GENERAL ASSEMBLY

CLUSTERING

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LEARNING OBJECTIVES

- Supervised vs unsupervised algorithms
- Understand and apply k-means clustering
- Density-based clustering: DBSCAN
- Silhouette Metric

OPENING

UNSUPERVISED LEARNING

UNSUPERVISED LEARNING

- So far all the algorithms we have used are *supervised*:
  - each observation (row of data) came with one or more *labels*,
  - either *categorical variables* (classes) or *measurements* (regression)

- **Unsupervised learning** has a different goal: **feature discovery**

- **Clustering** is a common and fundamental example of unsupervised learning

- Clustering algorithms try to find *meaningful groups* within data

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

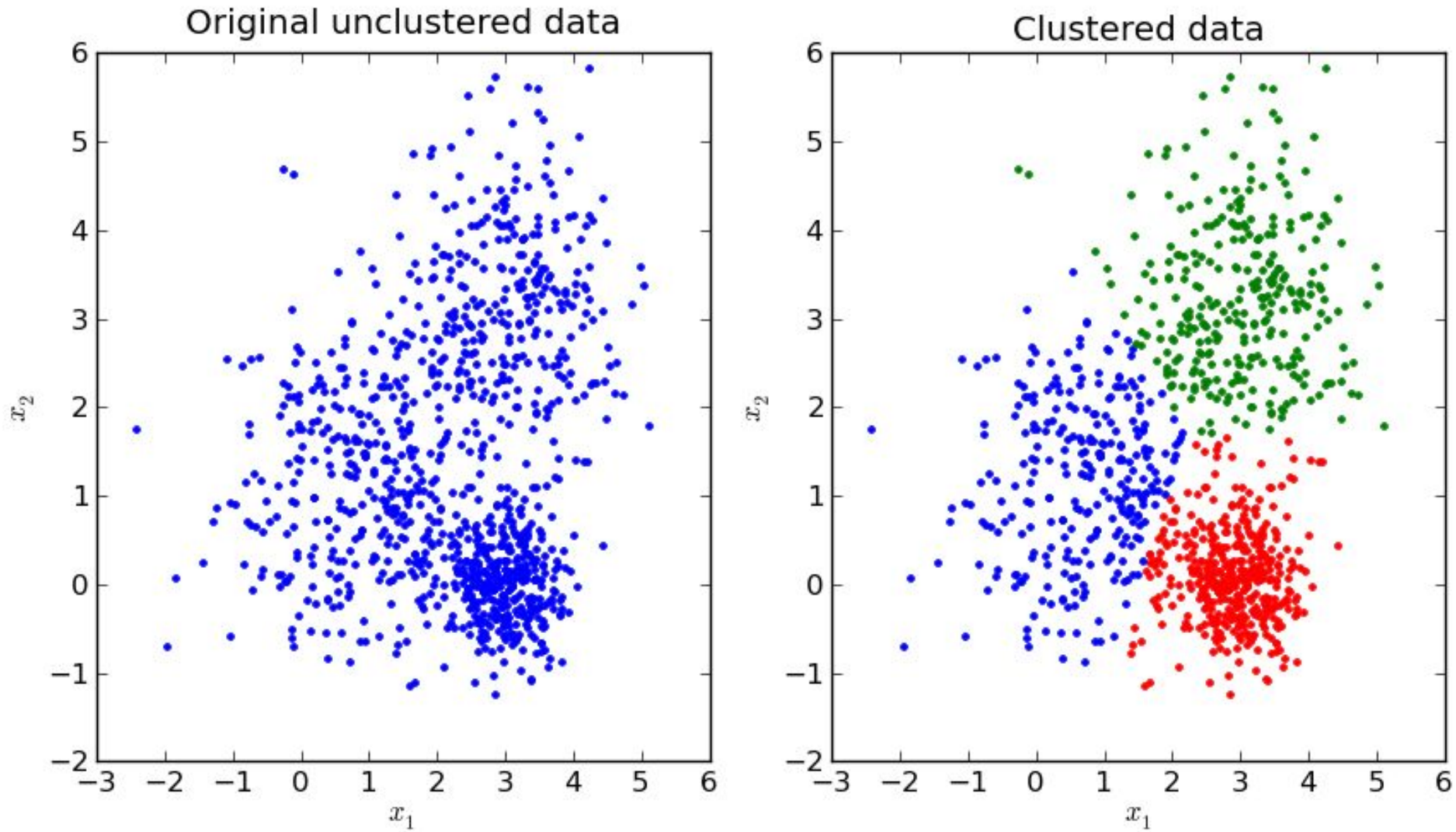
1. How is unsupervised learning different from classification?

