Clustering

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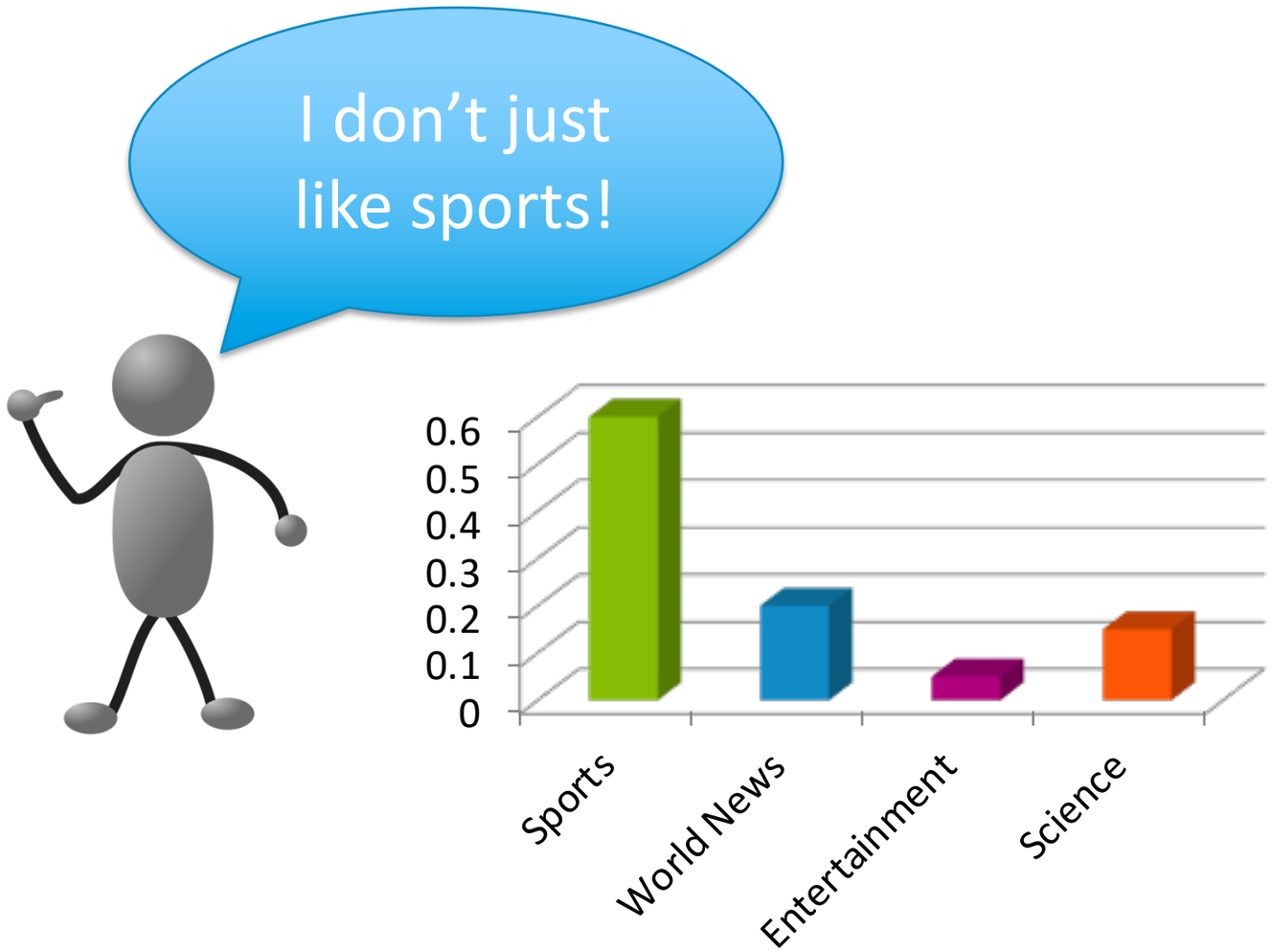
Clustering

SPORTS

WORLD NEWS

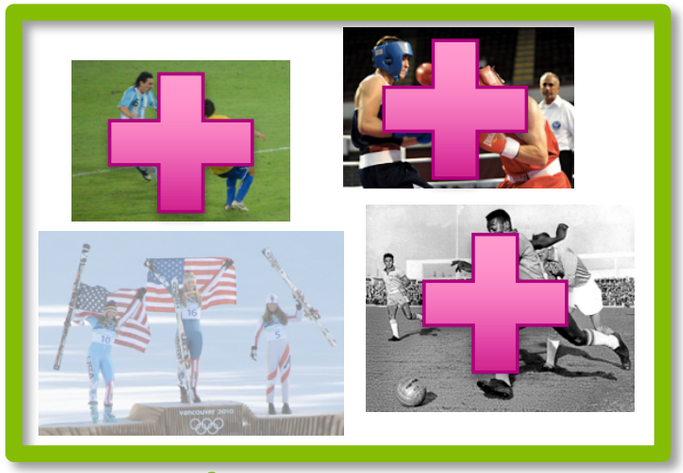
Why is clustering useful?

- User preference is important to learn, but challenging
- If we know a user's preference, we can recommend better



How do we learn a persons preference

- When the topics are not even pre-defined
- Let alone knowing which article falls into which group
- clustering: learns this from user feedback (rating, up/down)



Cluster 1

Cluster 2

Cluster 3

Cluster 4

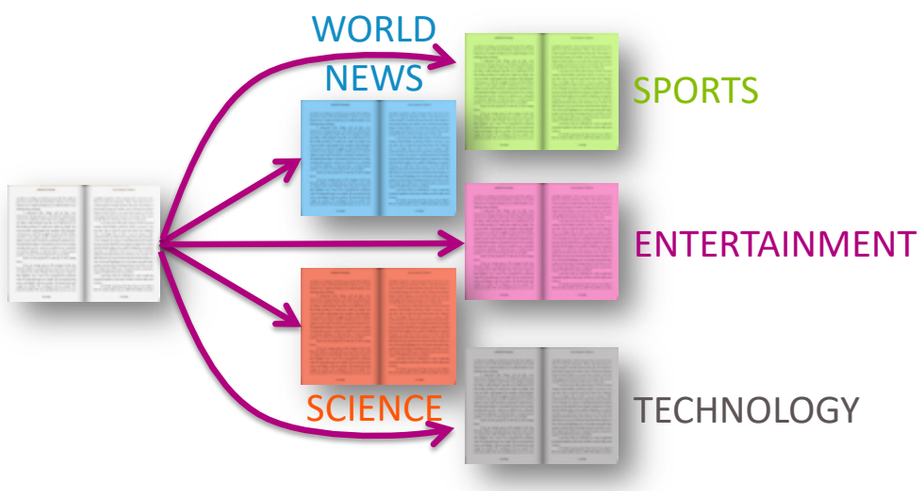
Use feedback to learn user preferences over topics

Clustering

- What if labels are known?

Training set of labeled docs

- Then we can use multiclass classification methods

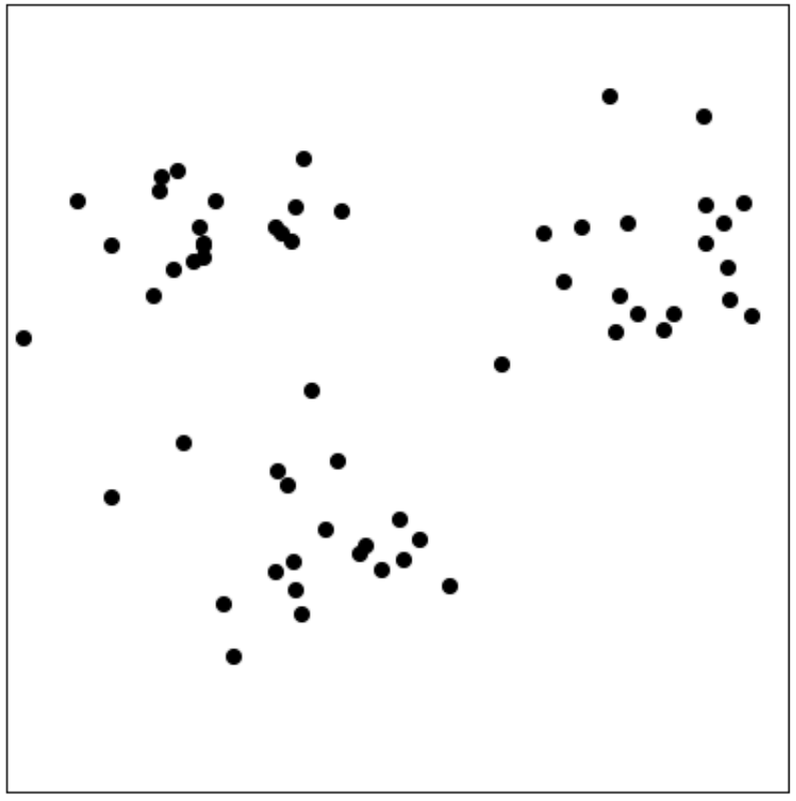


Example of
supervised learning

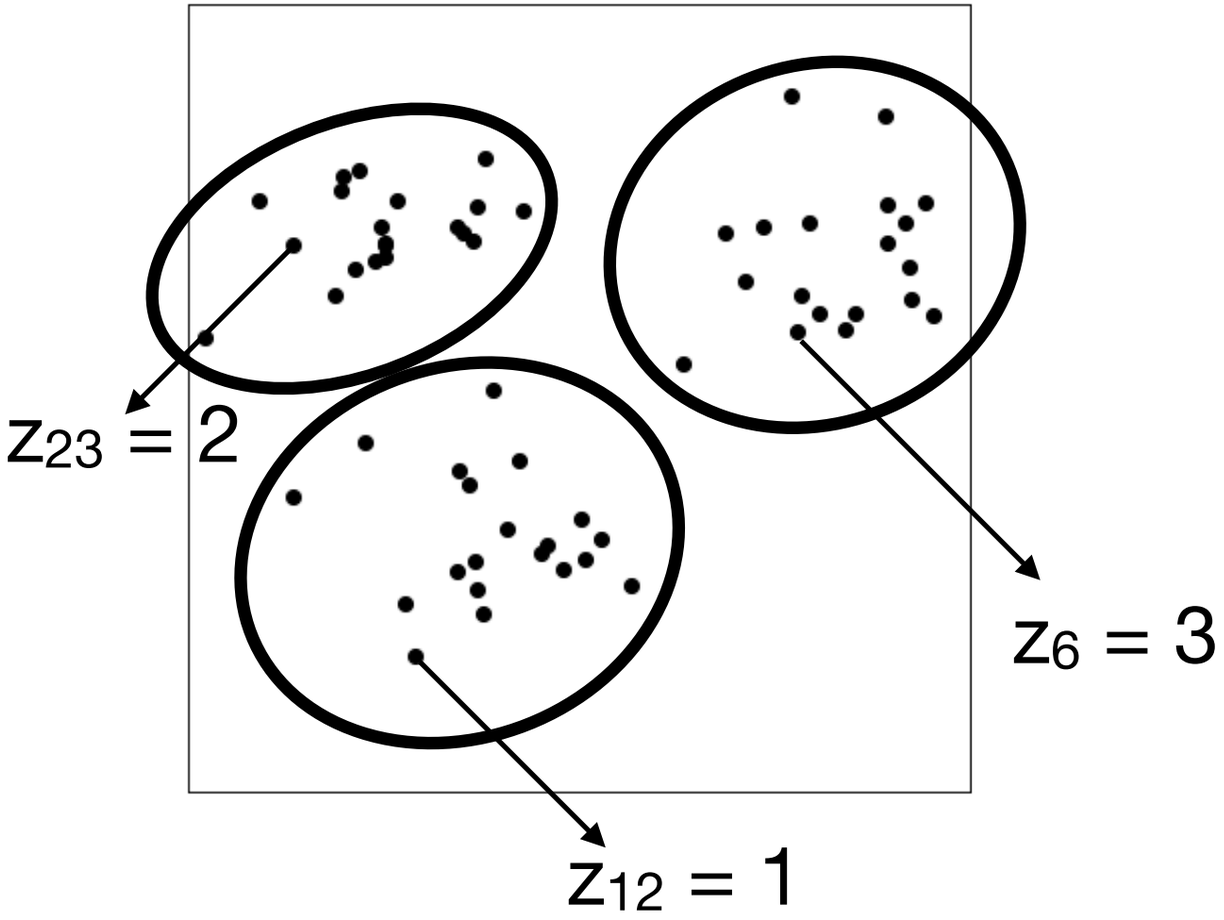
Clustering

- What if labels are unknown?
  - We need to uncover the structure (or pattern) from just x
  - ***Cluster*** is one of the most important patterns in real data
  - Finding clusters help, personalized medicine, targeted advertisement, scientific discovery, many other machine learning tasks

- Input: $x_1,\ldots,x_N$

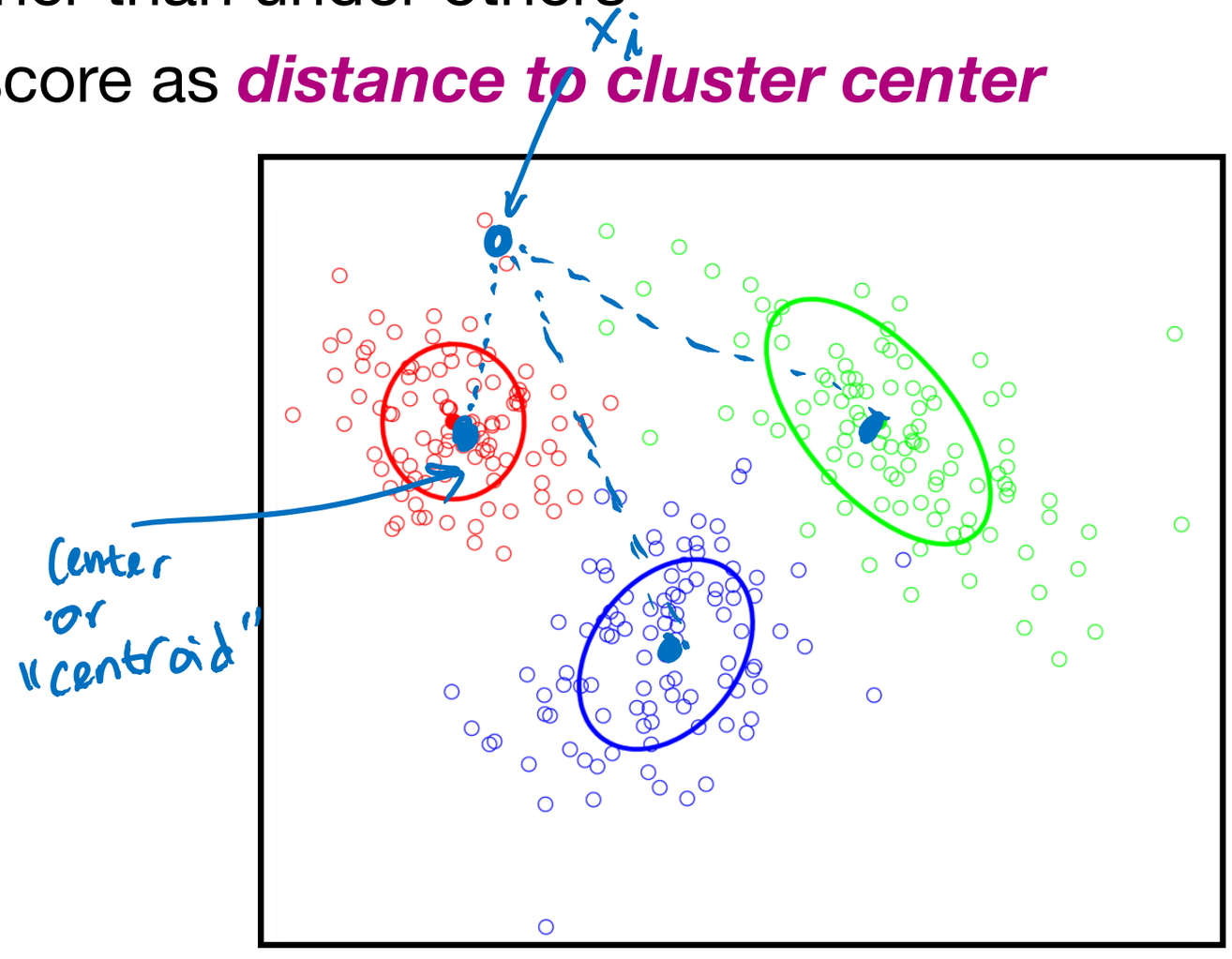


- Output: cluster label for each point z_i in {1,2,…,k}



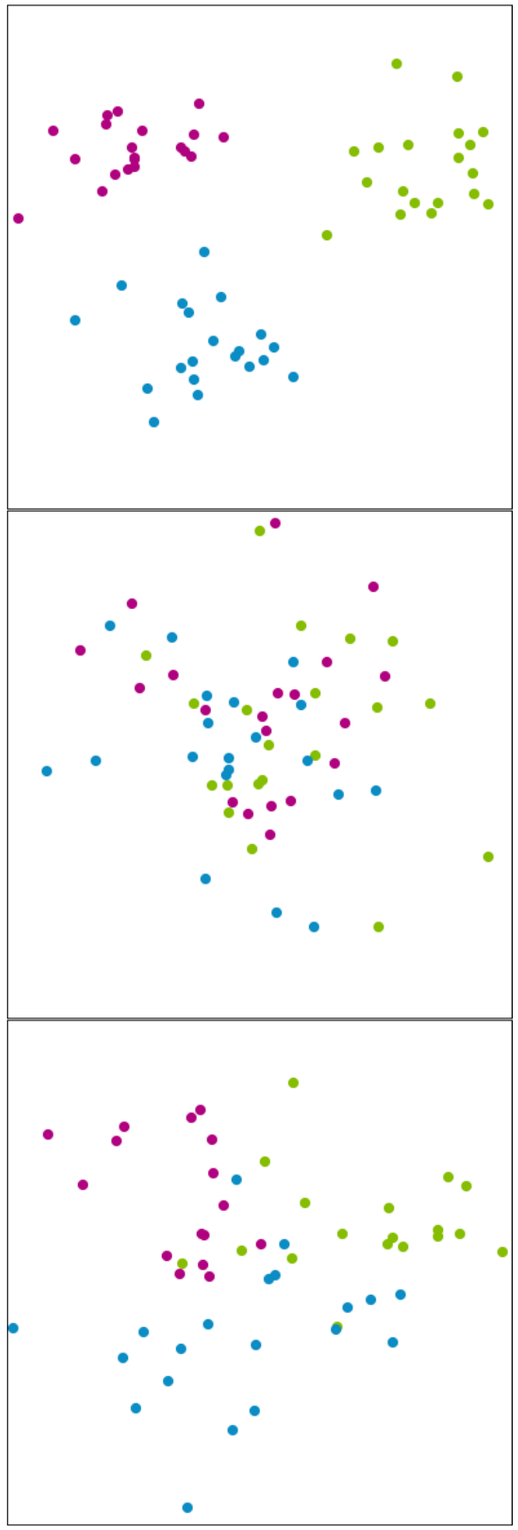
How is a cluster defined?

- In its simplest form, a cluster (on raw data) is defined by
  - The location of the ***center***
  - shape and size of the ***spread***
- An important step in defining what it means to be a cluster is
- Assign each observation x_i (doc) to cluster k (topic label) if
  - **Score** under cluster k is higher than under others
  - For simplicity, often define score as ***distance to cluster center*** (ignoring shape)



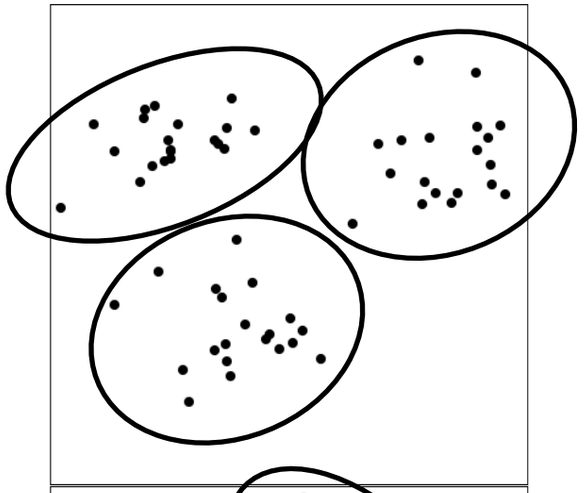
Clustering when distance of raw data captures the clusters

- Suppose the ground truth about the clusters is as follows.

