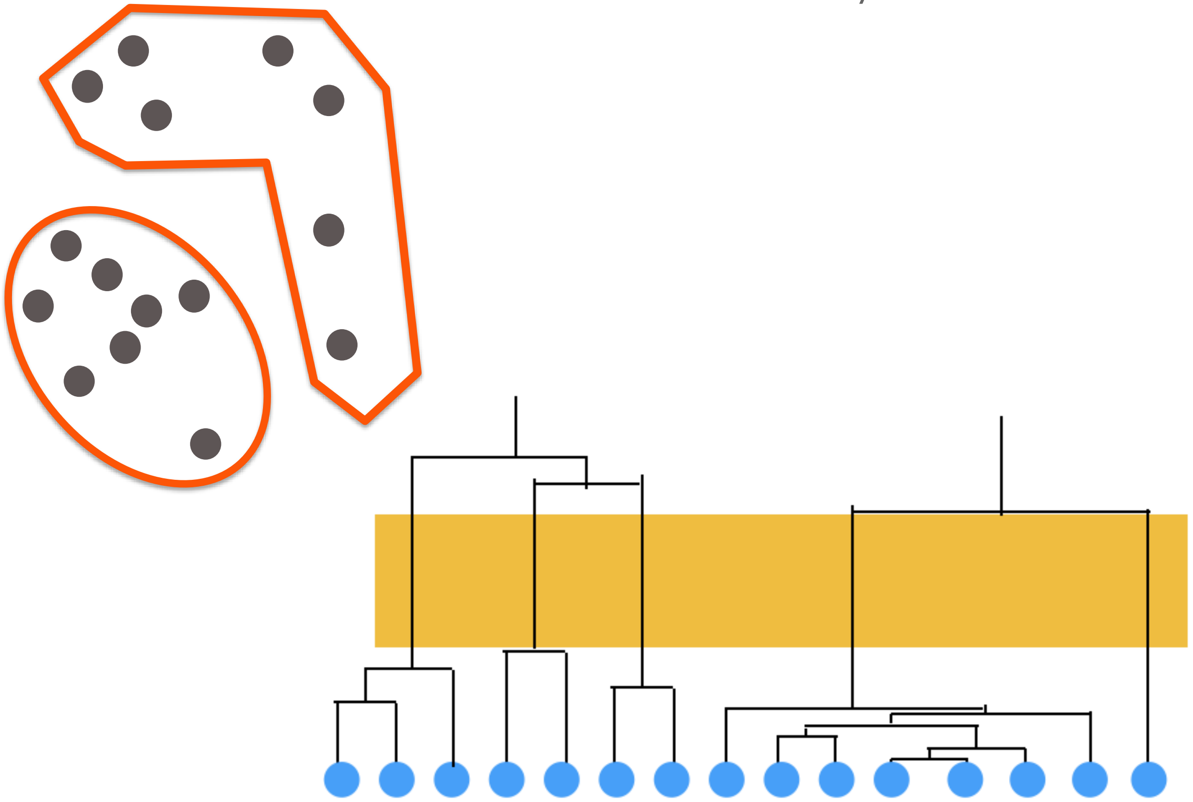
Looking at the dendrogram, we can see there is a bit of an outlier!

Can tell by seeing a point join a cluster with a really large distance.