DELIVERABLE

Answers to the above questions

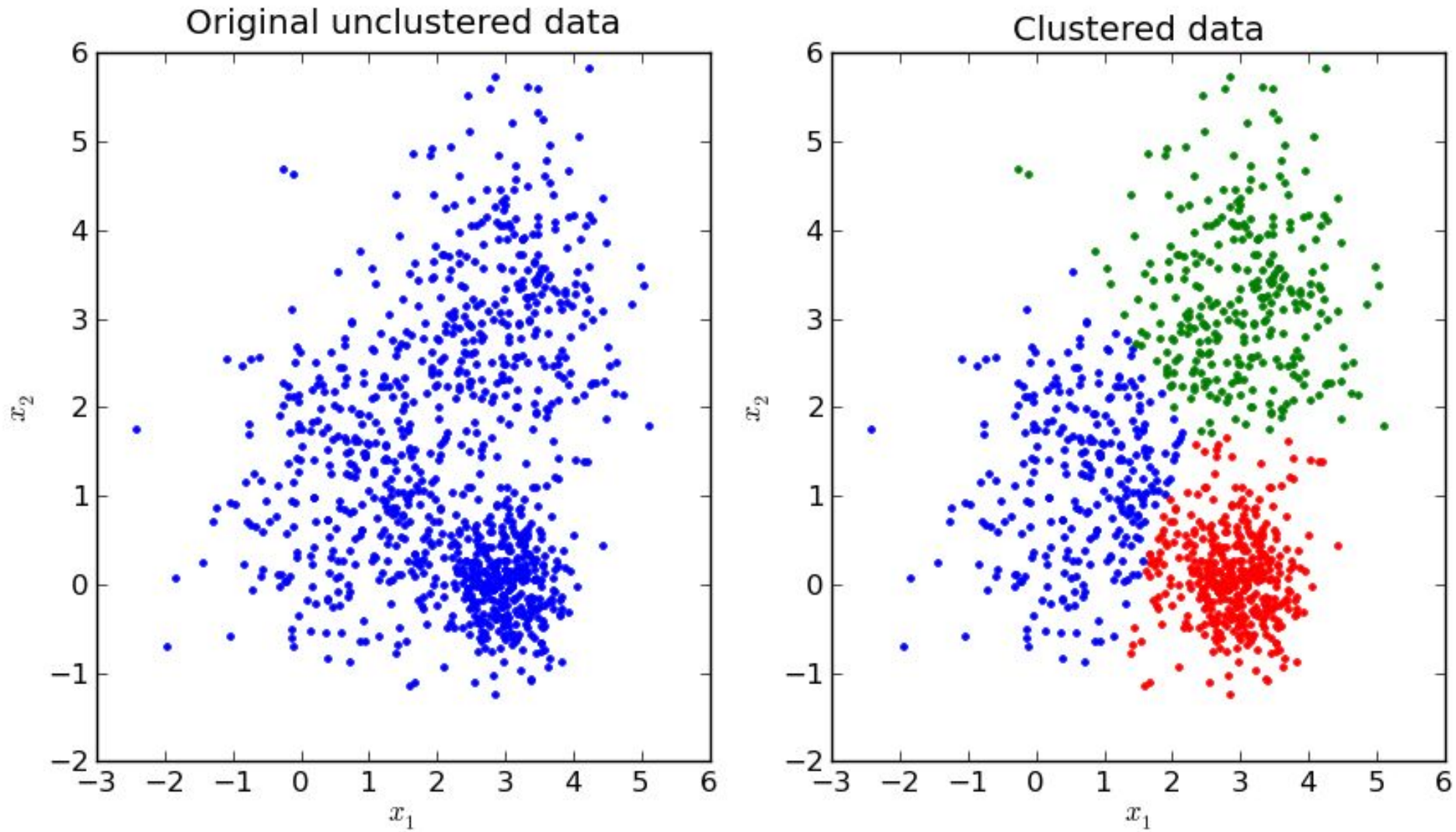
CLUSTERING

CLUSTERING: Centroids



Source: http://stackoverflow.com/questions/24645068/k-means-clustering-major-understanding-issue

CLUSTERING: Centroids



Source: http://stackoverflow.com/questions/24645068/k-means-clustering-major-understanding-issue