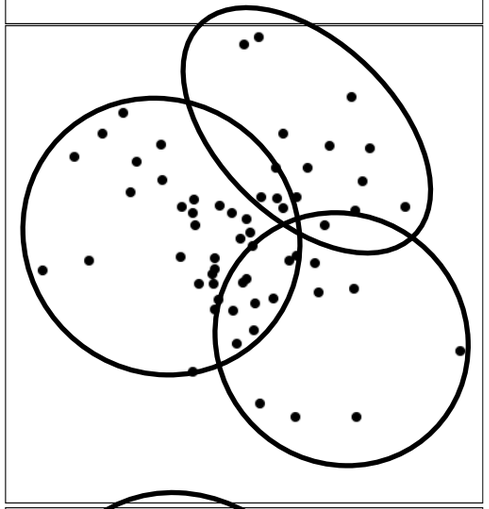


- But data we are given do not have the ground truth labels

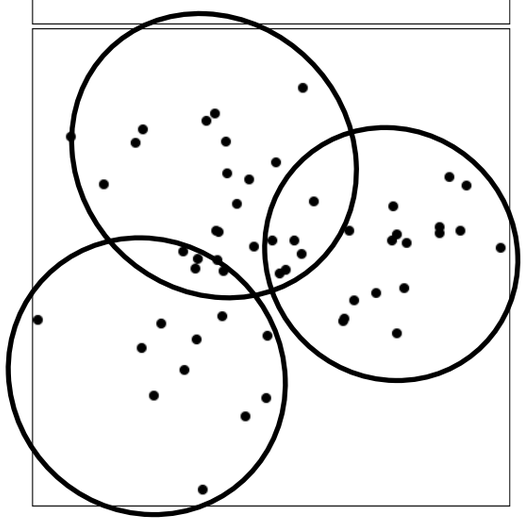
Easy



Impossible

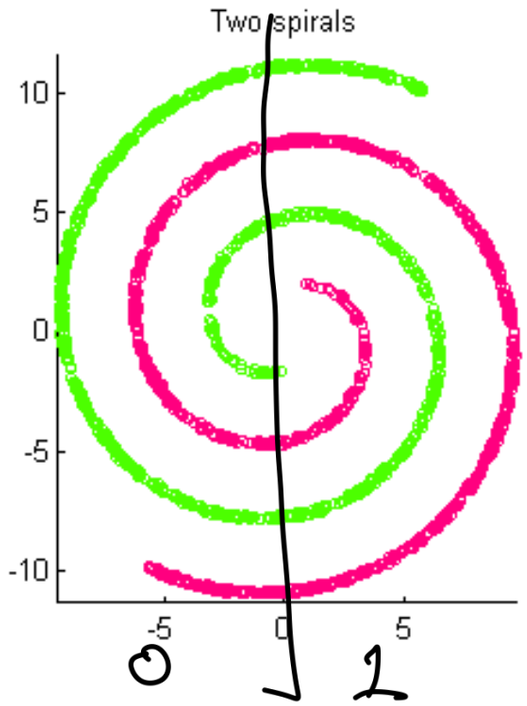


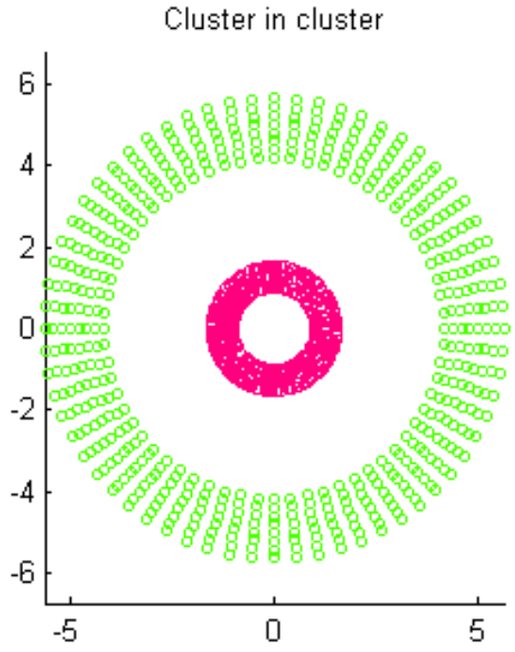
In between

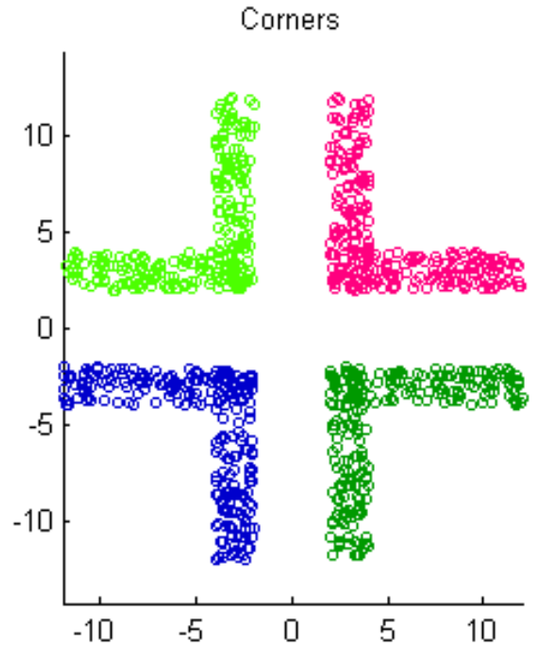


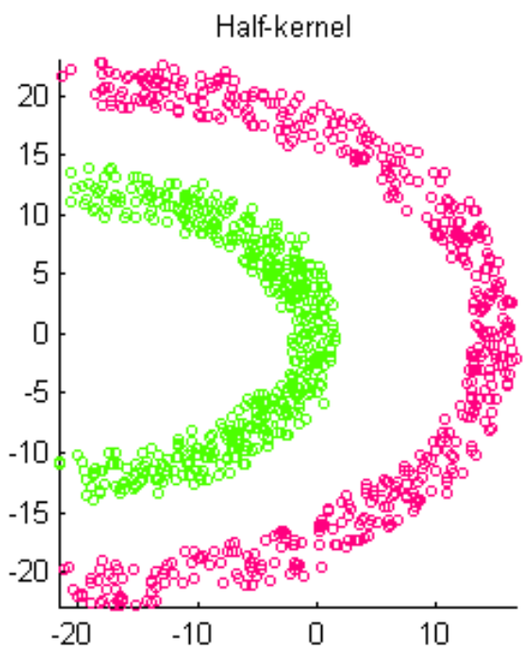
The structure we are looking for can be quite complicated

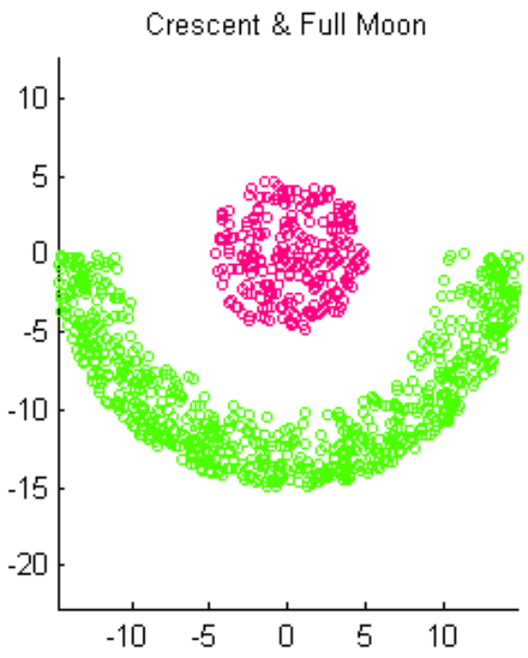
- If the distance in the raw data does not reflect cluster structure

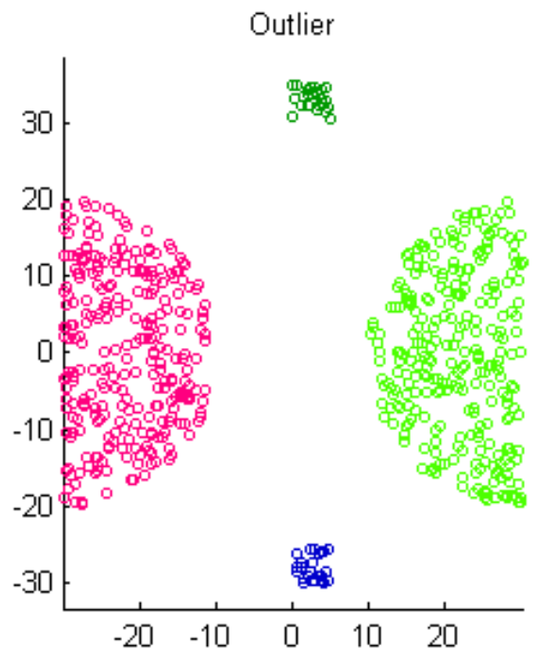


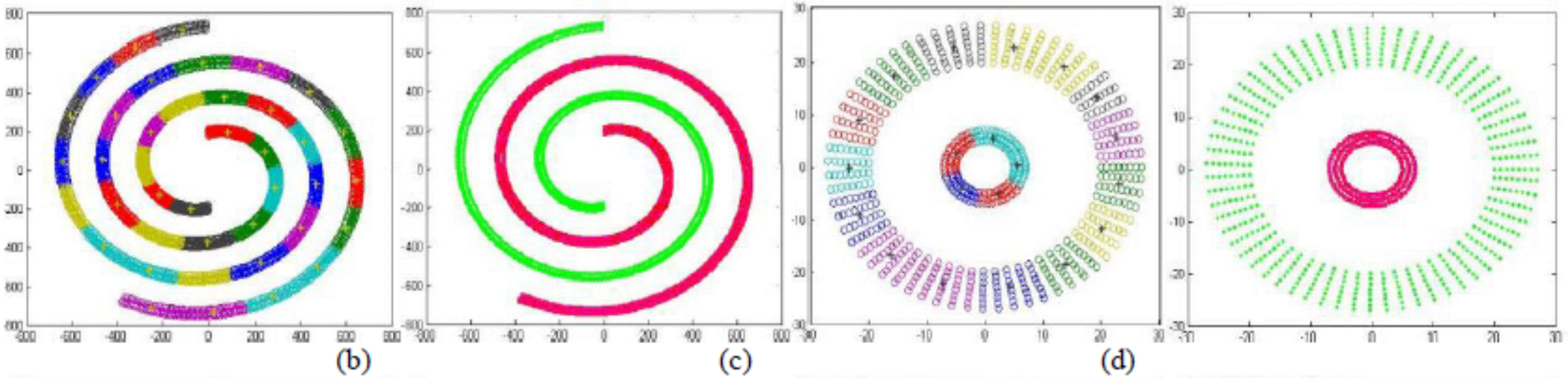




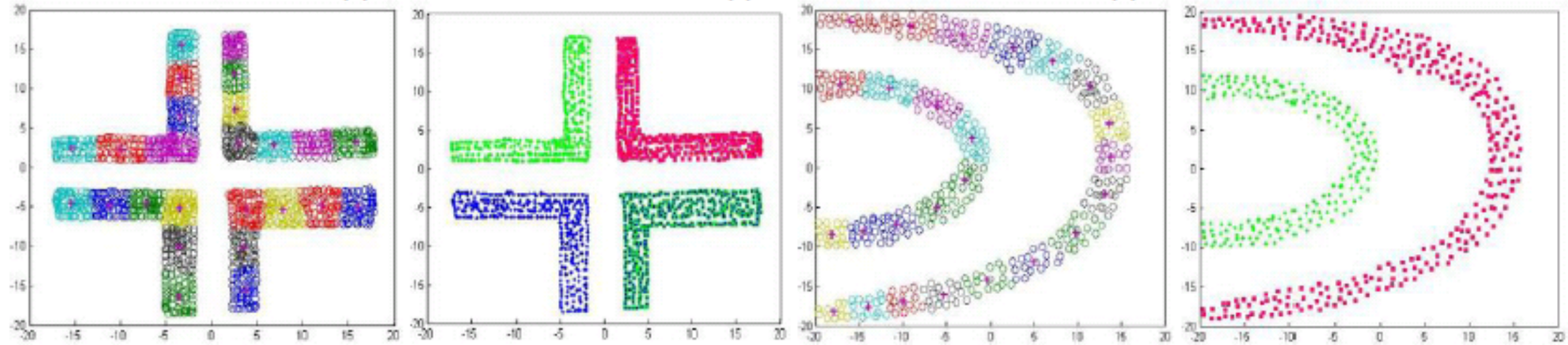




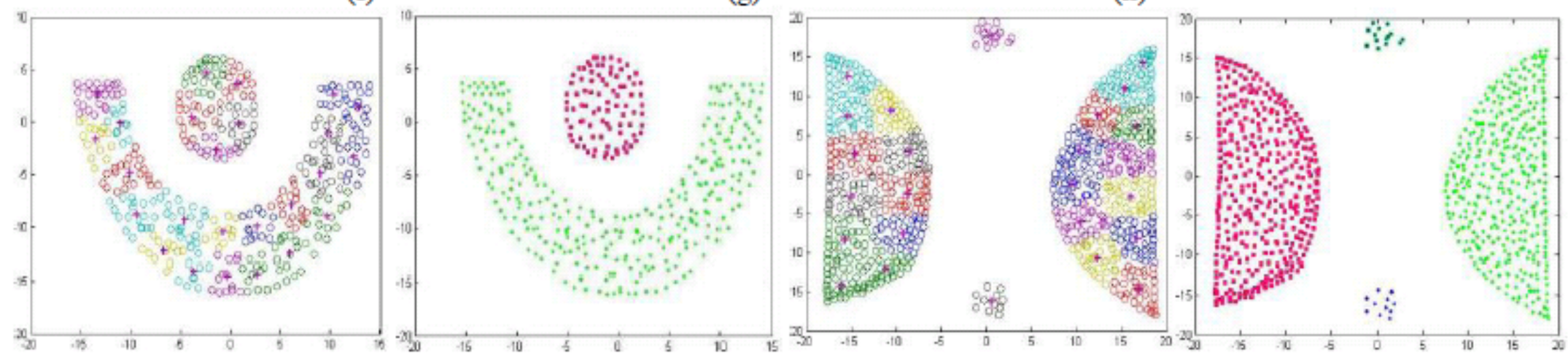




(b) (c) (d)



(f) (g) (h)

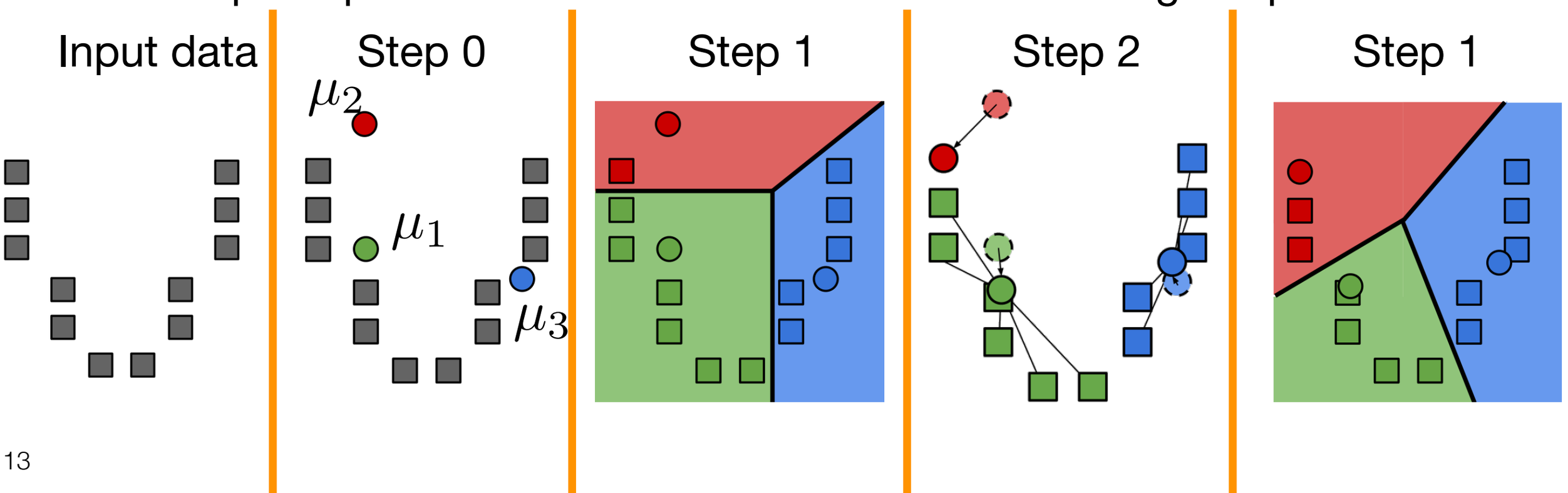


K-means clustering

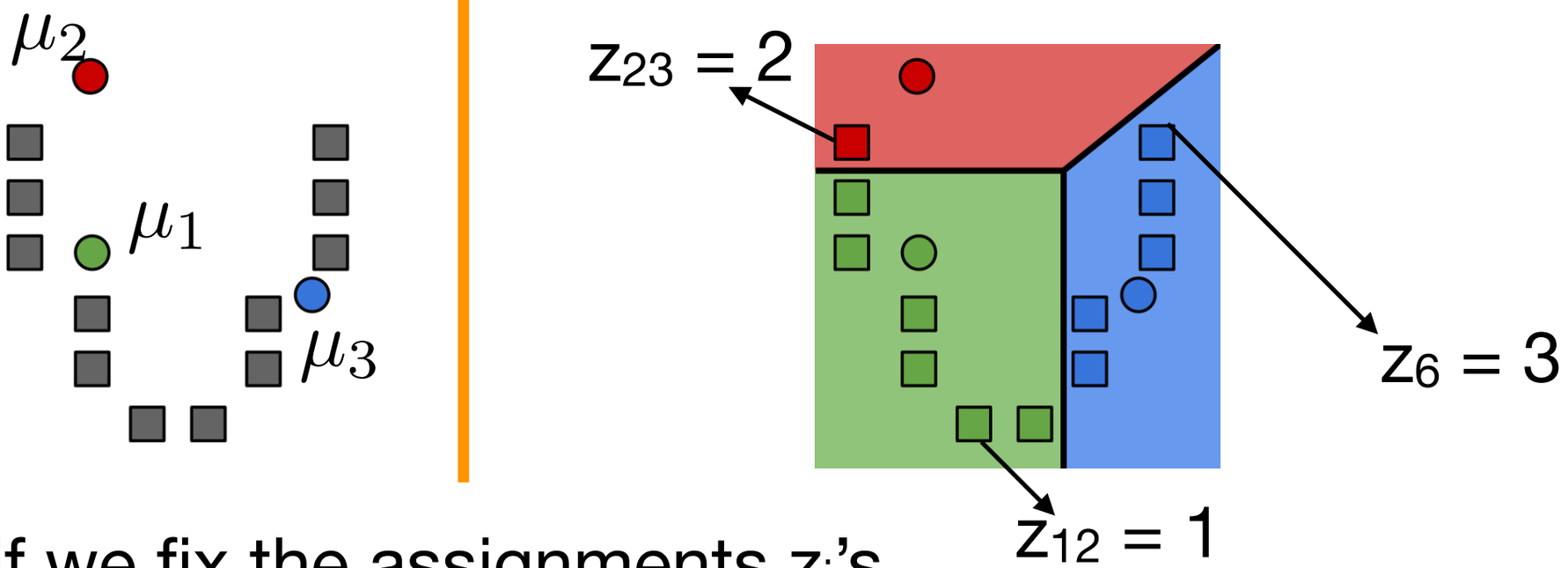
K-means algorithm

- k-means uses the **Score** between
  a data point x_i, for some ***i*** in {***1,…,N***} and
  a center μ_j, for some cluster index ***j*** in {***1,…,k***} which is
  score(x_i, μ_j) = distance (x_i, μ_j)
- Smaller score is better

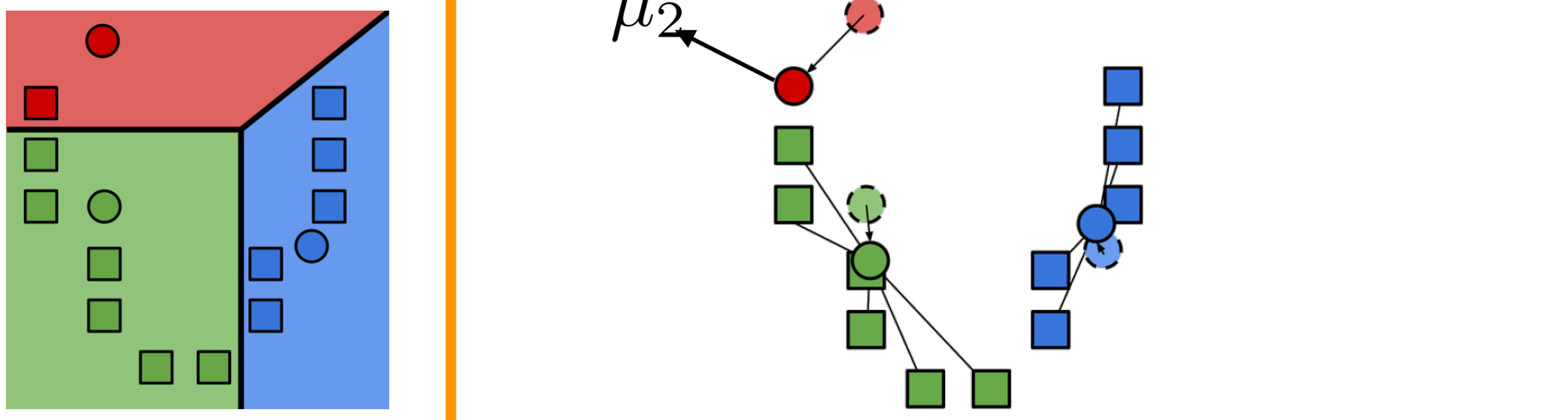
- Step 0: initialize cluster centers
- Repeat
  - Step 1: closest cluster to each **data point**
  - Step 2: update **cluster center** as the mean of assigned points