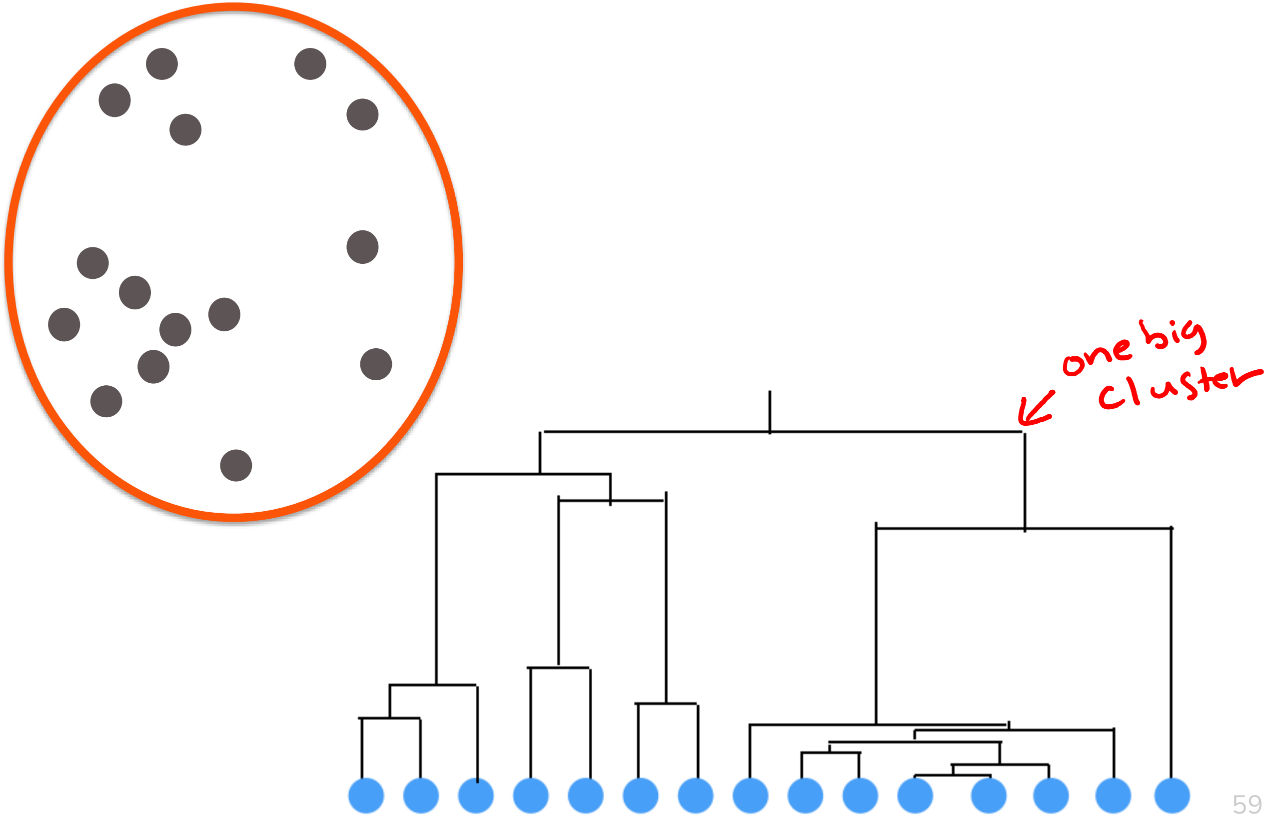
Repeat

The tall links in the dendrogram show us we are merging clusters that are far away from each other