ACTIVITY: KNOWLEDGE CHECK

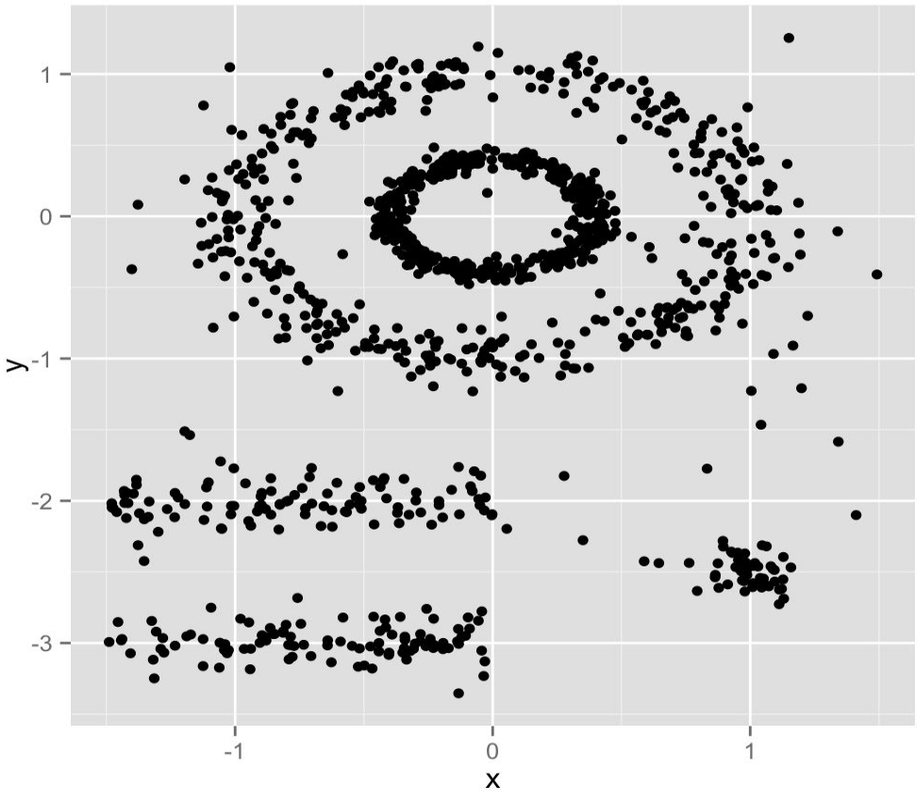
ANSWER THE FOLLOWING QUESTIONS

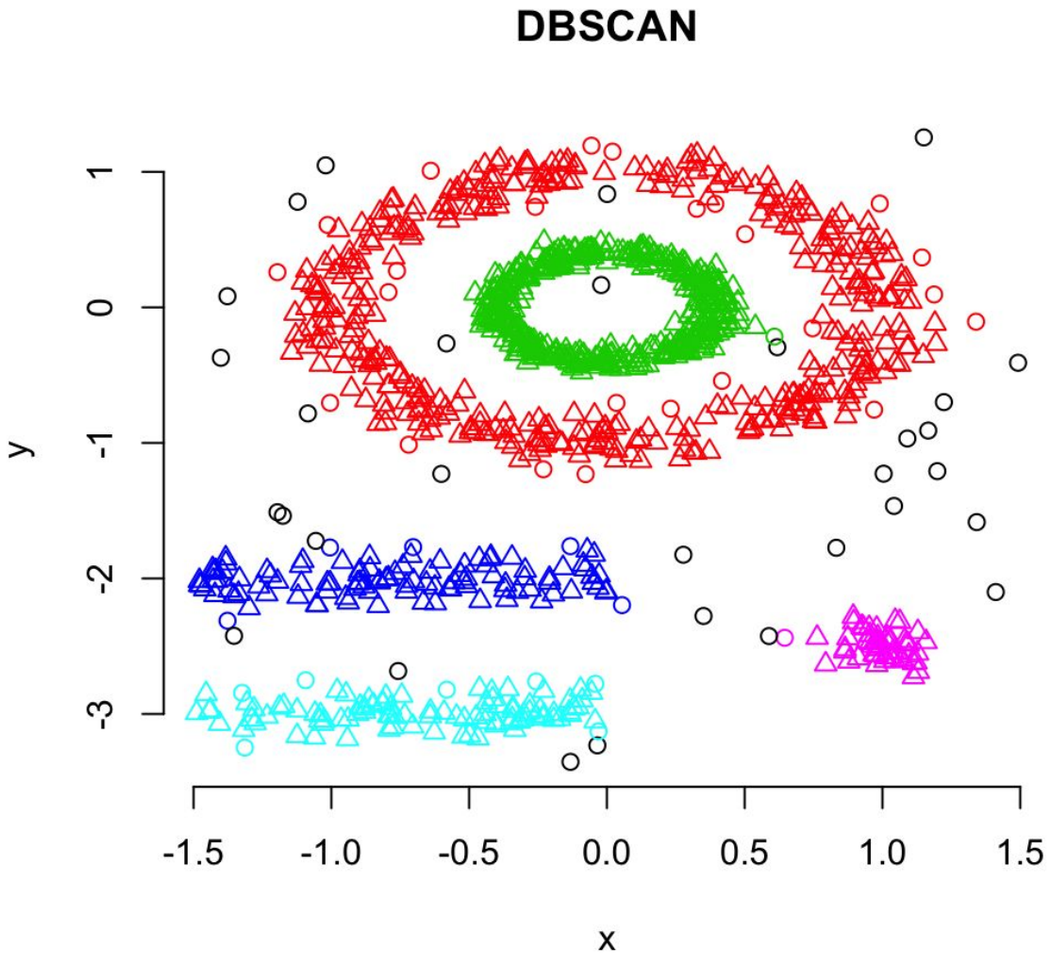
1. Why might data often appear in centered clusters?