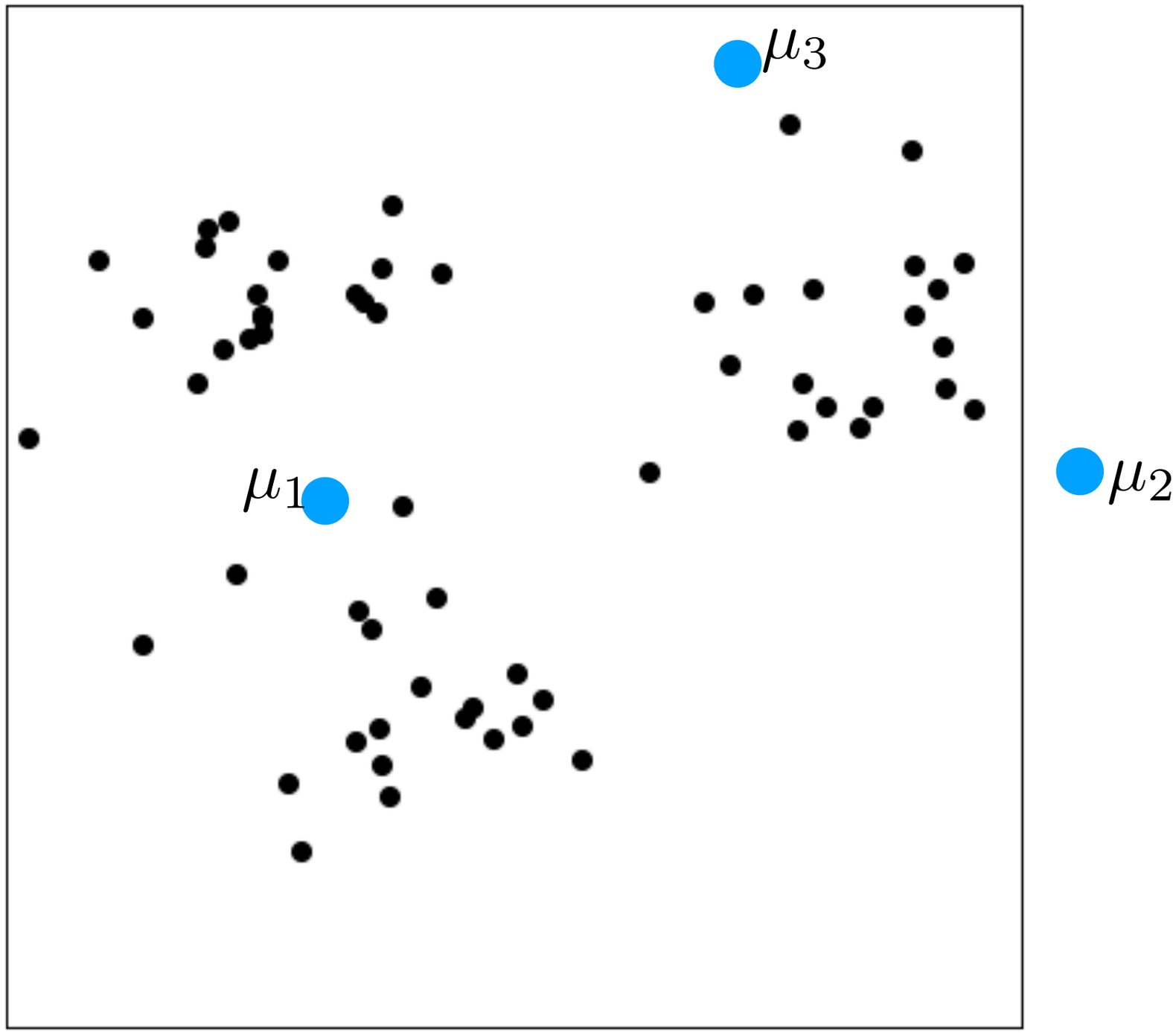
- idea: given that we use Euclidean distance as score
  - If we fix the current centers μ_j ,
    then the ***nearest neighbor clustering*** gives the best cluster assignments z_i's



- If we fix the assignments z_i's,
  then **finding center** gives the best cluster centers μ_j



K-means

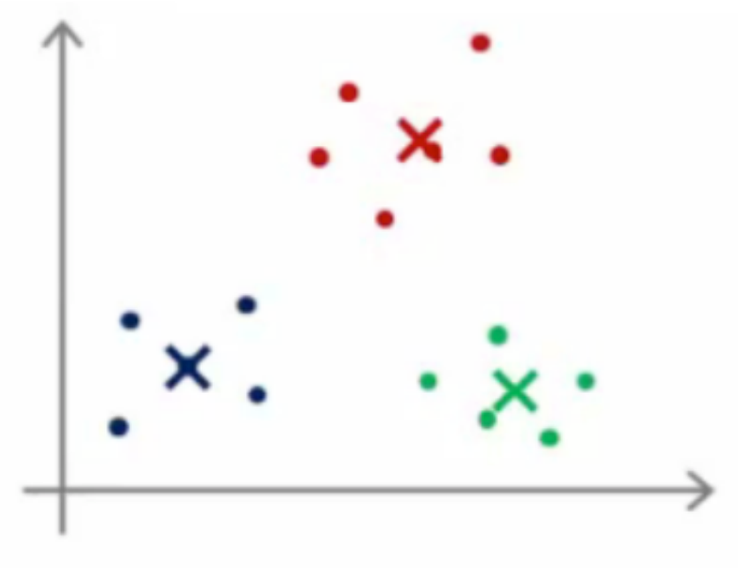


- If I give you a set of centers and assignments, can you tell if it resulted from running k-means until termination?

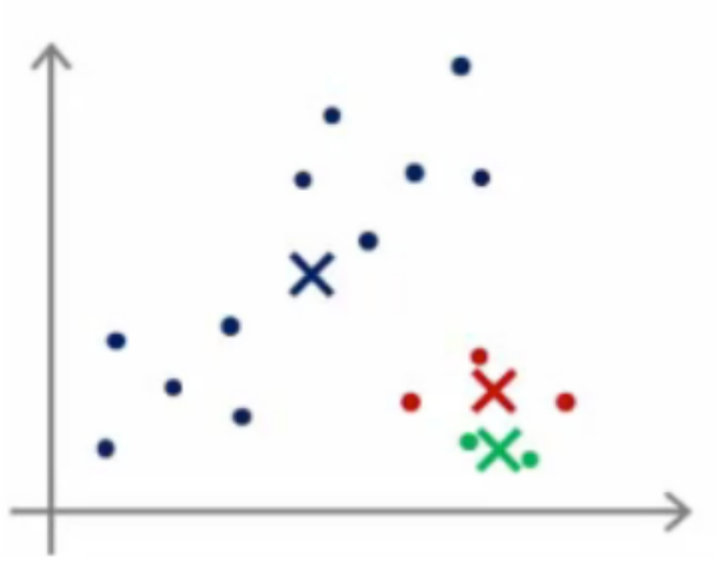
Which clustering can result from k-means?

- Can the algorithm run indefinitely? No.
- Let's say we ran k-means algorithm with some initial centers, until the center did not change any more.

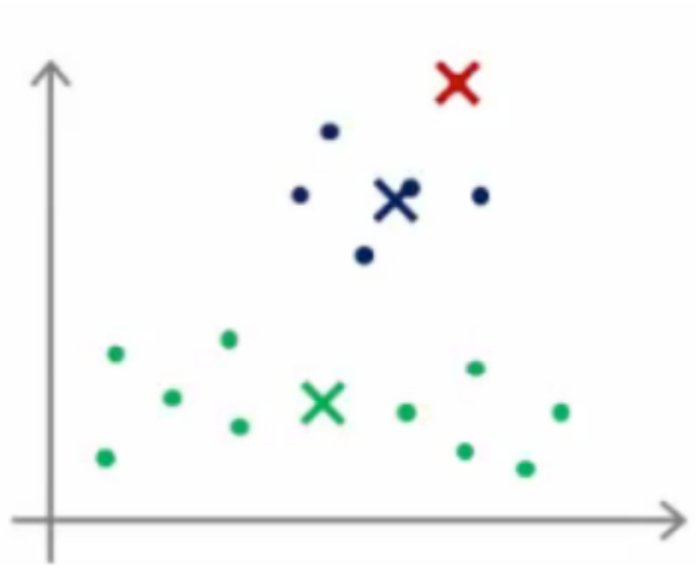
Clustering A



Clustering B



Clustering C



Convergence of k-means

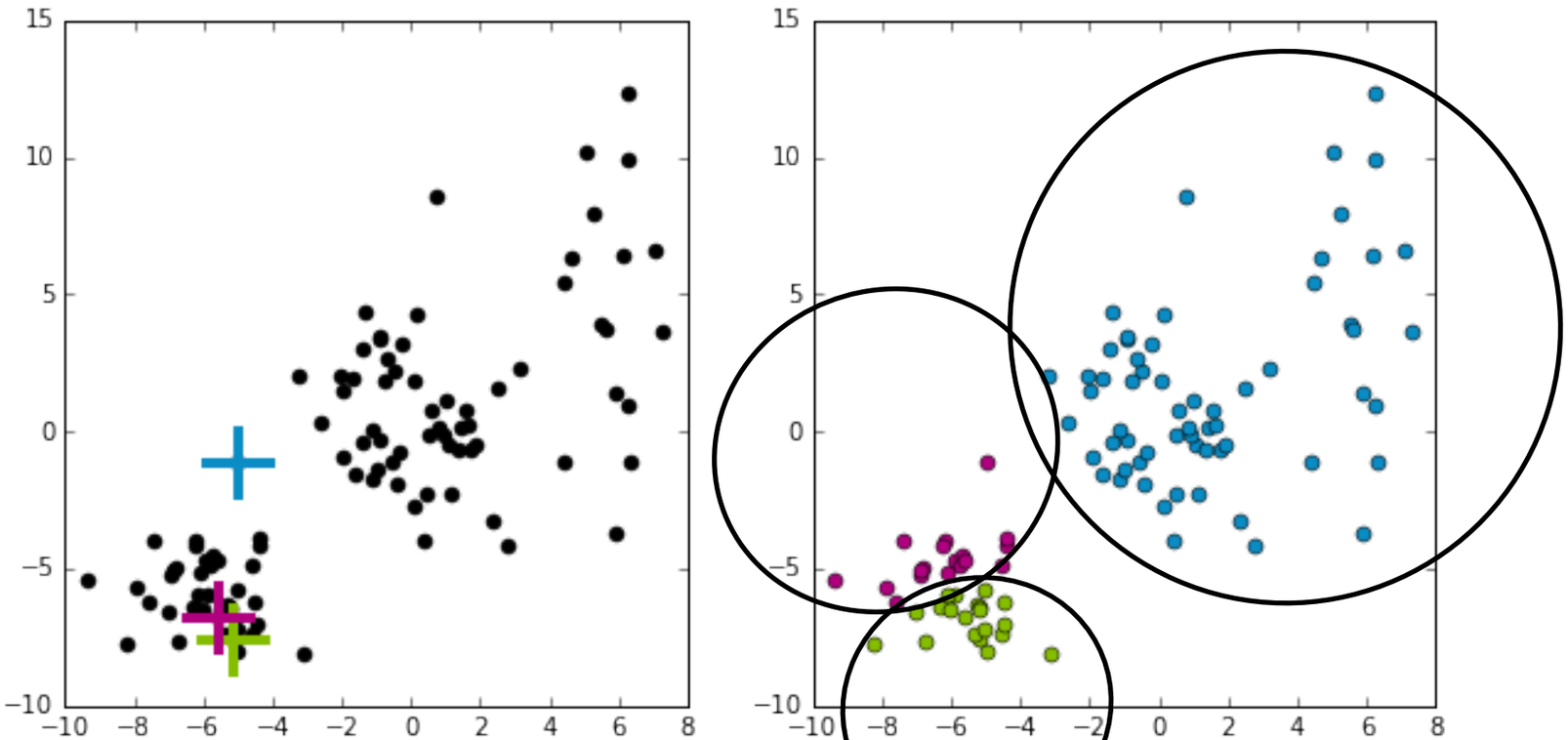
- Global optimum
- Local optimum
- Neither

Where k-mean converges, depends on the initialization

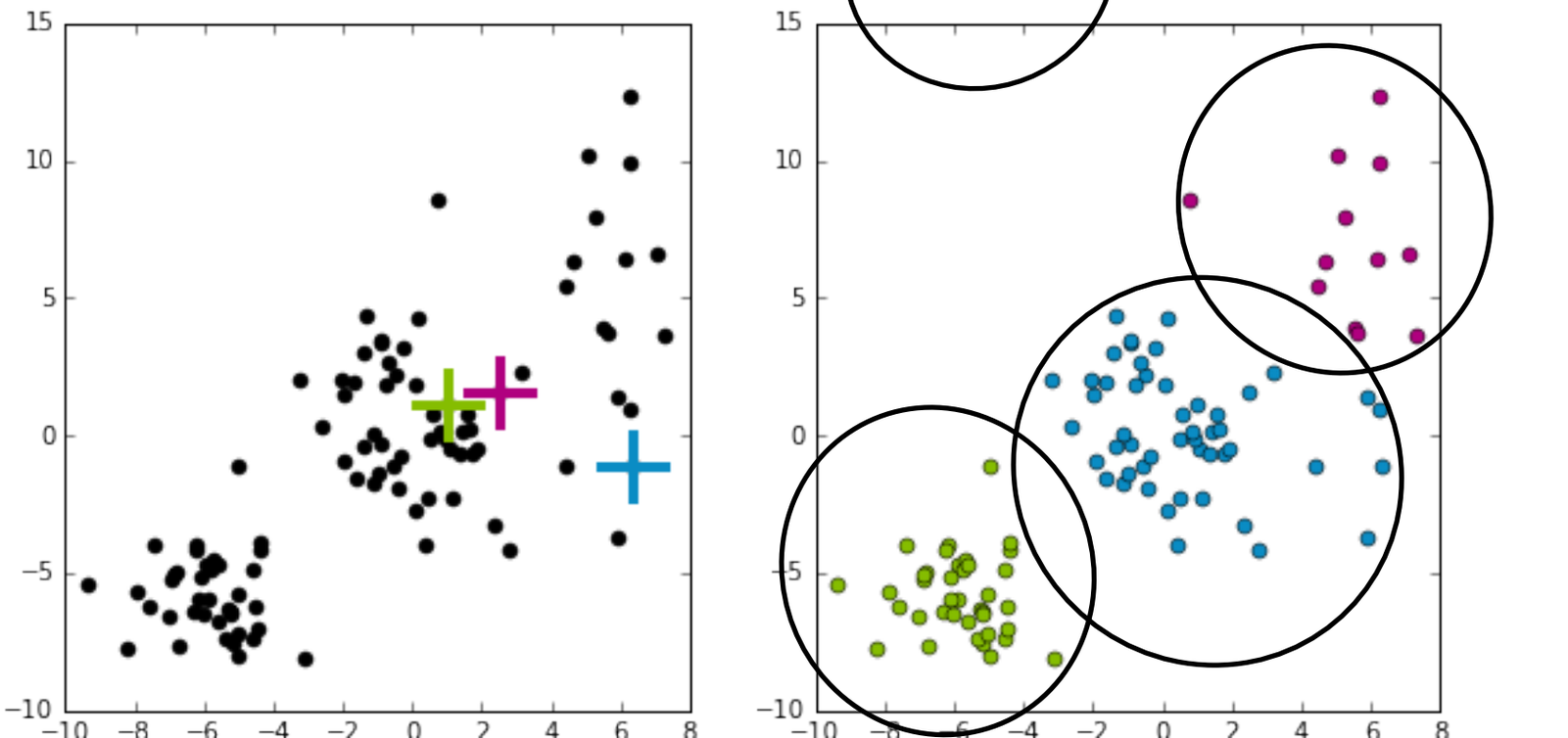
Initial position of centers

final converged assignment

Trial 1



Trial 2



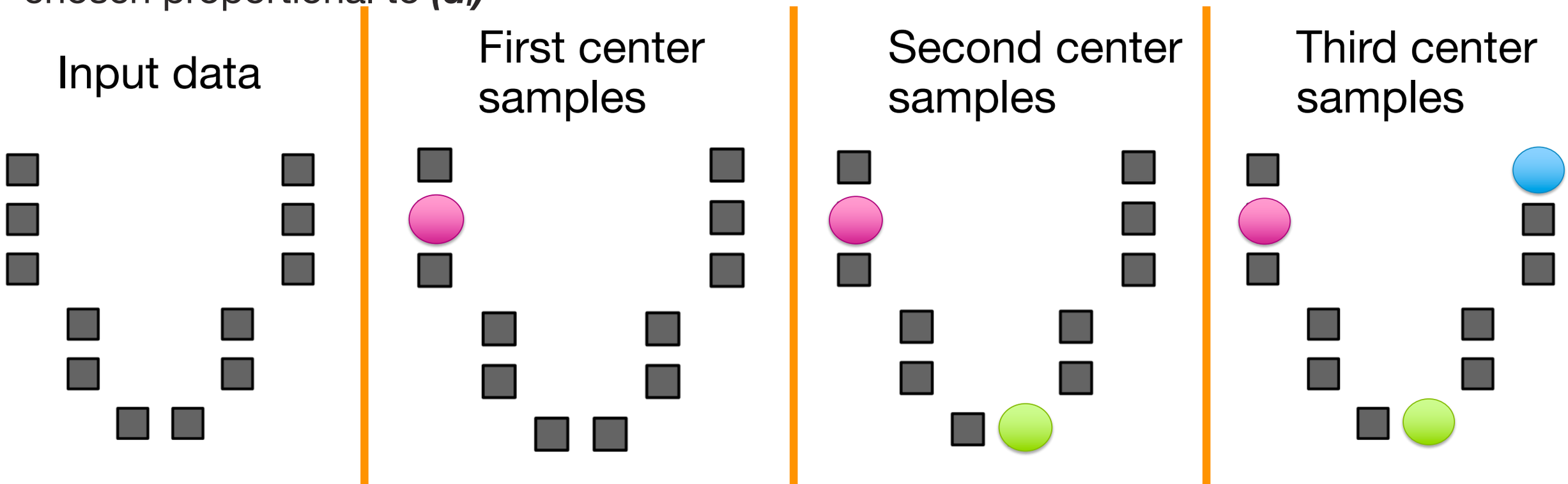
K-means ++
A smart initialization

k-means++

- Initialization of k-means algorithm is critical to quality of local optima found
- k-means++ proposes
  - Smart initialization
  - Followed by standard k-means algorithm

Smart initialization:

1. Choose first cluster center uniformly at random from data points
2. Repeat ***k*** times
   3. For each data point x_i, compute distance d_i to nearest cluster center
   4. Choose new cluster center from amongst data points, with probability of x_i being chosen proportional to $(d_i)^2$



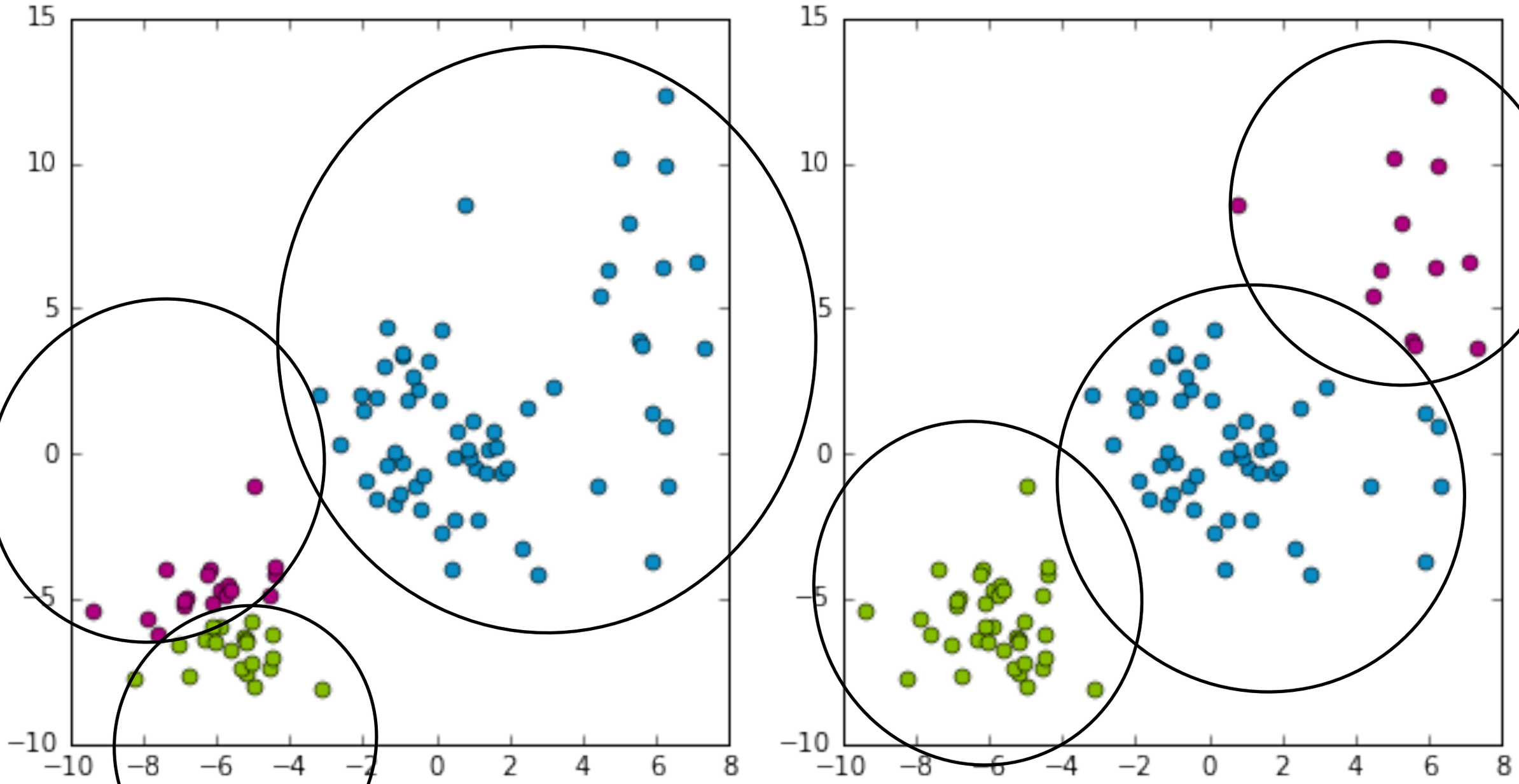
k-means++

- Compared to simple random initialization, where you pick ***k*** random data points as initial centers,
- smart initialization is computationally more costly
- But subsequent k-means algorithm converges faster

- overall, tends to find a better local optimum,
- And takes shorter time also

- insight about k-means++:
  - 1st step of randomly choosing on center tends to find one in the largest cluster, because there are more points
  - Subsequent sampling steps tend to find a center far from current centers

How do we measure which cluster is better?