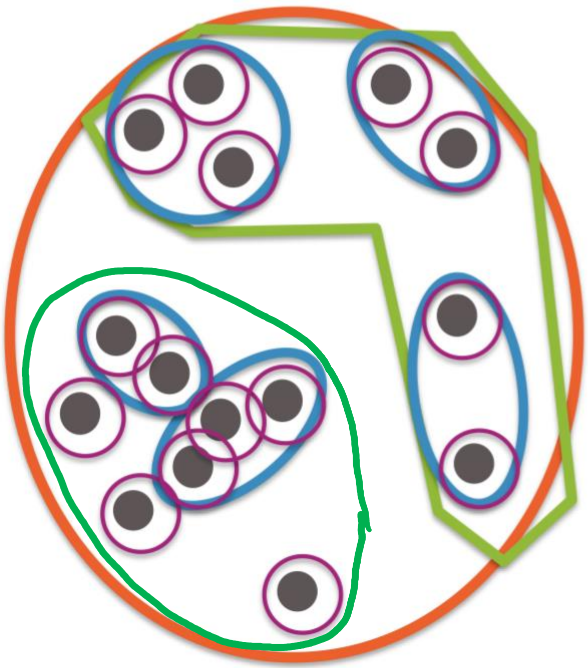


Repeat

Final result after merging all clusters



Final Result

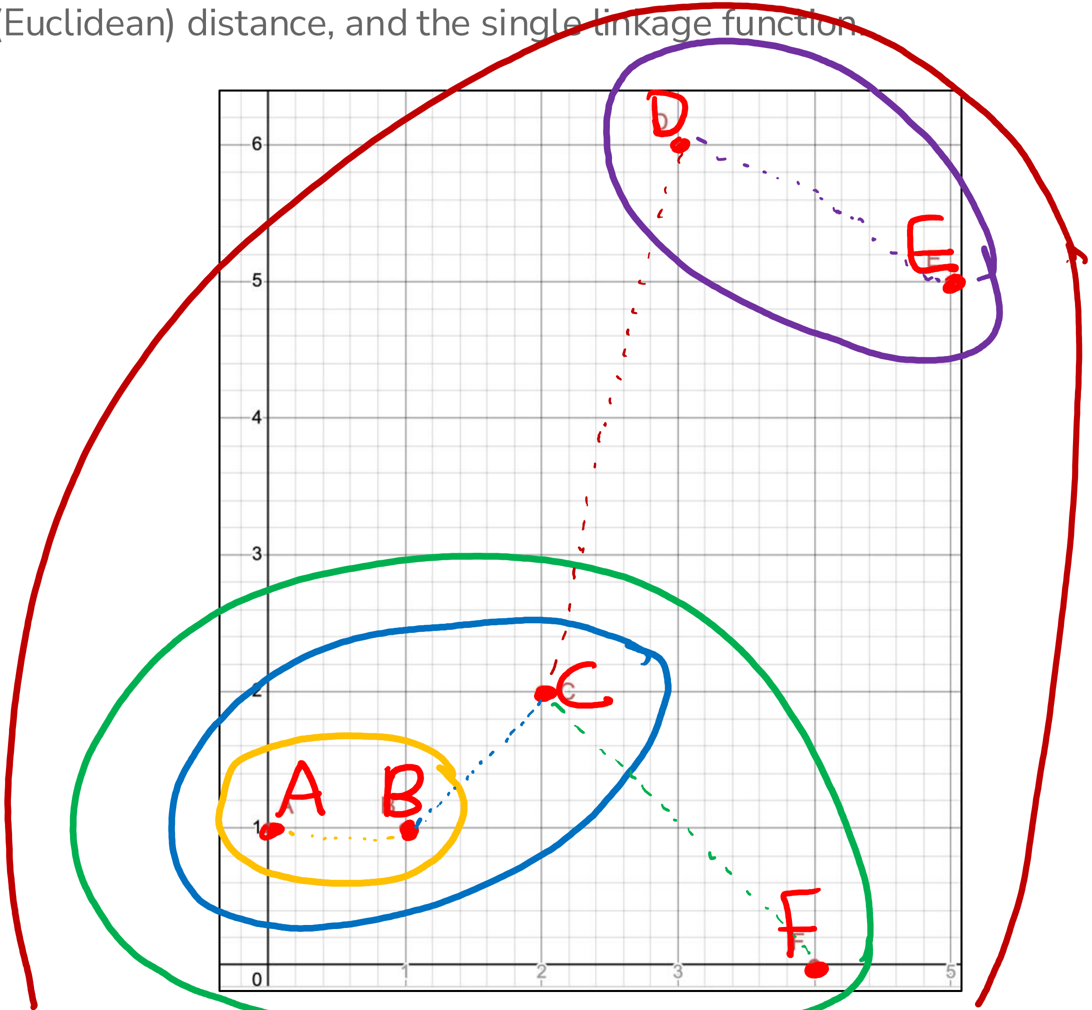


Poll Everywhere

Think

1 min

- In what order will the following points get merged into clusters? Use L2 (Euclidean) distance, and the single linkage function.



Brain Break

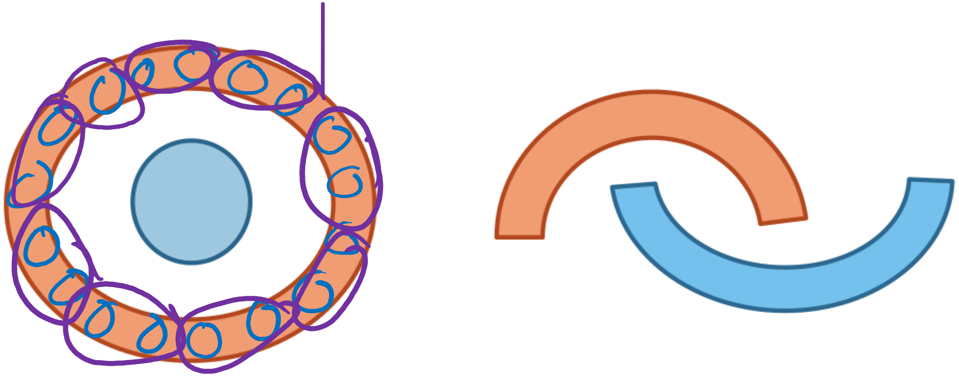
3:12

Dendrograms

Agglomerative Clustering

With agglomerative clustering, we are now very able to learn weirder clusterings like