DELIVERABLE

Answers to the above questions

CLUSTERING: Density-Based





Source: http://www.sthda.com/english/wiki/dbscan-density-based-clustering-for-discovering-clusters-in-large-datasets-with-noise-unsupervised-machine-learning

ACTIVITY: KNOWLEDGE CHECK

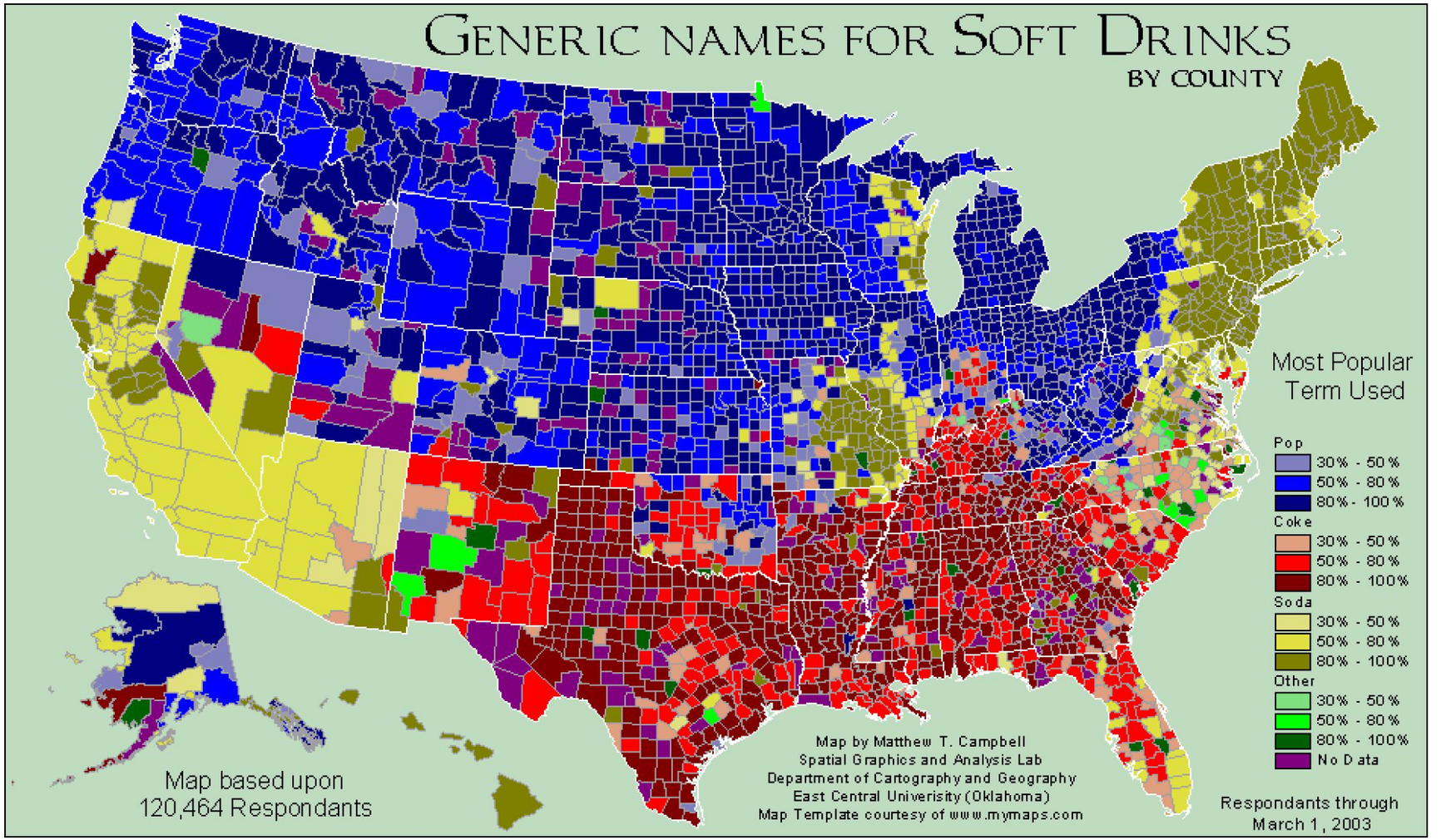