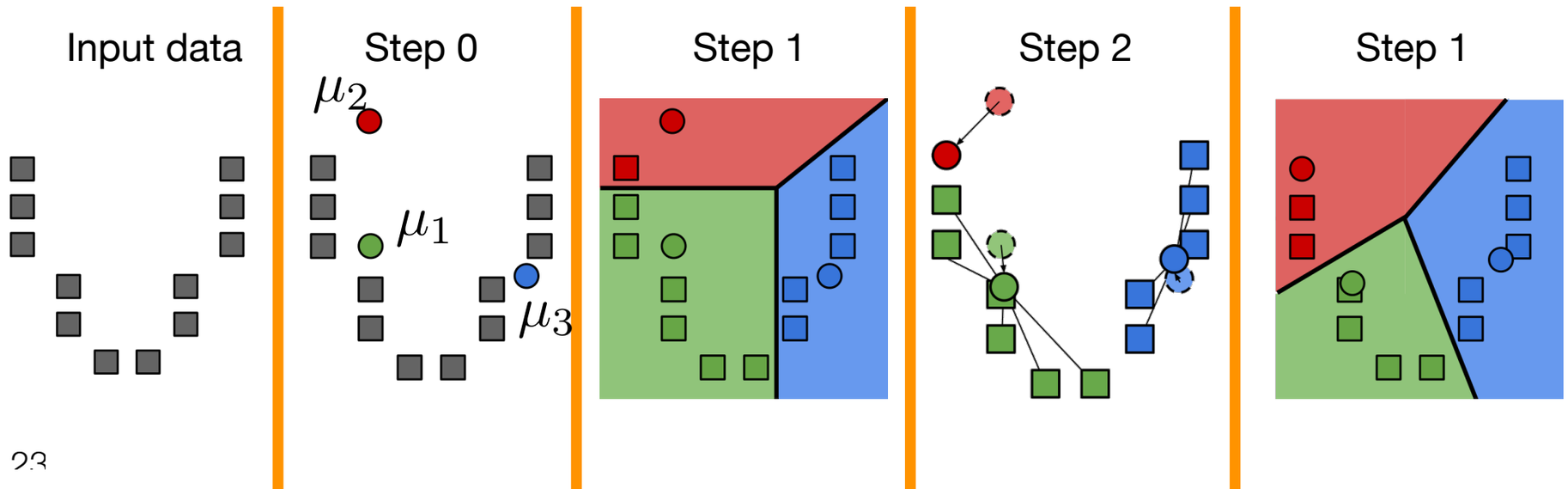
- What does k-means algorithm assume is a better cluster?
- k-means is one way of minimizing $\sum_{j=1}^{k} \sum_{i:z_i=j} ||\mu_j - \mathbf{x}_i||_2^2$

  which is how much you pay for **heterogeneity**

K-means as coordinate descent

$$\min_{\mu_1,\ldots,\mu_k,z_1,\ldots,z_N} \sum_{j=1}^{k} \sum_{i:z_i=j} \|\mu_j - x_i\|_2^2$$

- k-means
  - Start with random initialization of the centers (chosen from the data points)
  - Repeat
    - Fix centers and find optimal assignments (z_i's)
    - Fix assignments and find optimal centers (μ_j's)
- Note that we make the objective **strictly** smaller every step
- The algorithm converges in finite time



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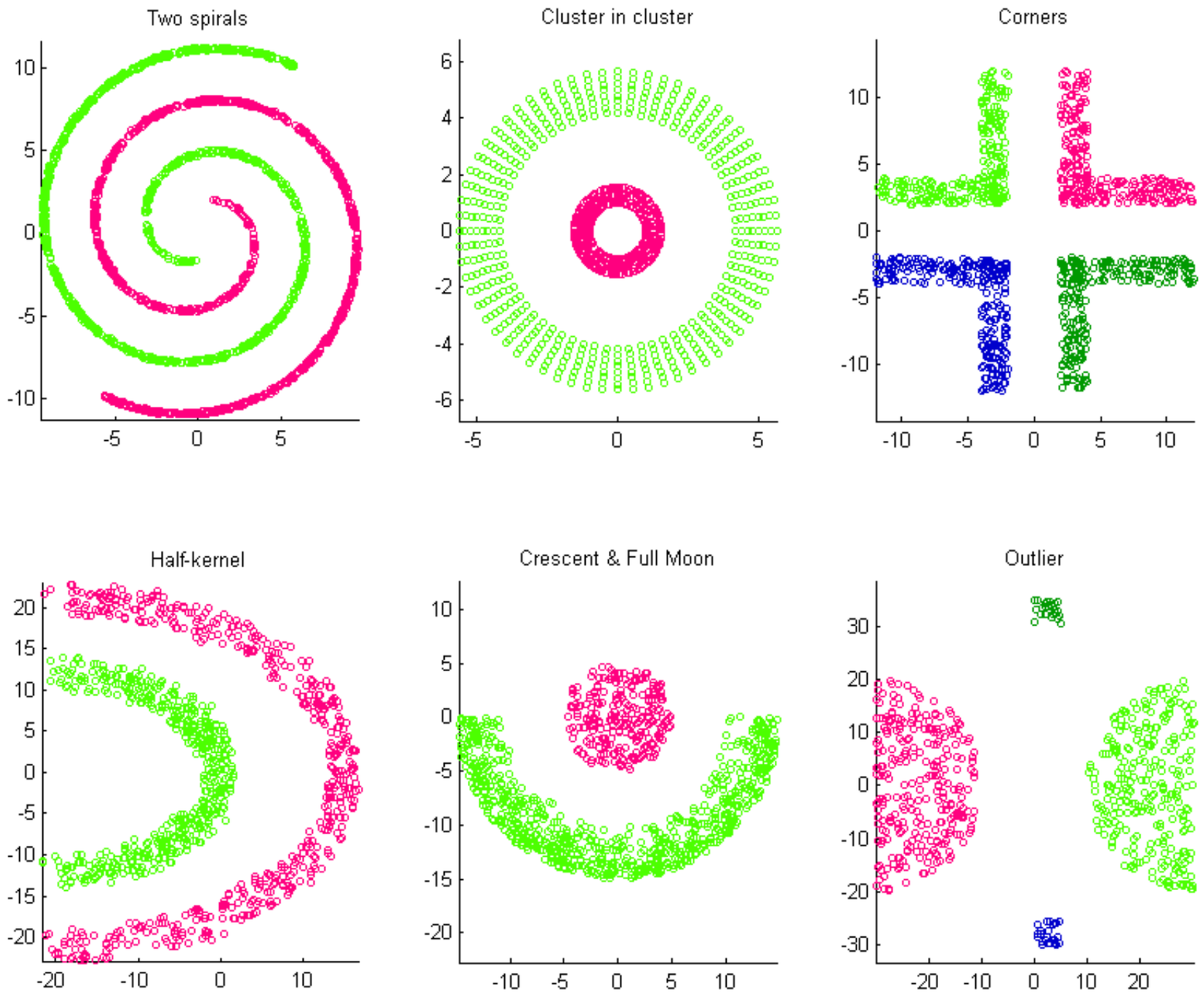
Is this the best measure of clustering error?

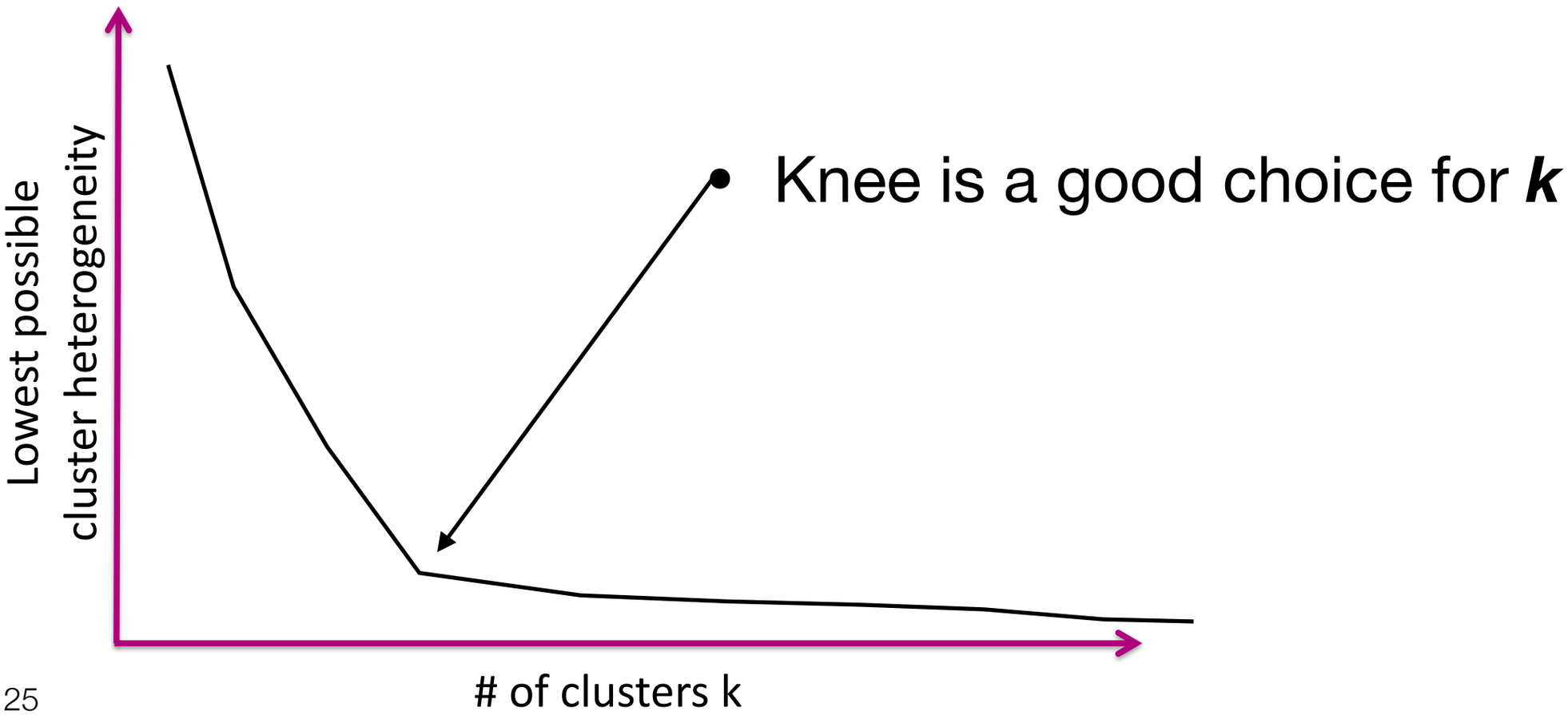
$$\min_{\mu_1,\ldots,\mu_k,z_1,\ldots,z_N} \sum_{j=1}^{k} \sum_{i:z_i=j} \|\mu_j - x_i\|_2^2$$



What *k* should we use?

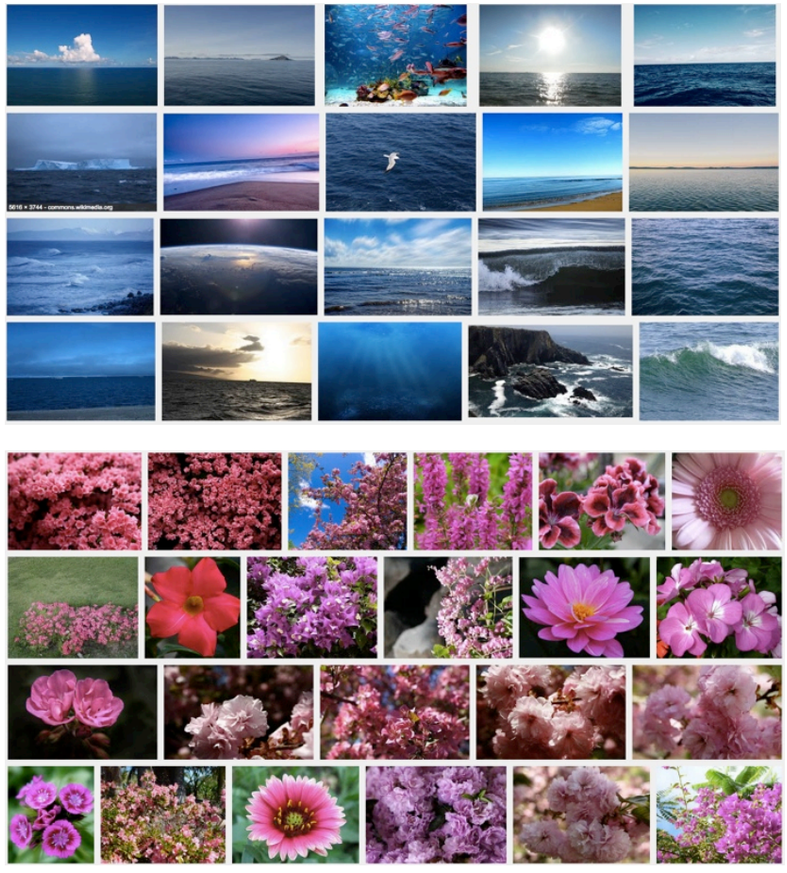
- Increasing ***k*** eventually overfits.

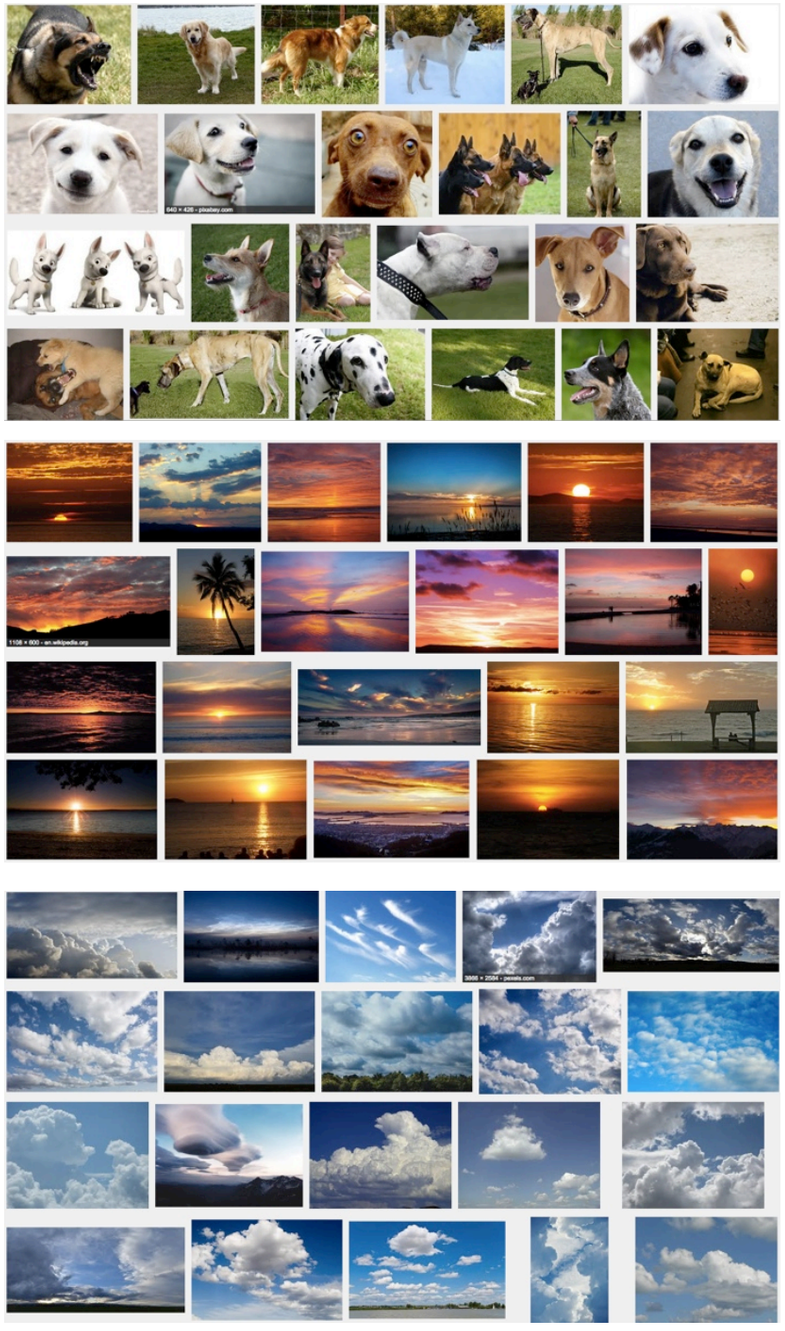
- One extreme, when ***k=N***
  - Each data point is its own cluster
  - Heterogeneity is zero, and we get the best score under k-means



Real world examples

- For search, group as:
  - Ocean
  - Pink flower
  - Dog
  - Sunset
  - Clouds
  - …



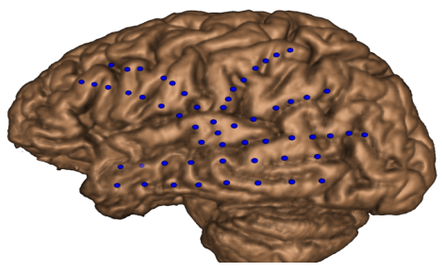


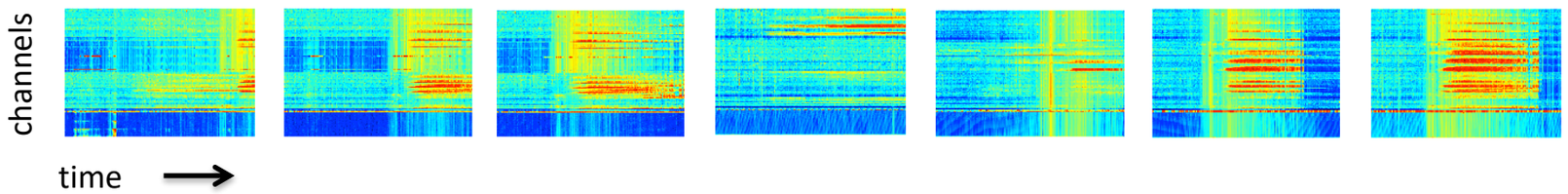
Structuring web search results

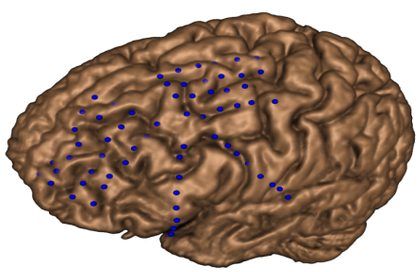
- Search terms can have multiple meanings
- Example: “cardinal”

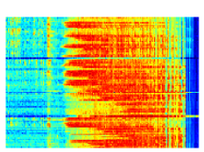
- Use clustering to structure output

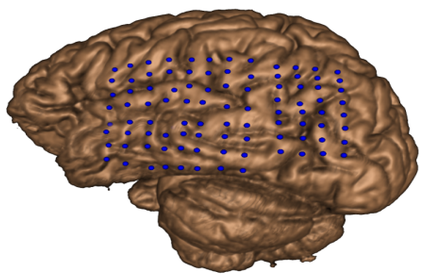
- You can use it to partition patients based on medical condition, to be used in more targeted studies
- Combinations of patients and seizures are diverse