Single Linkage: $\min_{x_i \in C_1, x_j \in C_2} dist(x_i, x_j)$

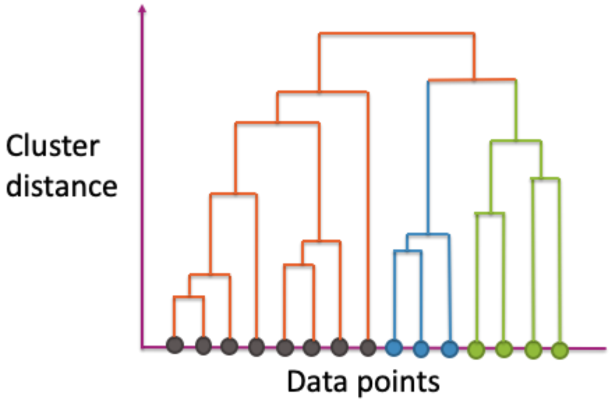


Single Linkage can merge long chains

Dendrogram

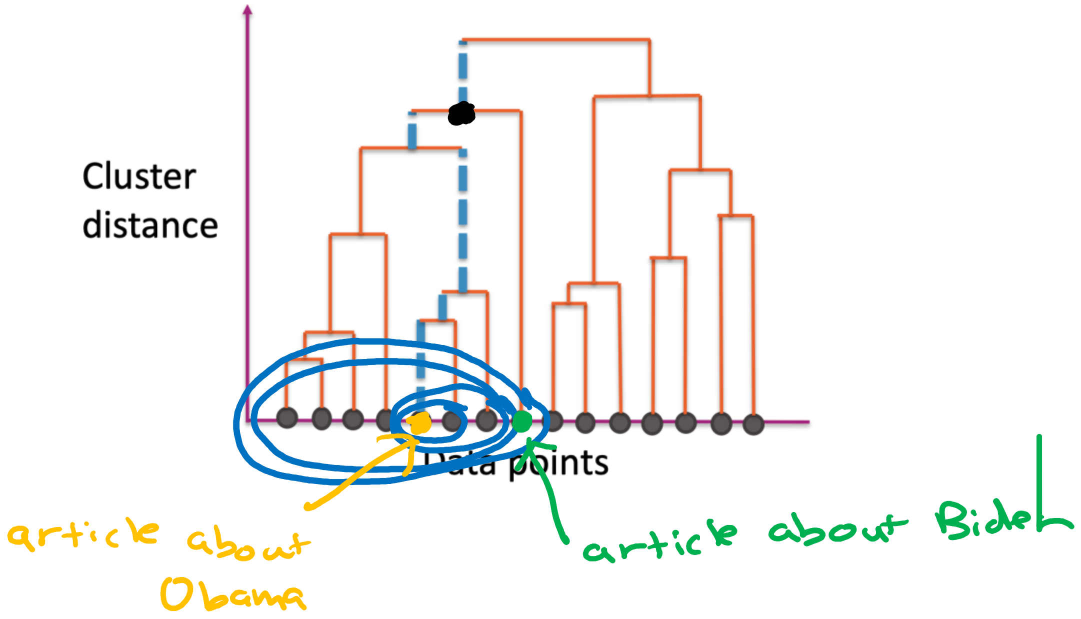
x-axis shows the datapoints (arranged in a very particular order)