ANSWER THE FOLLOWING QUESTIONS

1. Why might data often appear in density-based clusters?

DELIVERABLE

Answers to the above questions

ACTIVITY: KNOWLEDGE CHECK

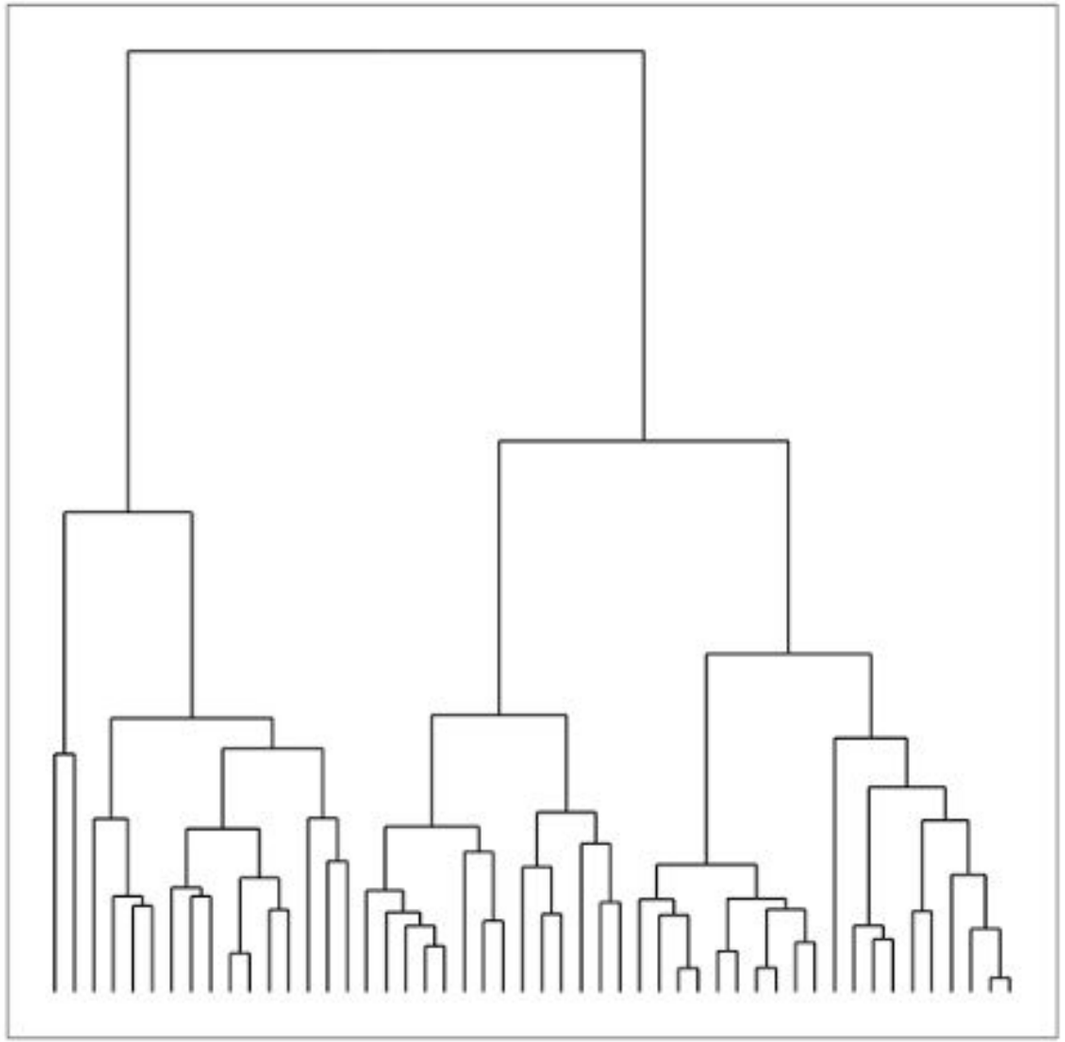


See also: http://www4.ncsu.edu/~jakatz2/files/dialectposter.png