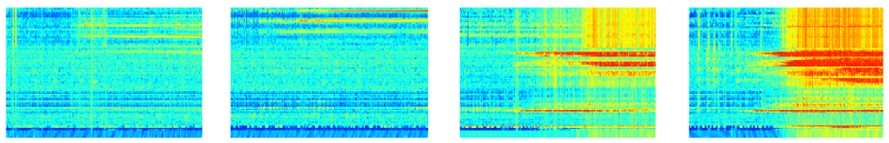






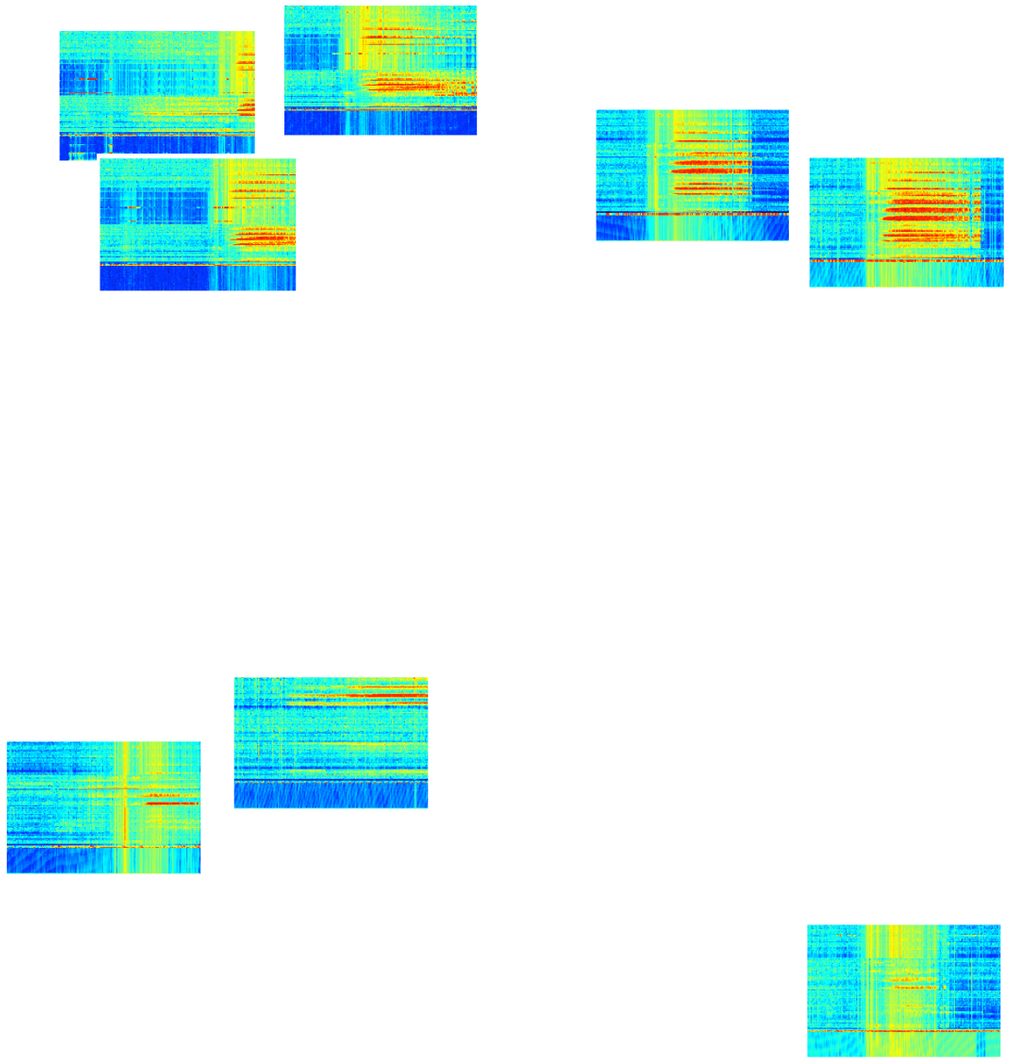






- The electrode placement is unique in each patient
- Each patient has a different number of seizures that themselves often display quite different dynamics within each seizure
- the thumbprint of each seizure with a colored box shows how a particular feature changes in each channel over the course of the seizure.

- We can place these observed signal in lower dimensional space according to their clusters, which provides important visualization and insights that can be used following clinical decisions and studies



Amazon

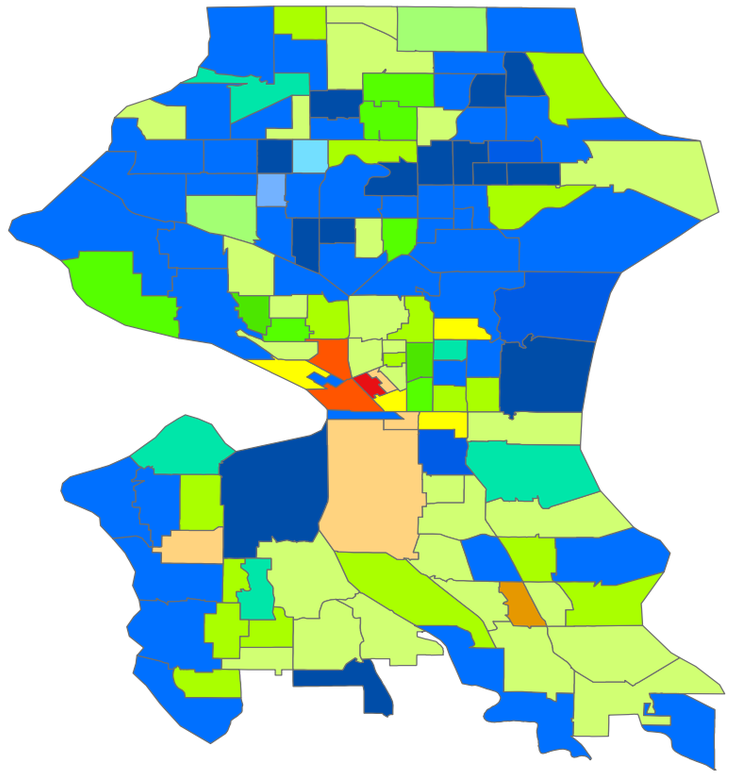
- Discover product categories from purchase histories

~~"furniture"~~
"baby"

- Or discovering groups of users

Discover similar neighborhoods

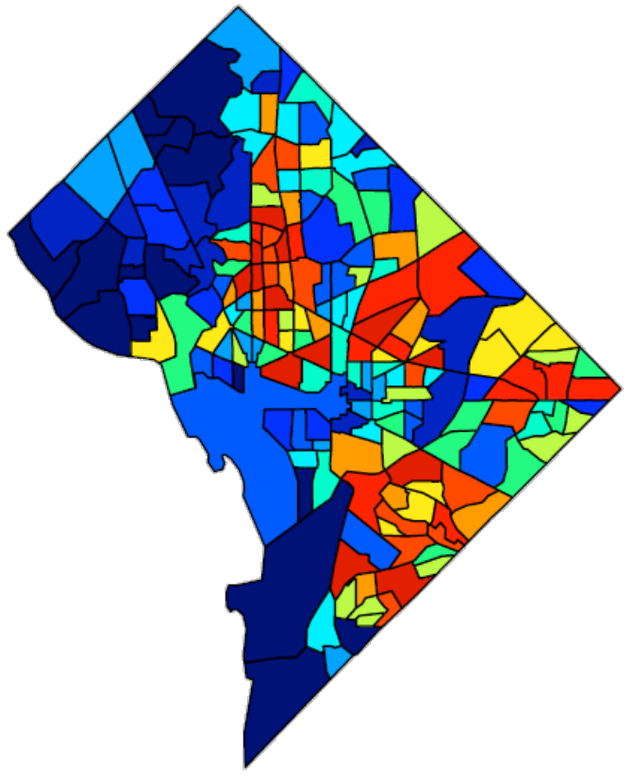
- Task 1: Estimate price at a small regional level
- Challenge:
  - Only a few (or no!) sales in each region per month
- Solution:
  - Cluster regions with similar trends and share information within a cluster



City of Seattle

Discover similar neighborhoods

- Task 2: Forecast violent crimes to better task police
- Again, cluster regions and share information!
- Leads to improved predictions compared to examining each region independently

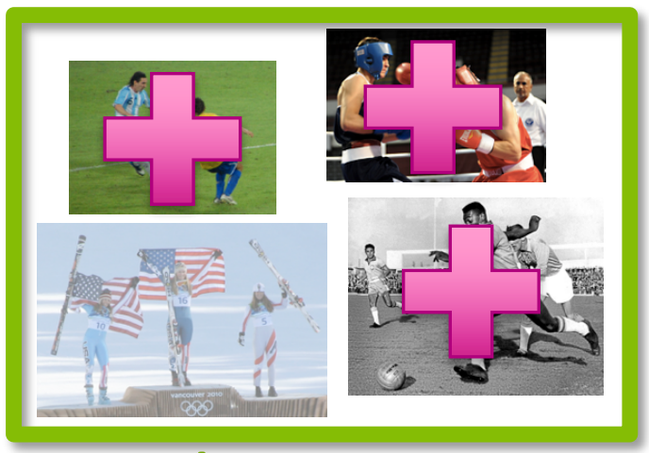


Washington, DC

Limitations and failure modes of k-means

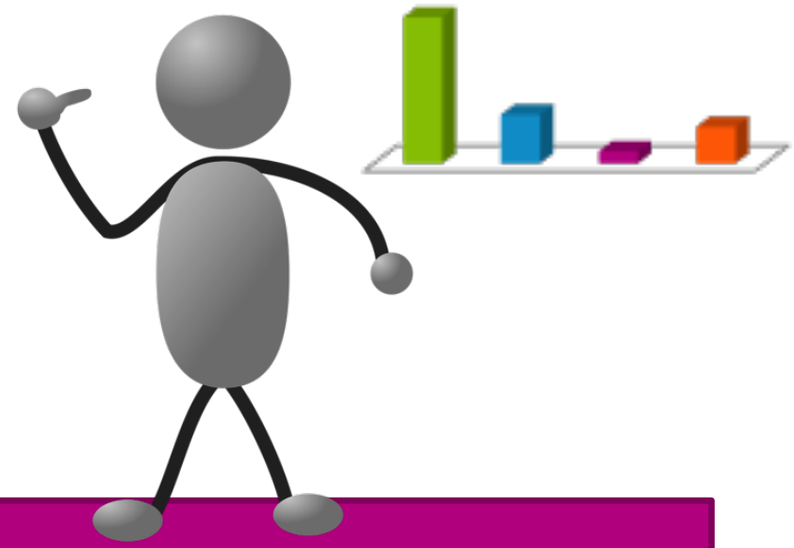
Learning user preferences

Set of clustered documents read by user



Cluster 1

Cluster 2



Use feedback to learn user preferences over topics

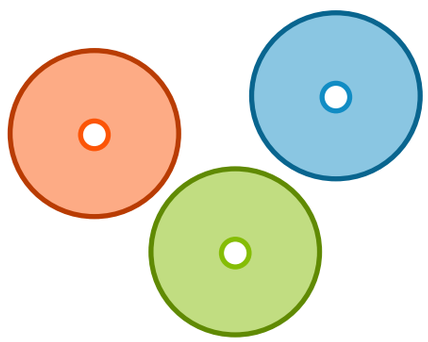
Cluster 3

Cluster 4

- In reality, articles are not about just one topic
- HARD clustering misses nuanced soft membership

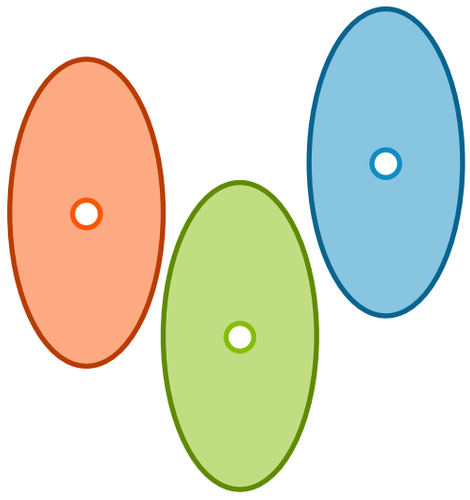
Shapes of the clusters

- K-means algorithm is essentially fitting or assuming spherically symmetric clusters
  because we use Euclidean distance, and
  all points at the same Euclidean distance are paying the same cost

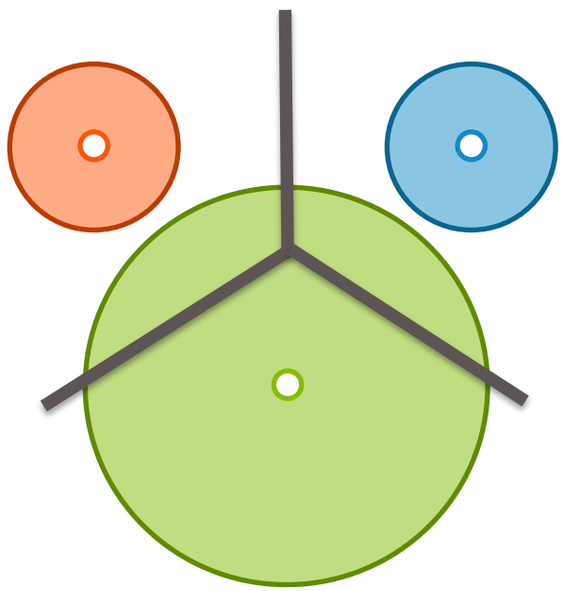


$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

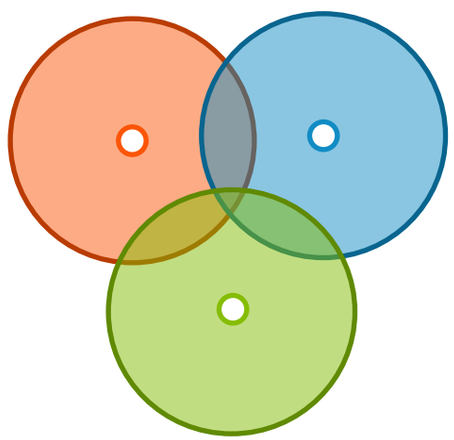
- How can we resolver this? Use wighted Euclidean distance



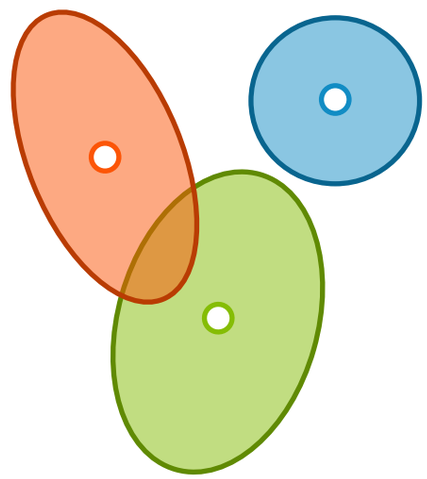
Typical failure modes



disparate cluster sizes



overlapping clusters



different shaped/oriented clusters

•Provides soft assignments of observations to clusters (uncertainty in assignment)

−e.g., 54% chance document is world news, 45% science, 1% sports, and 0% entertainment

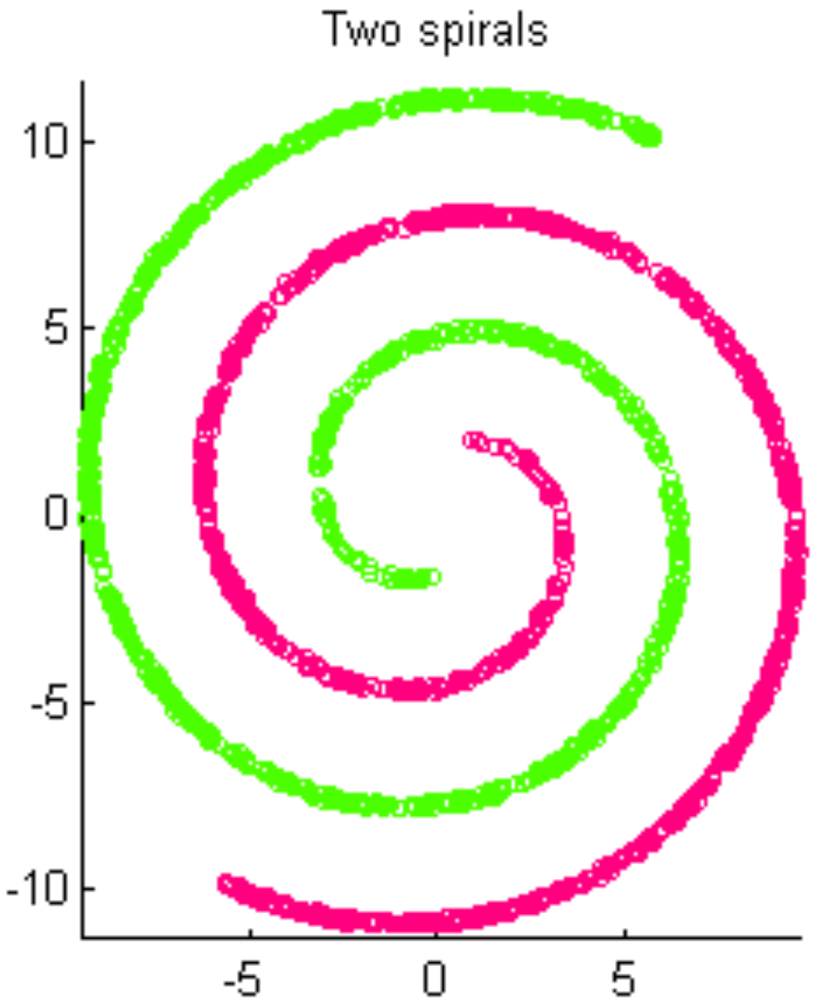
•Accounts for cluster shapes not just centers

•Enables learning weightings of dimensions

−e.g., how much to weight each word in the vocabulary when computing cluster assignment