y-axis shows distance between merged clusters



Dendrogram

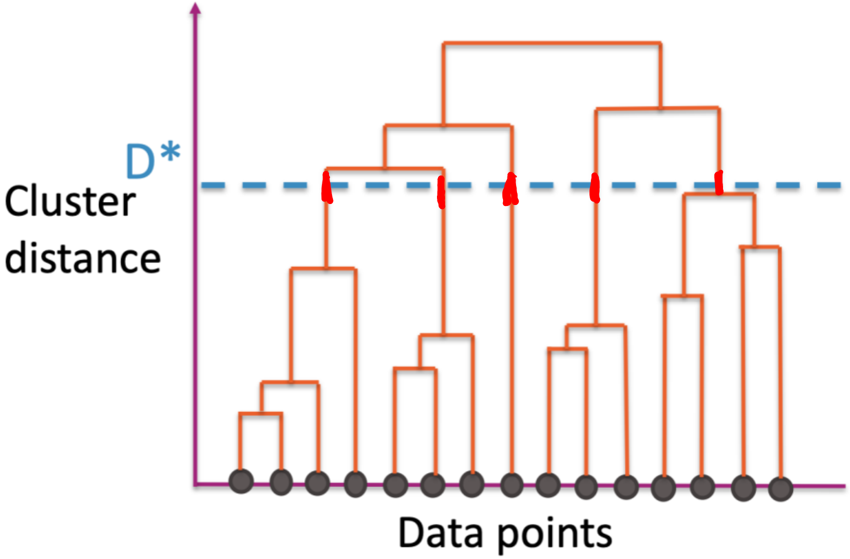
The path shows you all clusters that a single point belongs and the order in which its clusters merged



Cut Dendrogram

Choose a distance D^* to "cut" the dendrogram

- Use the largest clusters with distance $< D^*$
- Usually ignore the idea of the nested clusters after cutting



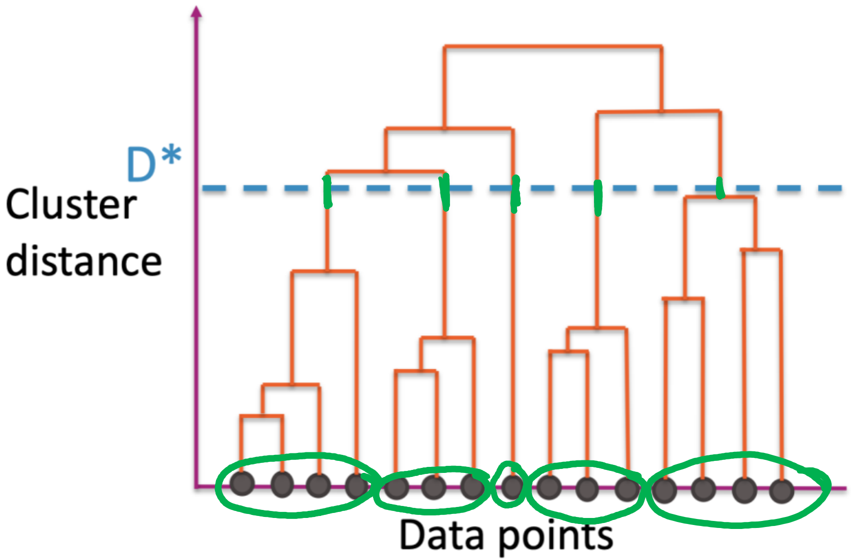
Poll Everywhere

Think

1 min

pollev.com/cs416

How many clusters would we have if we use this threshold?