CLUSTERING: Hierarchical

- Goal: Build hierarchies that form clusters

- Based on **classification trees** (next lesson)



ACTIVITY: KNOWLEDGE CHECK

ANSWER THE FOLLOWING QUESTIONS

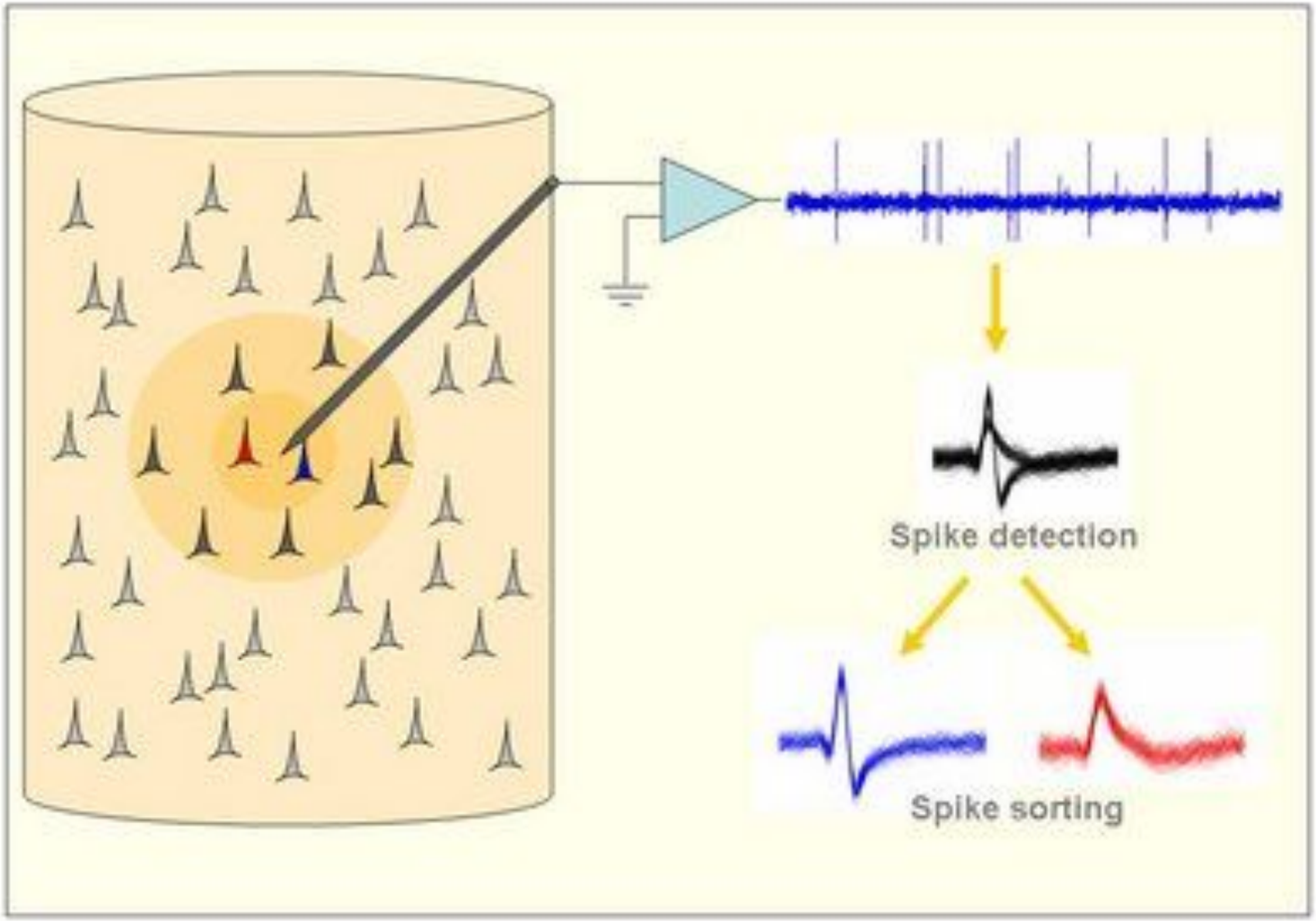
1. Can you think of a real-world clustering application?