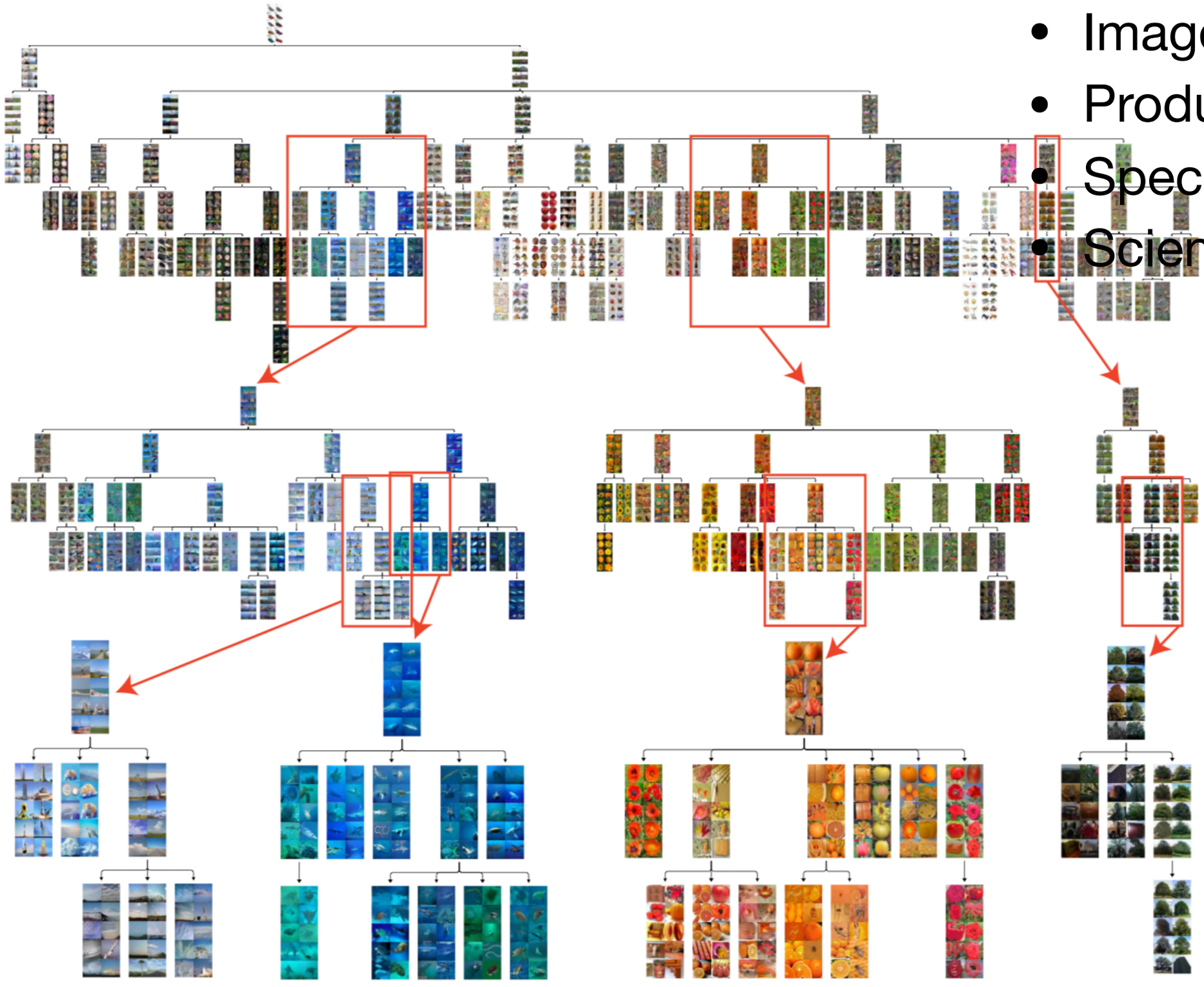
Diffusion maps

- Non-linear dimensionality reduction
-



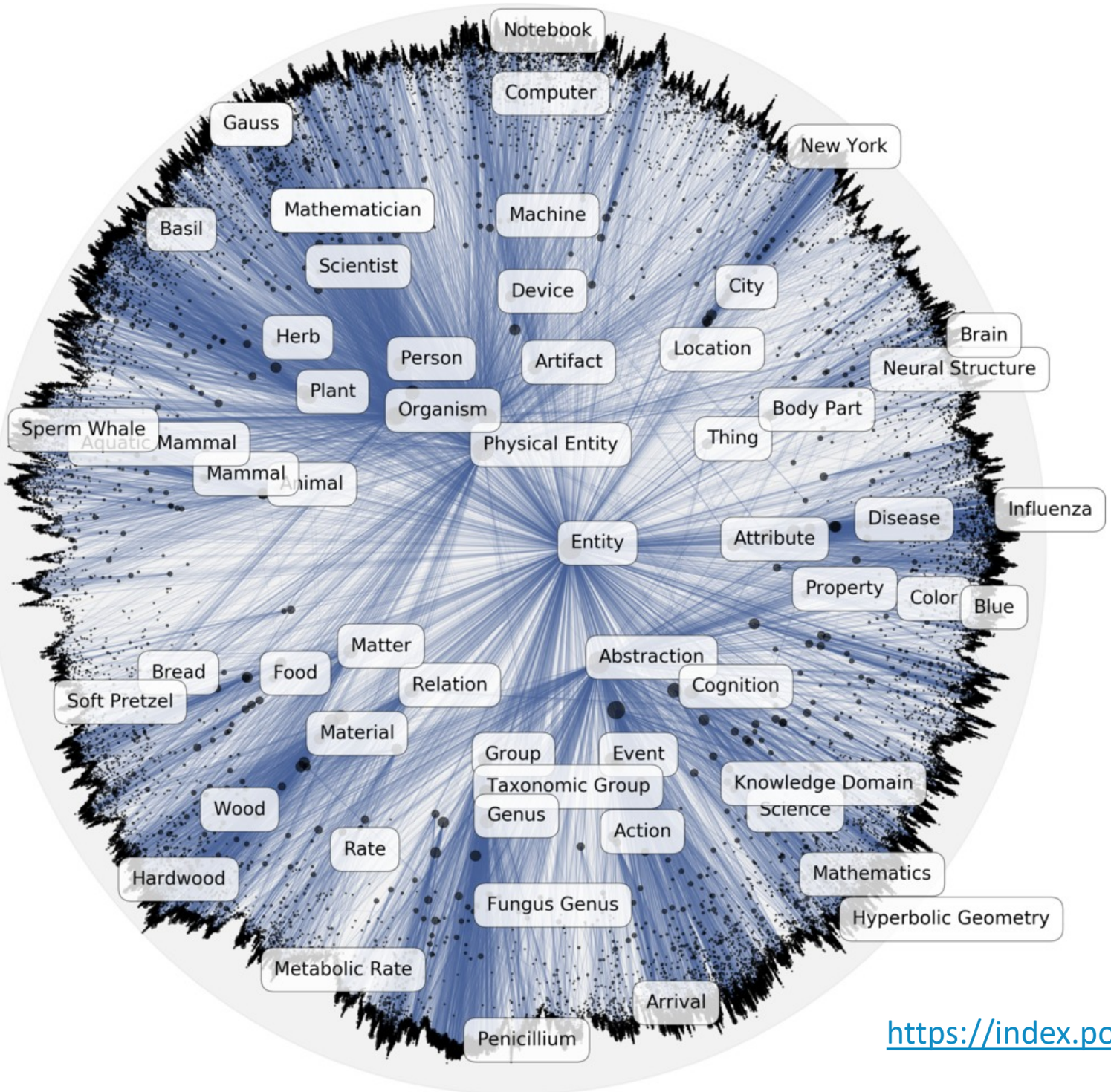
Hierarchical clustering

Lots of data are hierarchical in nature



- Image types
- Product categories
- Species
- Scientific concepts

- Nouns



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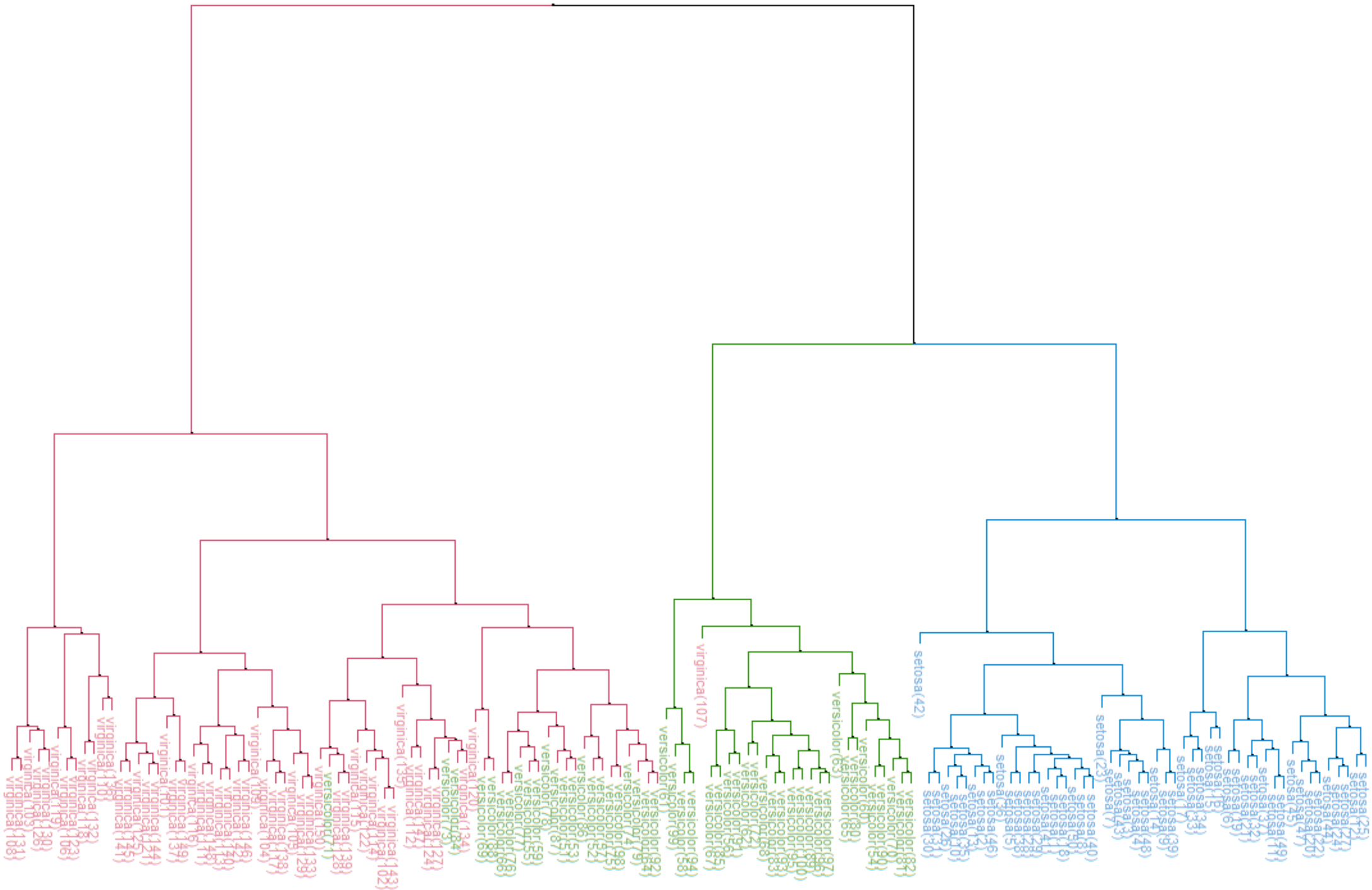
- Species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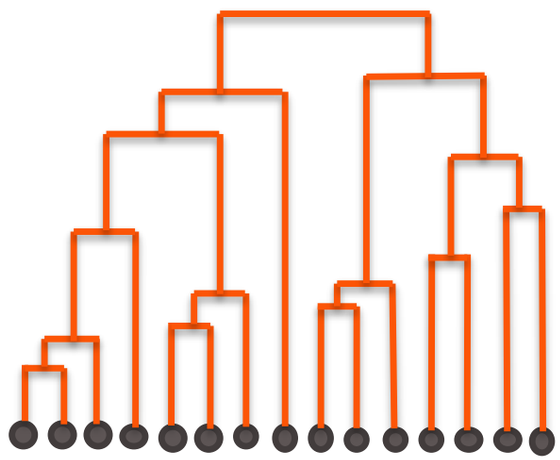
Other motivations for hierarchical clustering

- Avoid choosing # clusters beforehand

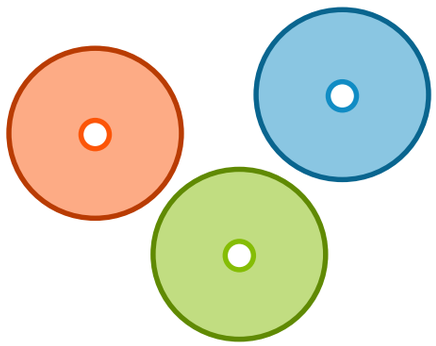
- Dendrograms help visualize different clustering granularities
  - No need to rerun algorithm



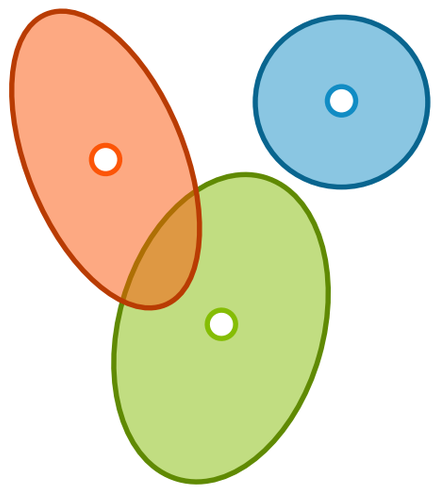
- Most algorithms allow user to choose any distance metric
  - k-means restricted us to Euclidean distance

Can often find more complex shapes than k-means or Gaussian mixture models

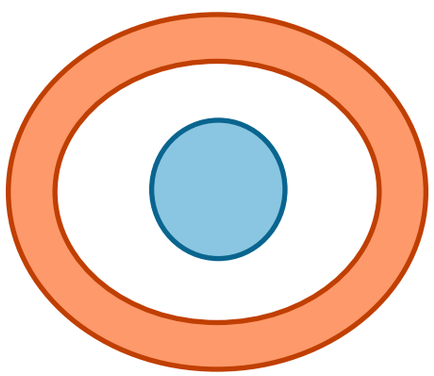
k-means: spherical clusters

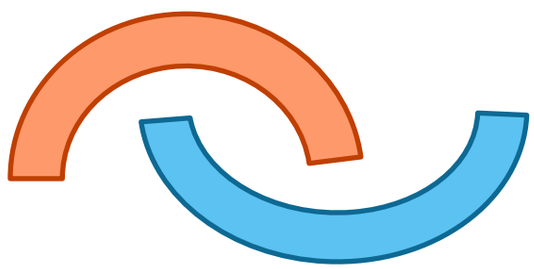


Gaussian mixtures: ellipsoids



What about these?





Two-types of apporaches

Divisive, *a.k.a. top-down:* Start with all data in one big cluster and recursively split.

–Example: recursive k-means

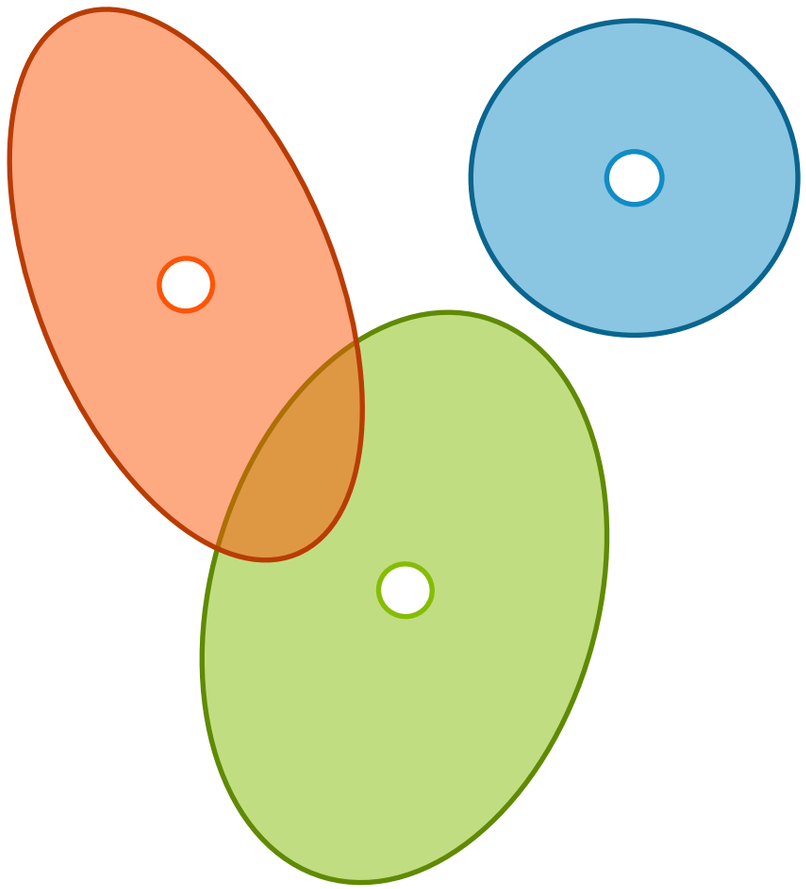
Agglomerative *a.k.a. bottom-up*: Start with each data point as its own cluster. Merge clusters until all points are in one big cluster.

–Example: single linkage

Divisive clustering

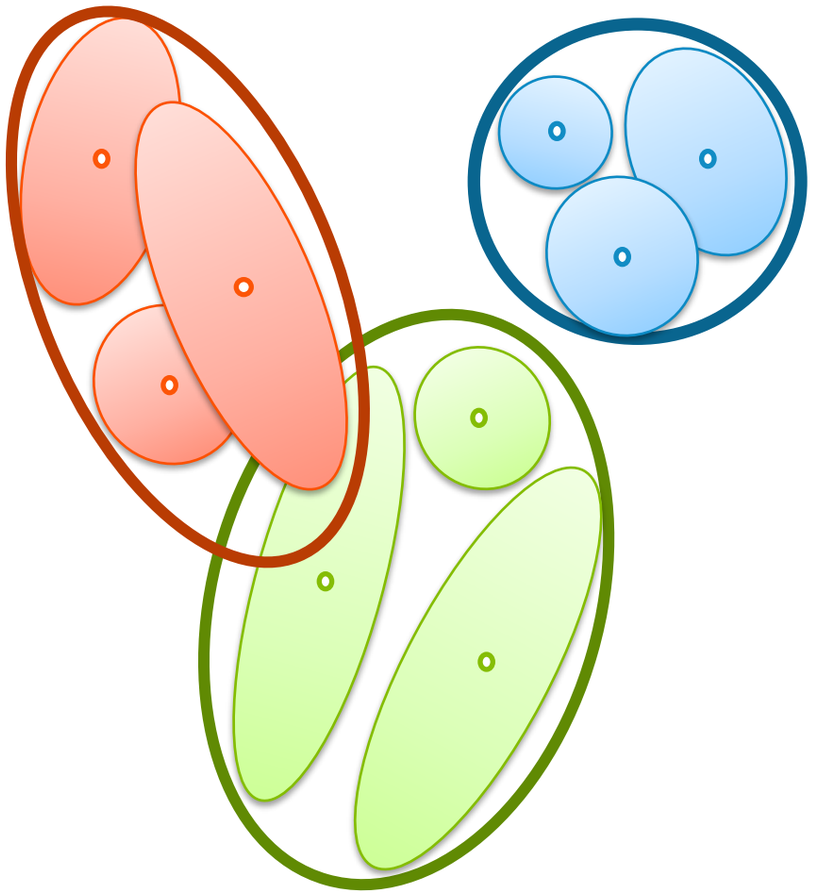
Divisive in pictures – level 1

- Cluster all the data into, say, 3 clusters first



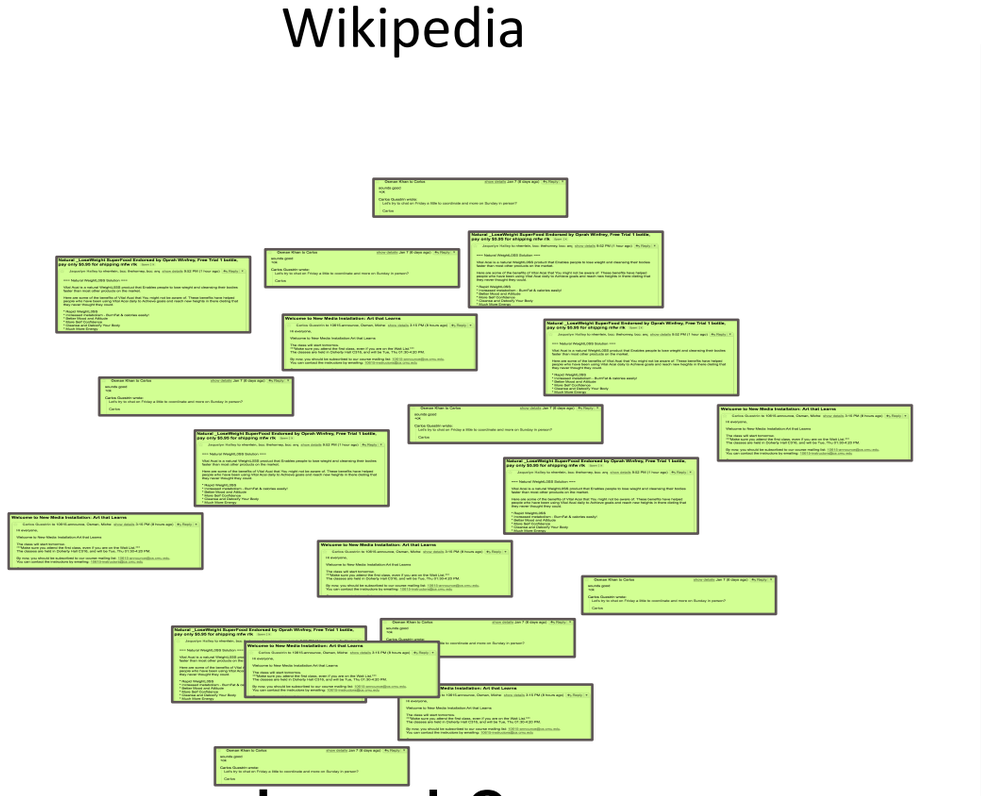
Divisive in pictures – level 2

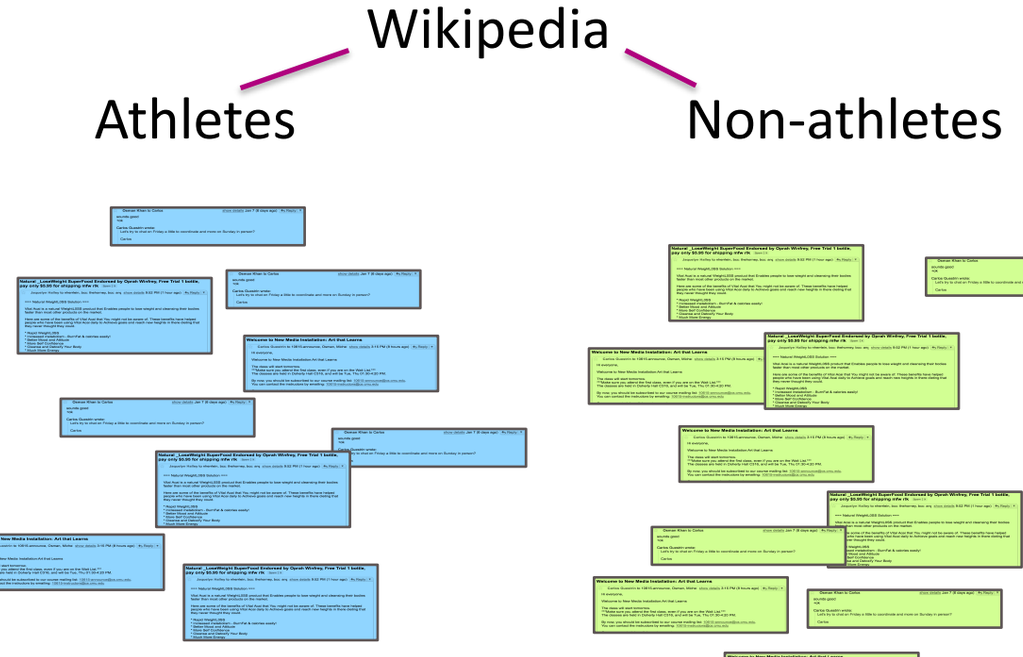
- For data in each cluster, run a new clustering algorithm of choice