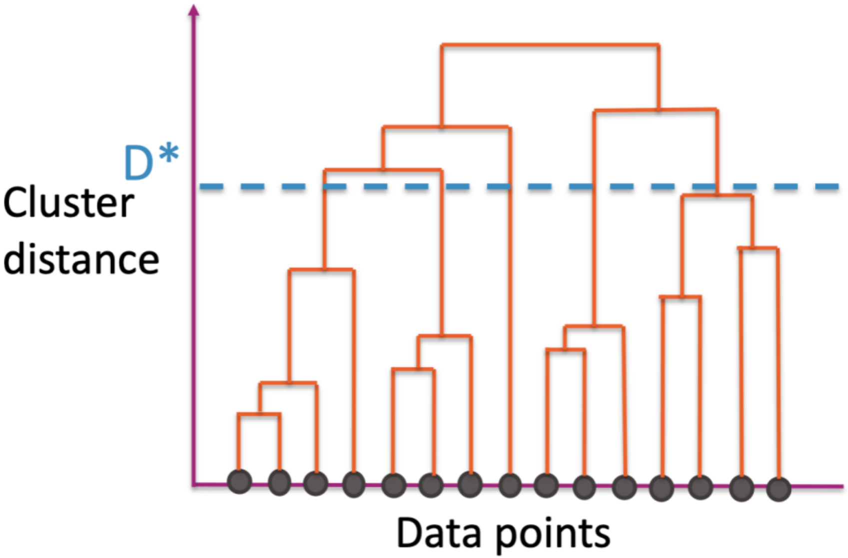
Poll Everywhere

Think

2 min

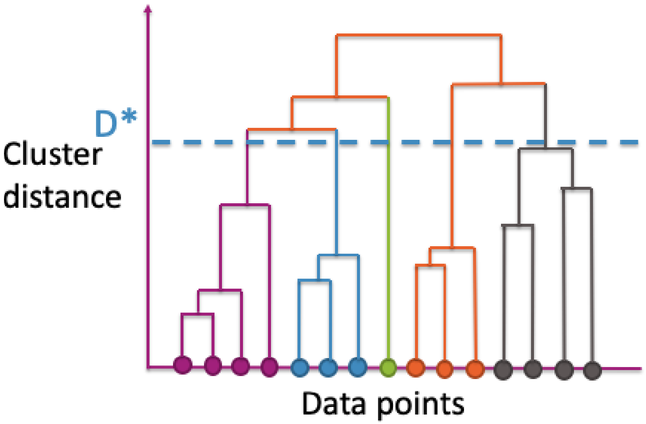
pollev.com/cs416

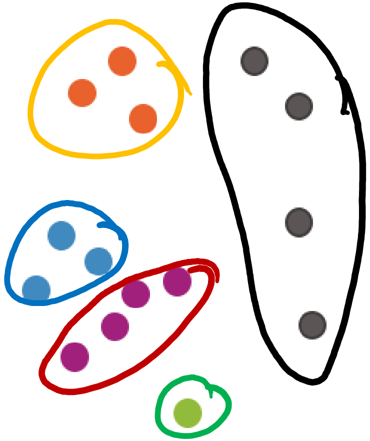
How many clusters would we have if we use this threshold?



Cut Dendrogram

Every branch that crosses D^* becomes its own cluster





Choices to Make

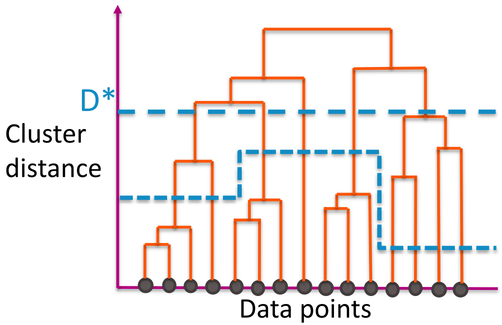
For agglomerative clustering, you need to make the following choices:

- Distance metric $d(x_i, x_j)$
- Linkage function
  - Single Linkage:

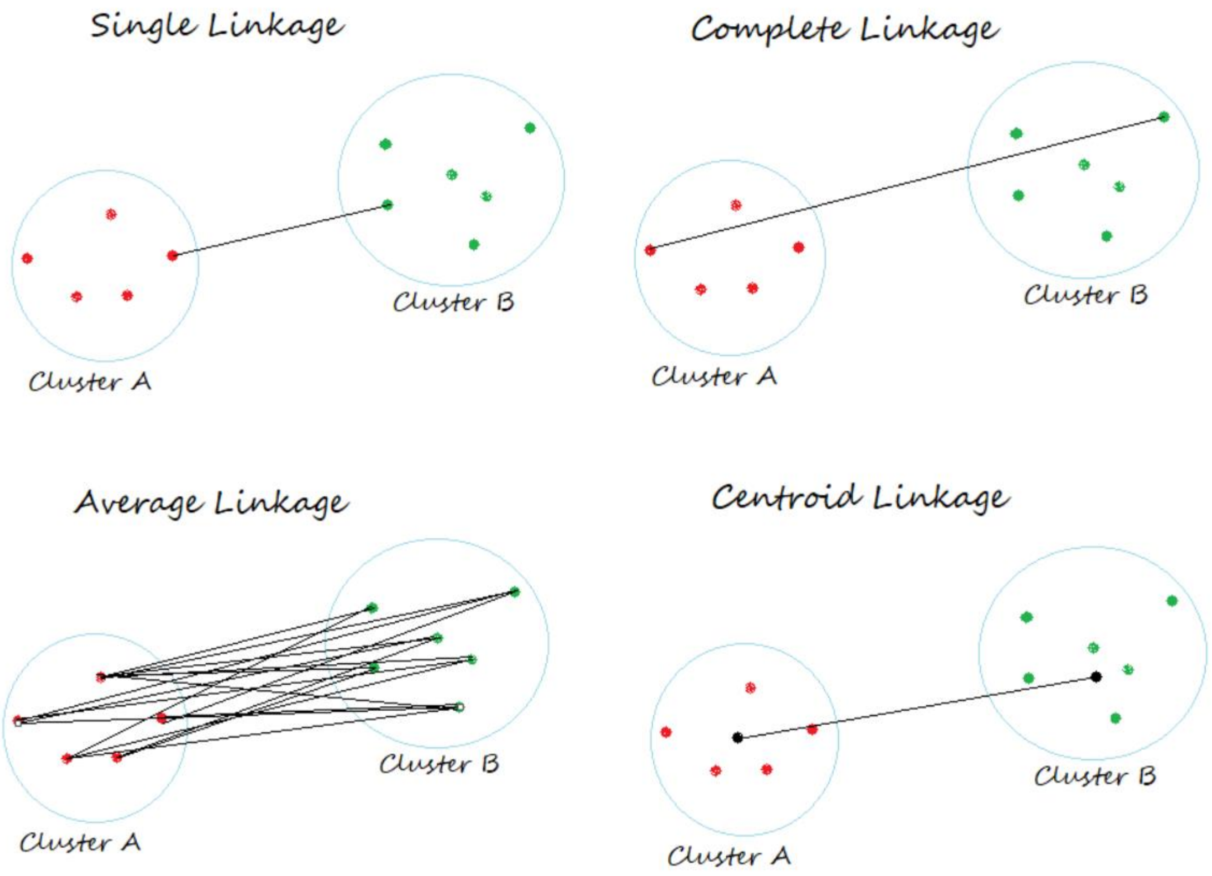
    $$\mathrm{D}(\mathrm{C}_1, \mathrm{C}_2) = \min_{x_i \in C_1, x_j \in C_2} d(x_i, x_j)$$
  - Complete Linkage:

    $$D(C_1, C_2) = \max_{x_i \in C_1, x_j \in C_2} d(x_i, x_j)$$
  - Centroid Linkage

    $$\mathrm{D}(C_1, C_2) = d(\mu_1, \mu_2)$$
  - Others
- Where and how to cut dendrogram



Linkage Functions



Practical Notes

For visualization, generally a smaller # of clusters is better

For tasks like outlier detection, cut based on:

- Distance threshold
- Or some other metric that tries to measure how big the distance increased after a merge

No matter what metric or what threshold you use, no method is "incorrect". Some are just more useful than others.

Computational Cost of Agglomerative Clustering

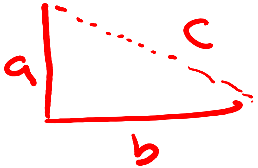
Computing all pairs of distances is pretty expensive!

- A simple implementation takes $\mathcal{O}(n^2 \log(n))$

Can be much implemented more cleverly by taking advantage of the **triangle inequality**

- "Any side of a triangle must be less than the sum of its sides"

Best known algorithm is $\mathcal{O}(n^2)$



$c \leq a+b$

k-means vs. Agglomerative Clustering

- K-means is more efficient on big data than hierarchical clustering.
- Initialization changes results in k-means, not in agglomerative clustering has reproducible results.
- K-means works well only for hyper-spherical clusters, agglomerative clustering can handle more complex cluster shapes.
- K-means requires selecting a number of clusters beforehand. In agglomerative clustering, you can decide on the number of clusters afterwards using the dendrogram.

Concept Inventory

This week we want to practice recalling vocabulary. Spend 10 minutes trying to write down all the terms for concepts we have learned in this class and try to bucket them into the following categories.

Regression

Classification

Deep Learning

Document Retrieval

Misc – For things that fit in multiple places or none of the above

You don't need to define/explain the terms for this exercise, but you should know what they are!

Try to do this for at least 5 minutes from recall before looking at your notes!

Recap

- Problems with k-means
- Mixture Models
- Hierarchical clustering
- Divisive Clustering
- Agglomerative Clustering
- Dendrograms