DELIVERABLE

Answers to the above questions

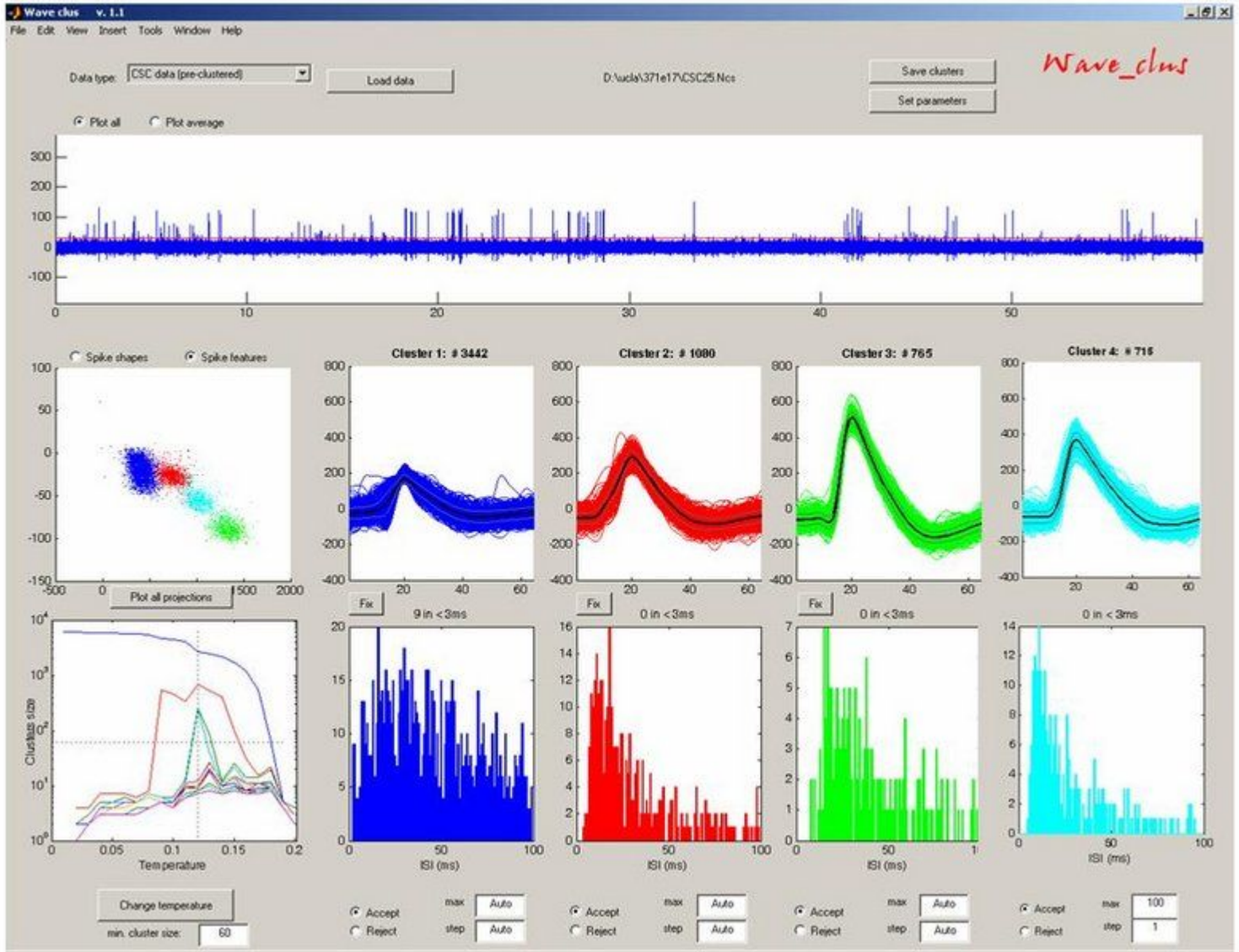
ACTIVITY: KNOWLEDGE CHECK

EXERCISE



ACTIVITY: KNOWLEDGE CHECK

EXERCISE



ACTIVITY: KNOWLEDGE CHECK

ANSWERS

1. Recommendation Systems e.g. Netflix genres
2. Medical Imaging: differentiate tissues
3. Identifying market segments
4. Discover communities in social networks
5. Lots of applications for genomic sequences (homologous sequences, genotypes)
6. Earthquake epicenters
7. Fraud detection