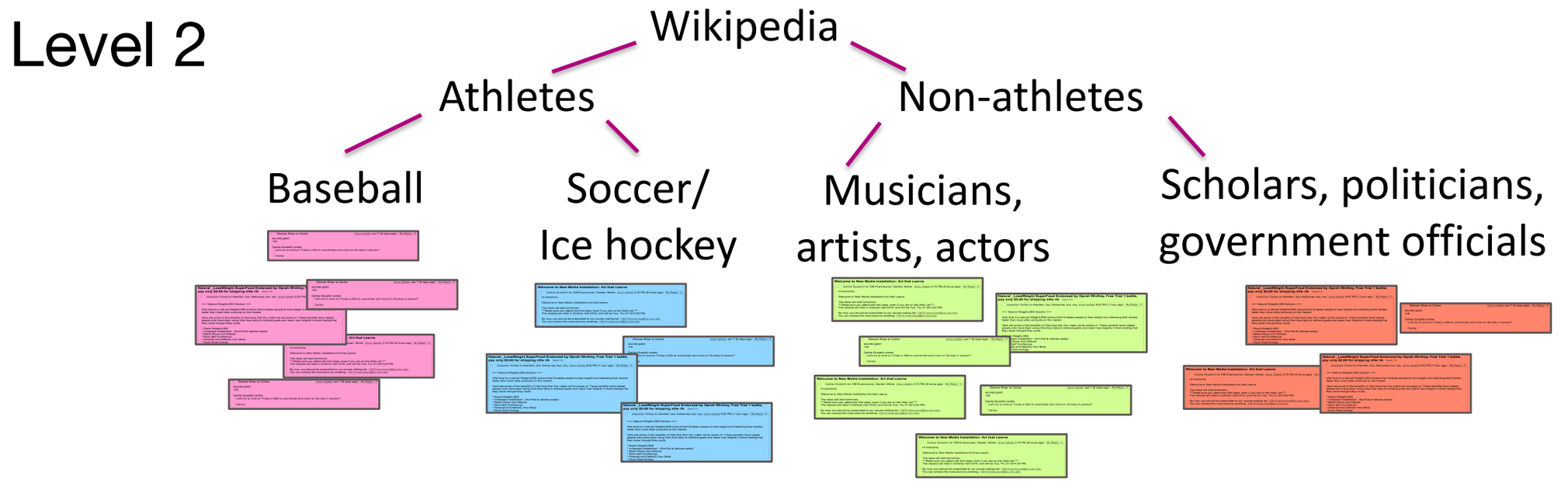


Divisive: Recursive k-means

- For example, we could run k-means, recursively







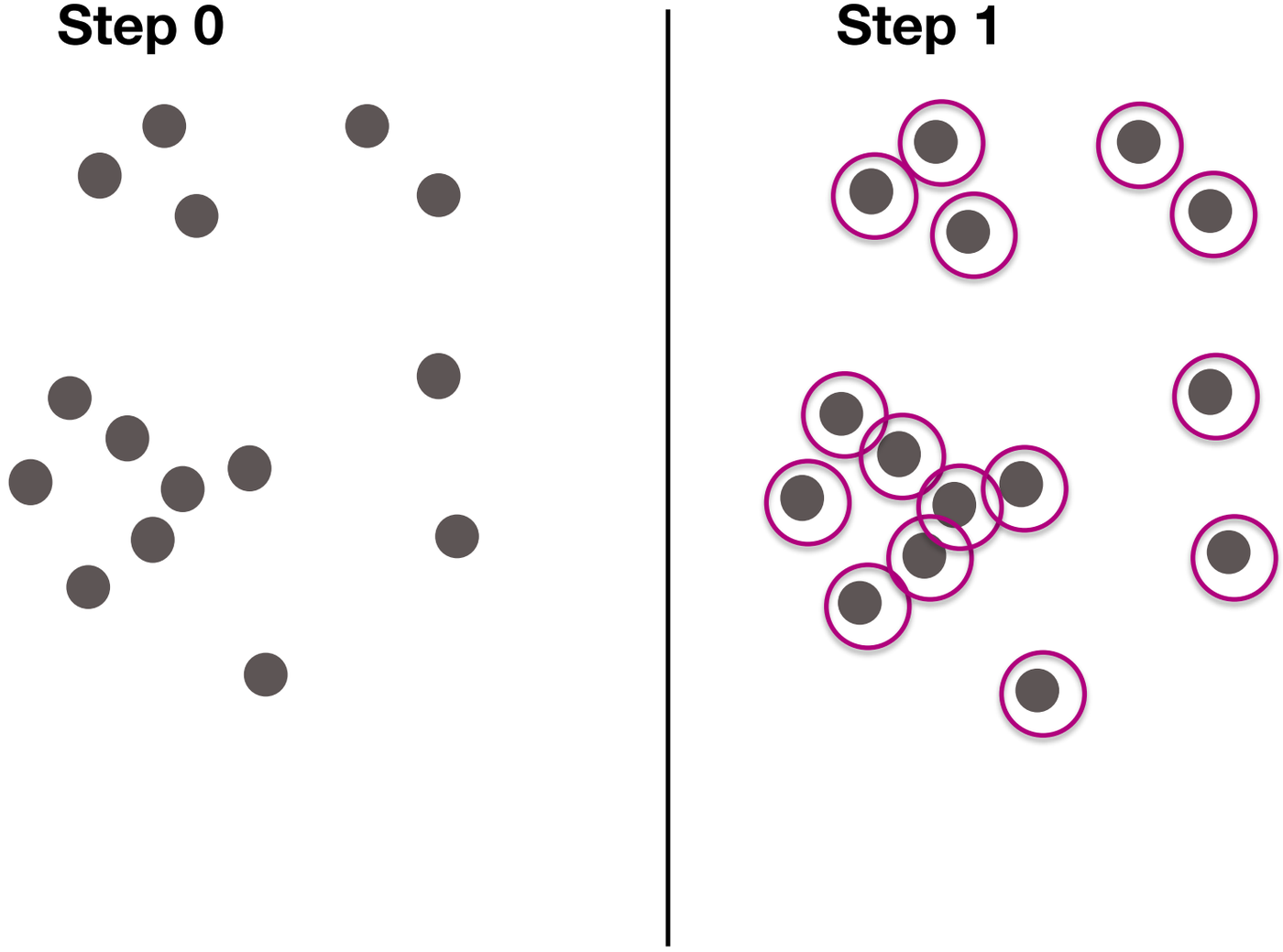
Divisive choices to be made

- Which algorithm to recurse
- How many clusters per split
- When to split vs. stop
  - Max cluster size:
    number of points in cluster falls below threshold
  - Max cluster radius:
    distance to furthest point falls below threshold
  - Specified # clusters:
    split until pre-specified # clusters is reached

Agglomerative clustering

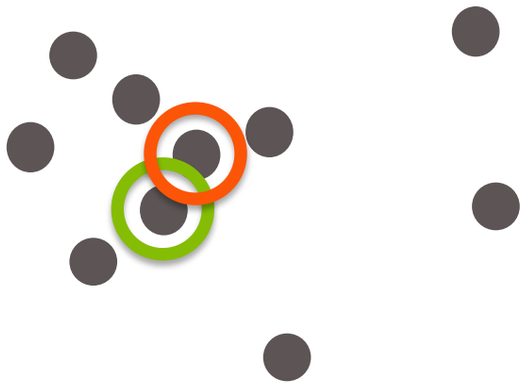
Agglomerative: Single linkage

1. Initialize each point to be its own cluster



Agglomerative: Single linkage

2. Define distance between clusters to be:



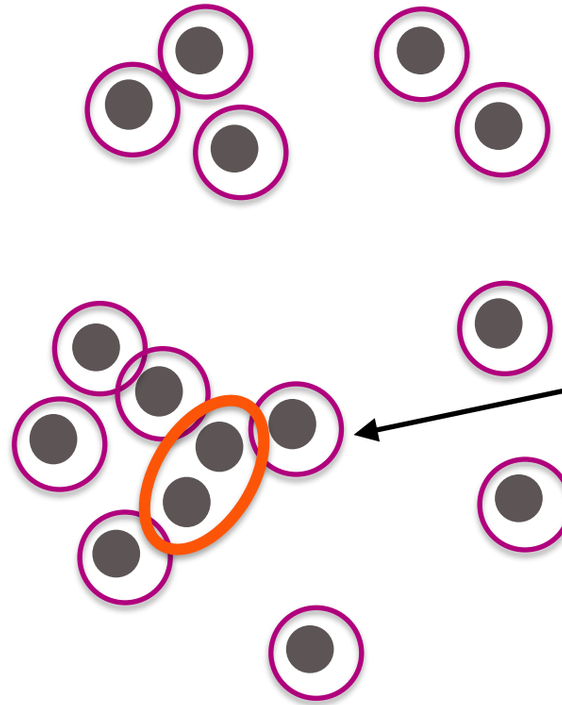
$$distance(C_1, C_2) = \min d(x_i, x_j)$$

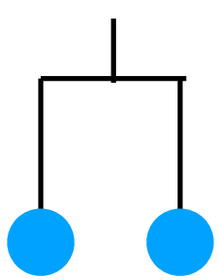
specified pairwise distance function

Linkage criteria

Agglomerative: Single linkage

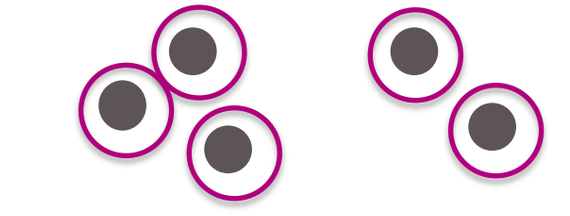
3. Merge the two closest clusters

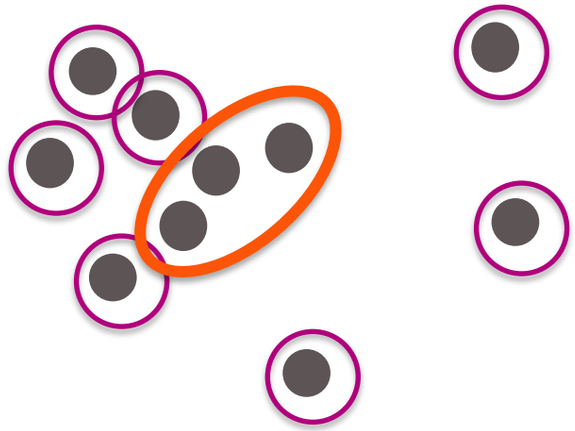


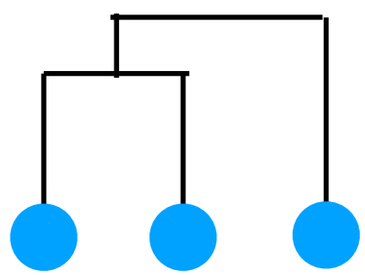


Agglomerative: Single linkage

4. Repeat step 3 until all points are in one cluster

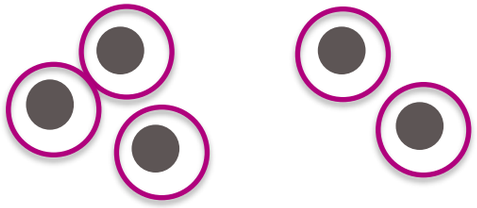


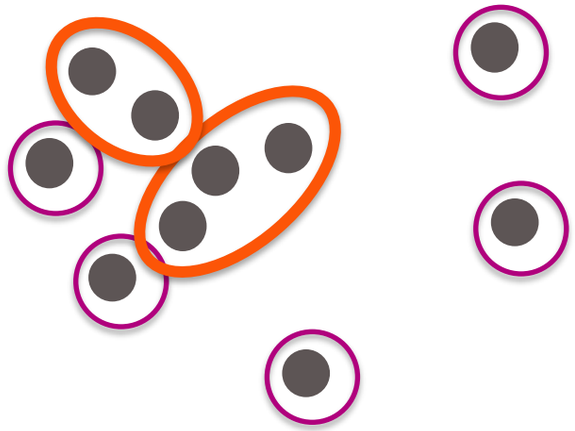


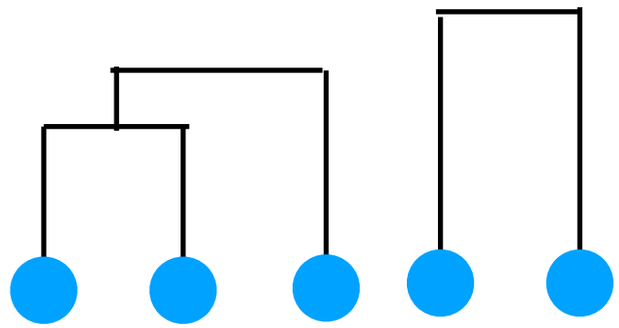


Agglomerative: Single linkage

4. Repeat step 3 until all points are in one cluster

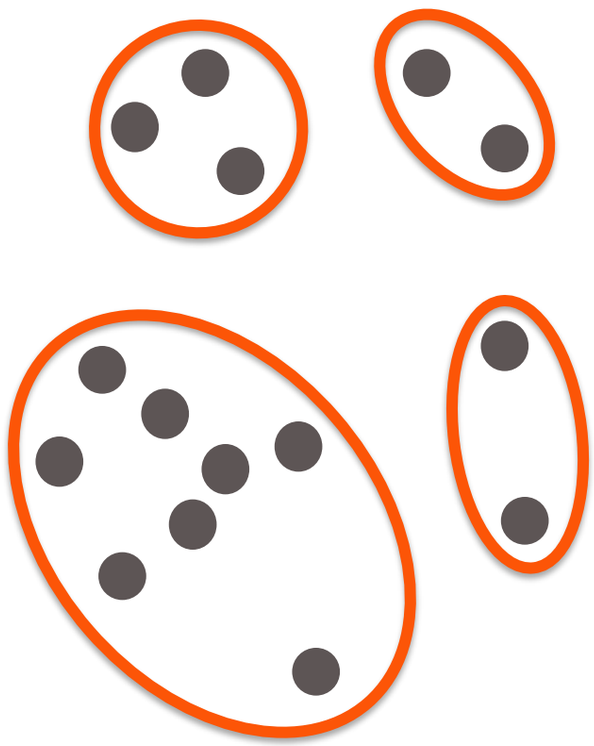






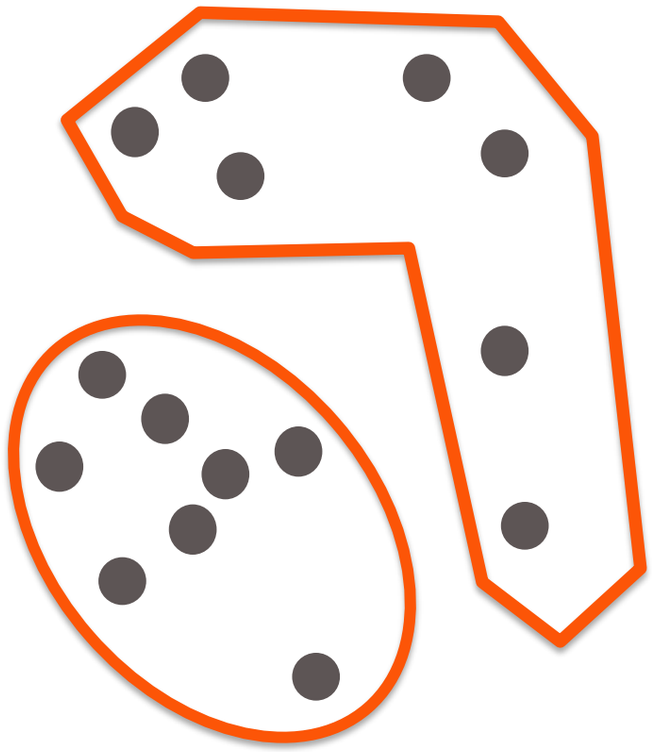
Agglomerative: Single linkage

4. Repeat step 3 until all points are in one cluster



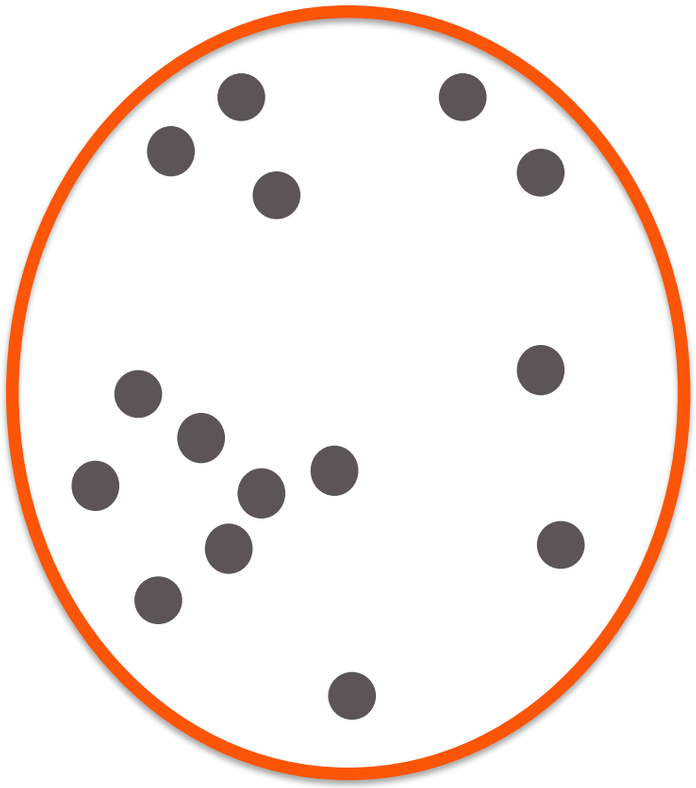
Agglomerative: Single linkage

4. Repeat step 3 until all points are in one cluster



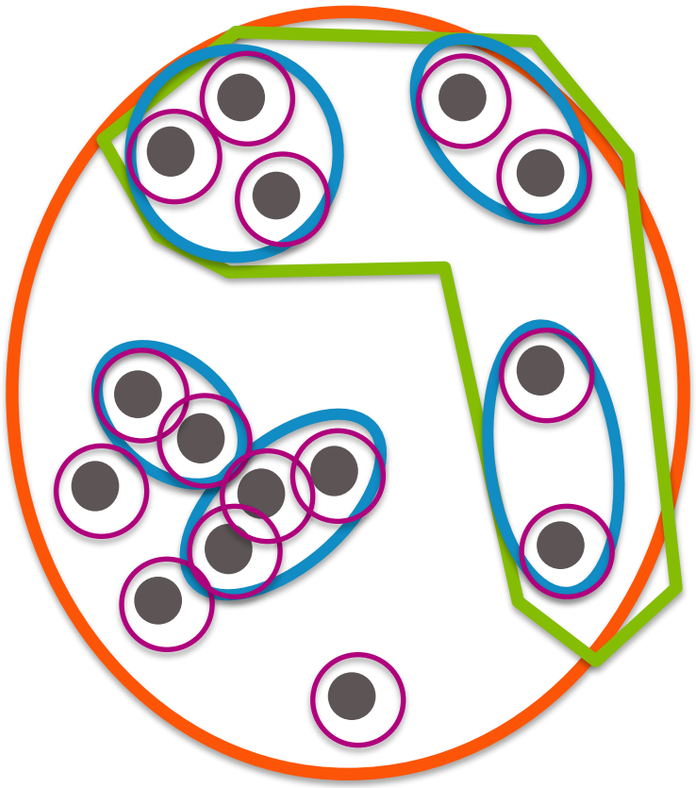
Agglomerative: Single linkage

4. Repeat step 3 until all points are in one cluster



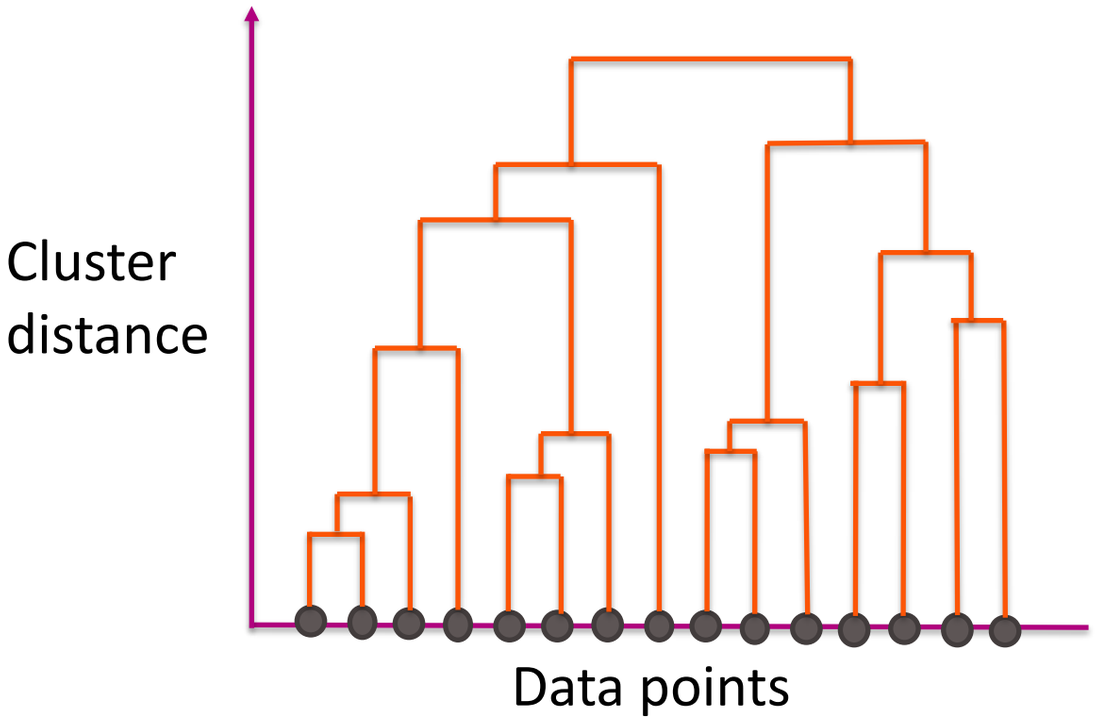
Clusters of clusters

Just like our picture for divisive clustering…



The dendrogram

- x axis shows data points (carefully ordered)
- y-axis shows distance between pair of clusters



The dendrogram

- x axis shows data points (carefully ordered)
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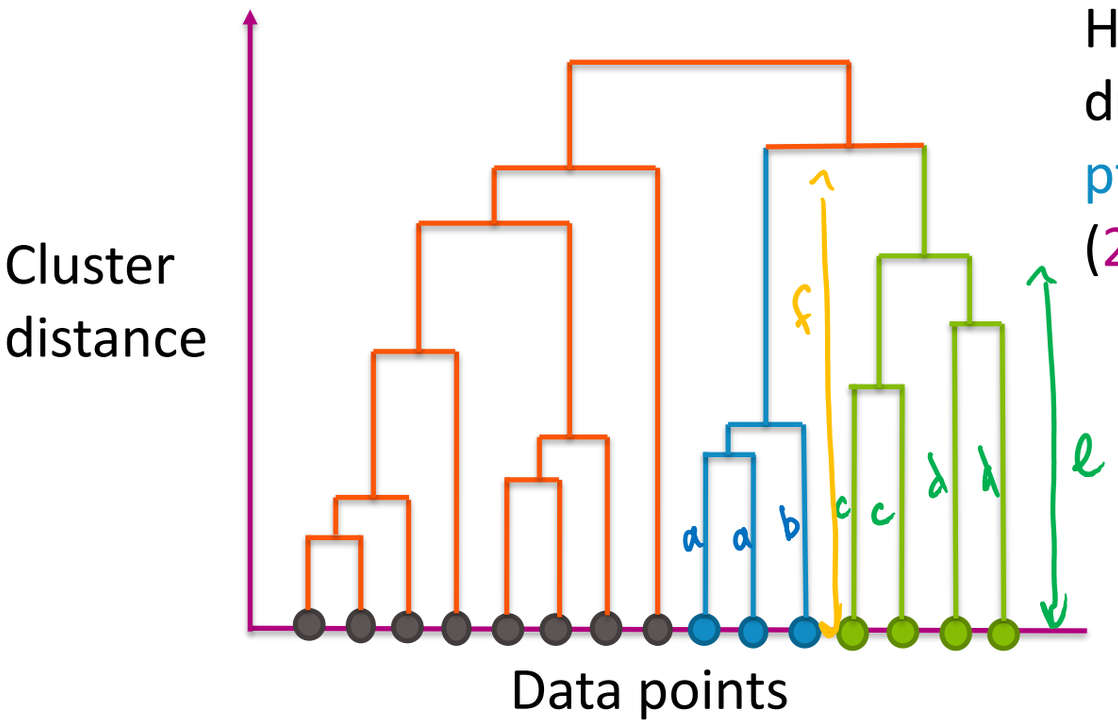
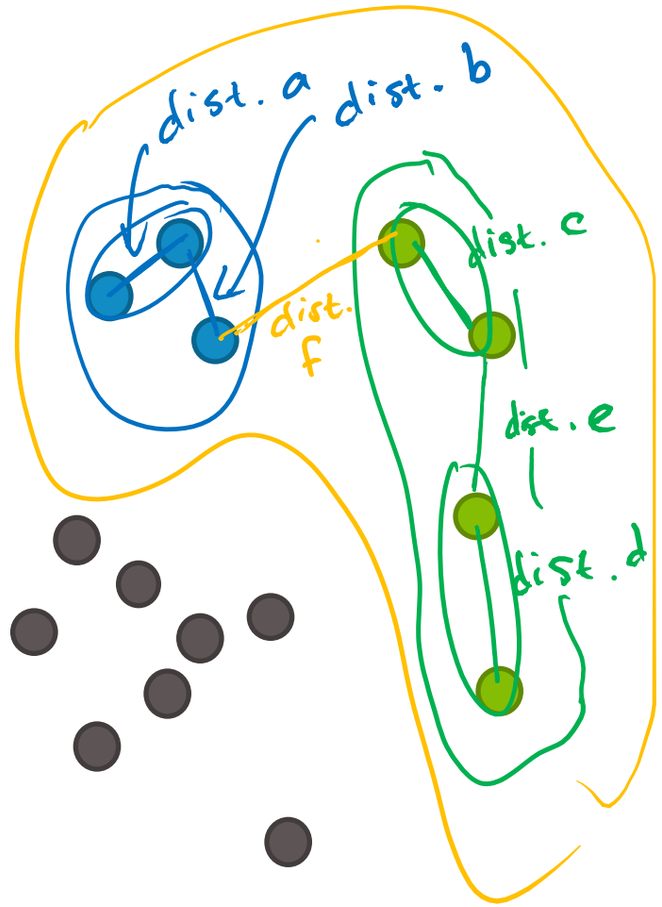
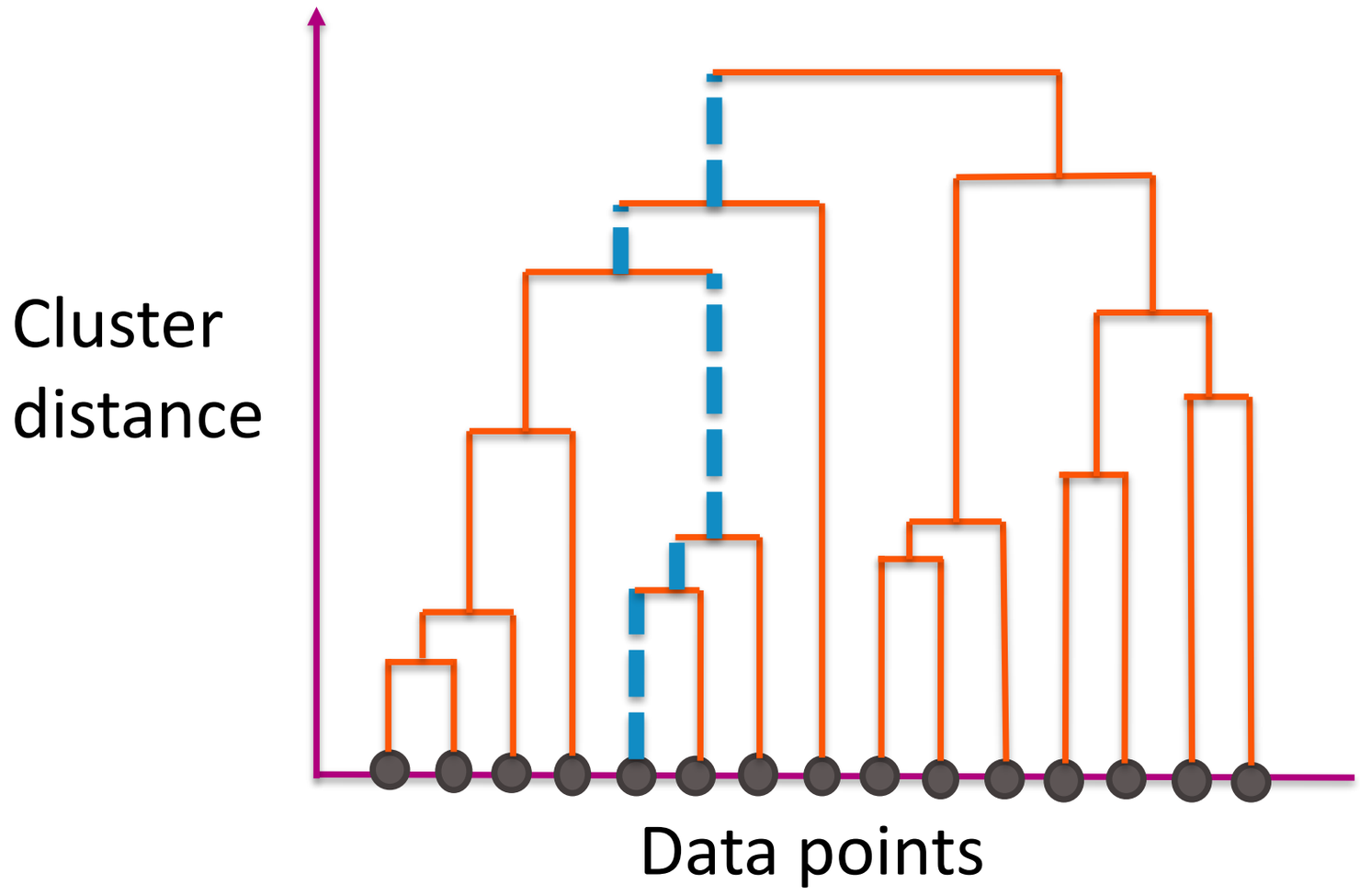


Height here indicates min distance between blue pts and green pts (2 clusters)



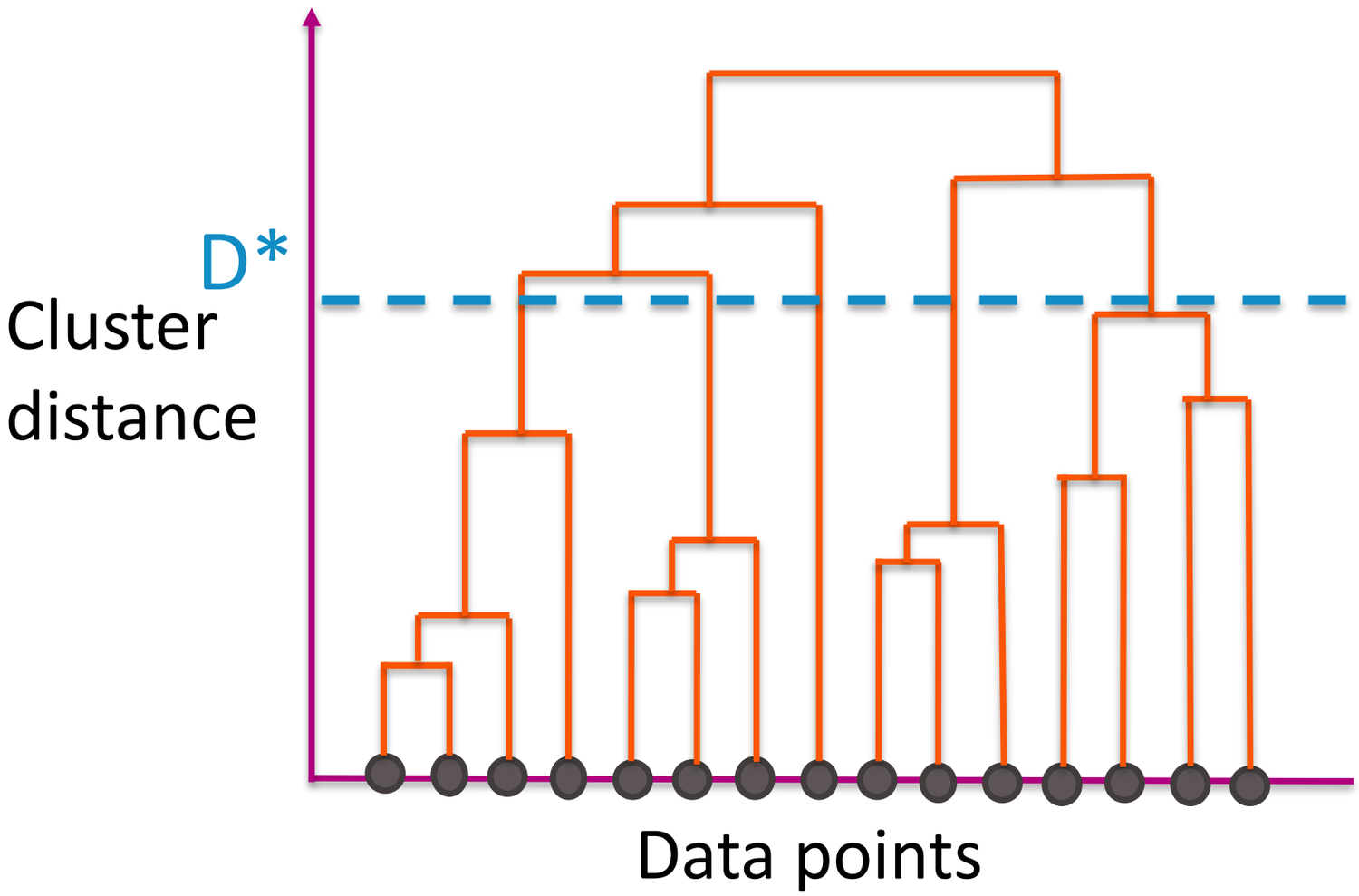
The dendrogram

Path shows all clusters to which a point belongs and the order in which clusters merge



Extracting a partition

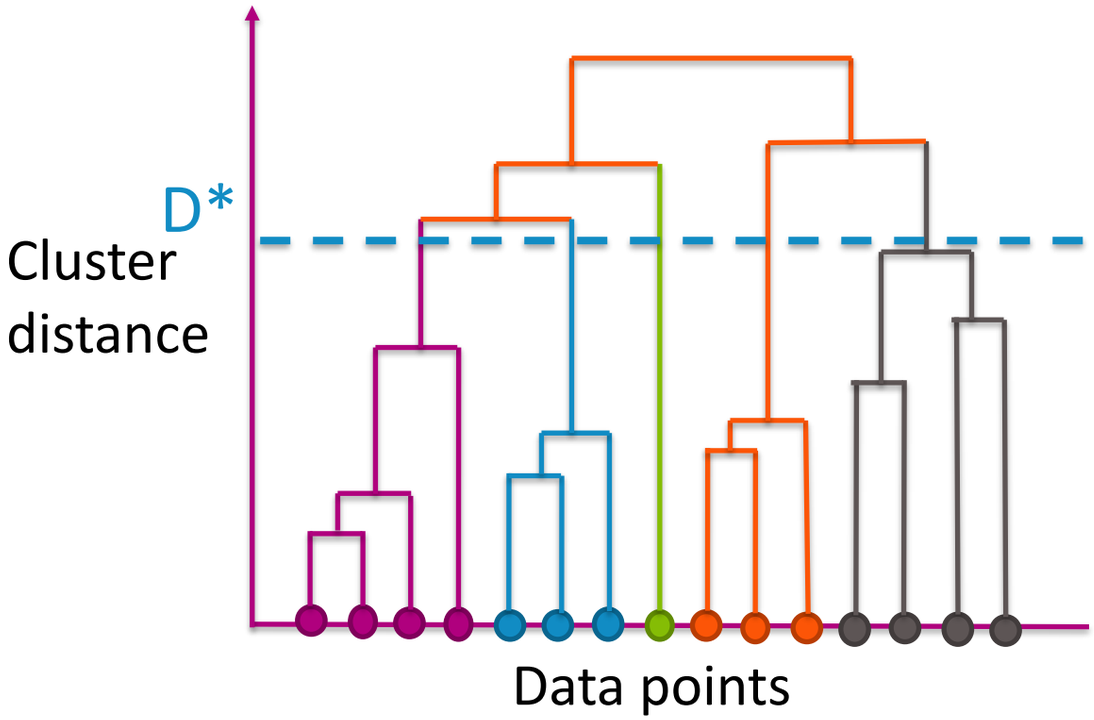
Choose a distance D* at which to cut dendogram



How many clusters do we get, with threshold D*?

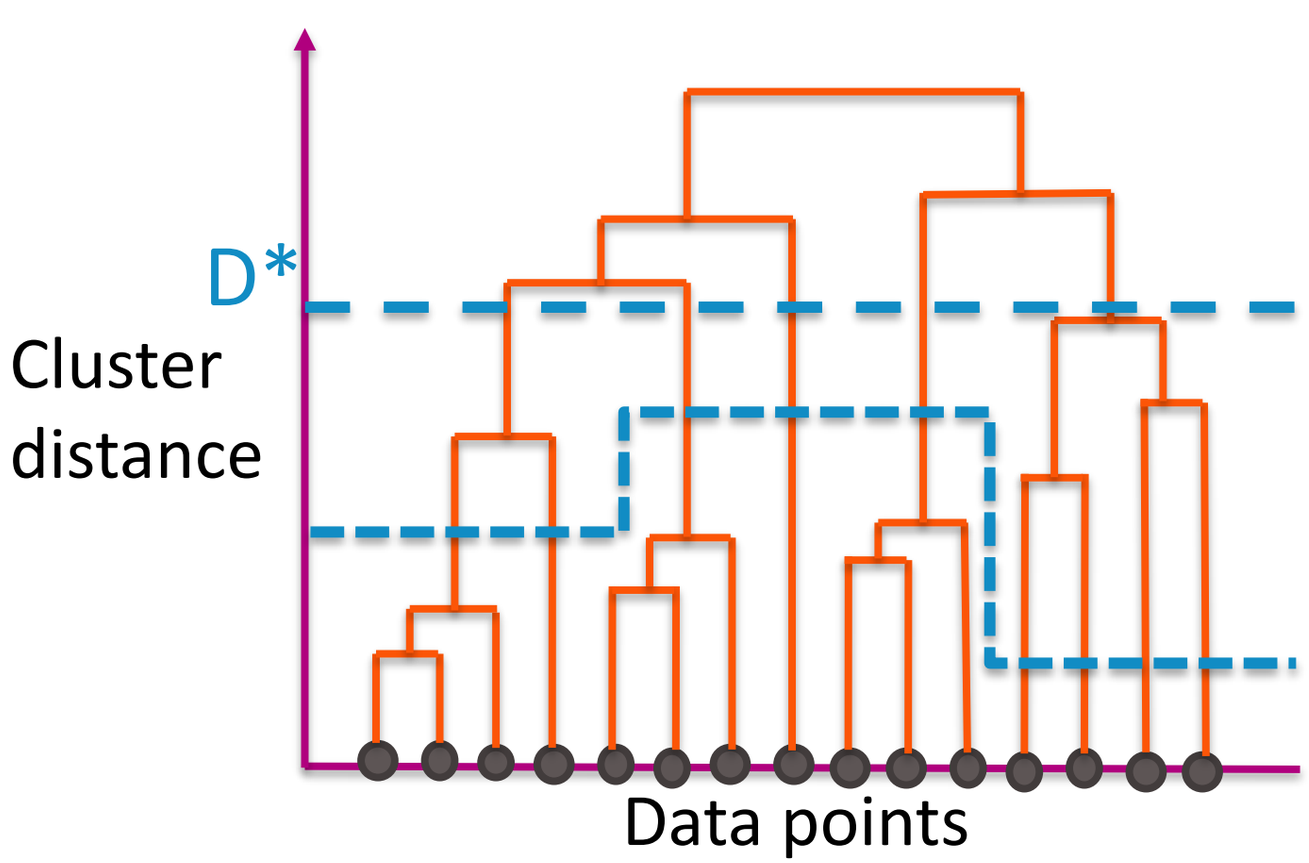
Extracting a partition

Every branch that crosses D* becomes a separate cluster



Agglomerative choices to be made

- Distance metric: d(x_i, x_j)
- Linkage function: e.g., $\min_{x_i \text{ in } C_1,\ x_j \text{ in } C_2} d(x_i, x_j)$
- Where and how to cut dendrogram



More on cutting dendrogram

- For visualization, smaller # clusters is preferable
- For tasks like outlier detection, cut based on:
  - Distance threshold
  - Inconsistency coefficient
    - Compare height of merge to average merge heights below
    - If top merge is substantially higher, then it is joining two subsets that are relatively far apart compared to the members of each subset internally
    - Still have to choose a threshold to cut at, but now in terms of "inconsistency" rather than distance
- No cutting method is "incorrect", some are just more useful than others

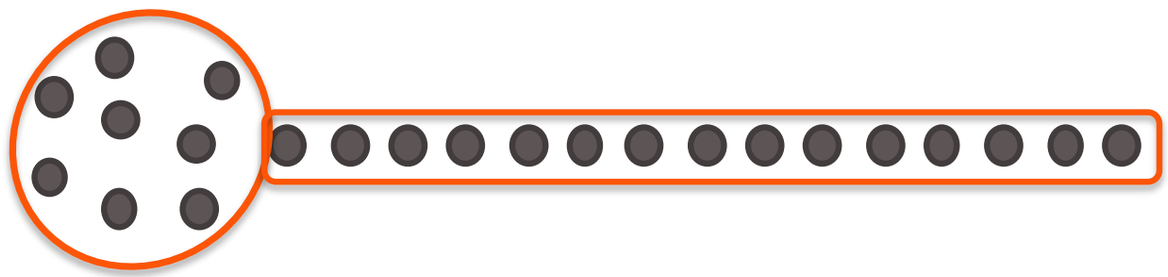
Computational considerations

- Computing all pairs of distances is expensive
  - Brute force algorithm is $O(N^2 \log(N))$

- Smart implementations use triangle inequality to rule out candidate pairs
-
- Best known algorithm is $O(N^2)$

Statistical issues

Chaining: Distant points clustered together if there is a chain of pairwise close points between



Other linkage functions can be more robust, but restrict the shapes of clusters that can be found

- Complete linkage:
  max pairwise distance between clusters
- Ward criterion:
  min increase in within-cluster variance at each merge