K-MEANS: CENTROID CLUSTERING

K-MEANS CLUSTERING

- k-Means clustering is a popular centroid-based clustering algorithm
- Basic idea: find *k* clusters in the data centrally located around various mean points
- Awesome Demo

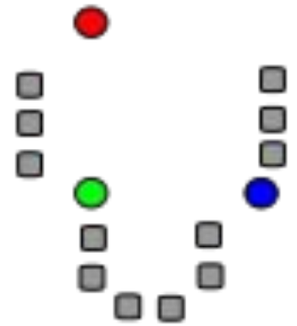
K-MEANS CLUSTERING

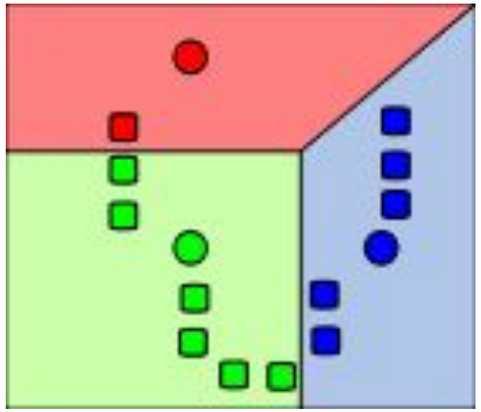
- This is a computationally difficult problem to solve so we rely on heuristics

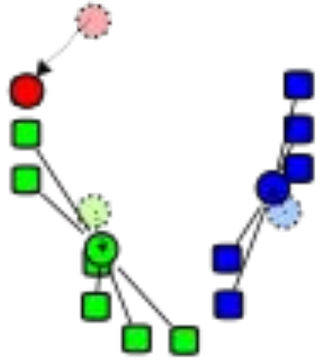
- The “standard” heuristic is called “Lloyd’s Algorithm”:
  - Start with k initial mean values
  - Data points are then split up into a Voronoi diagram
    - Each point is assigned to the “closest” mean
  - Calculate new means based on centroids of points in the cluster
  - Repeat until clusters do not change

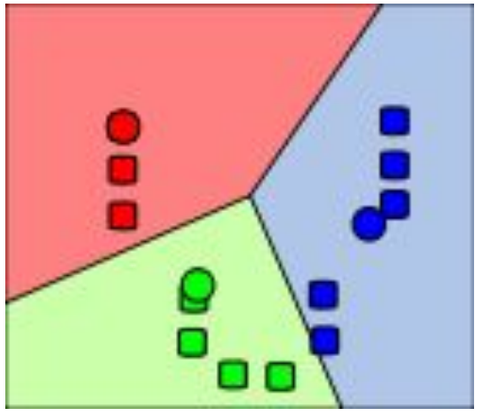
K-MEANS CLUSTERING

- Start with initial k mean values
- Data points are then split up into a Voronoi diagram
- Calculate new means based on centroids









K-MEANS CLUSTERING

- k-Means seeks to minimize the sum of squares about the means

- Precisely, find k subsets S_1, … S_k of the data with means mu_1, …, mu_k that minimizes:

$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \left\| \mathbf{x} - \boldsymbol{\mu}_i \right\|^2$$

K-MEANS CLUSTERING

- k-Means assumptions:
  - k is the correct number of clusters
  - the variance is the same for each variable
  - clusters are roughly the same size

ACTIVITY: KNOWLEDGE CHECK

ANSWER THE FOLLOWING QUESTIONS

1. What is **cluster analysis**?
2. How do we assign meaning to the clusters we find?
   - Do clusters always have meaning?

DELIVERABLE

Answers to the above questions

K-MEANS CLUSTERING

- Netflix prize: Predict how users will rate a movie
  - How might you do this with clustering?
  - Cluster similar users together and take the average rating for a given movie by users in the cluster (which have rated the movie)
  - Use the average as the prediction for users that have not yet rated the movie

- In other words, fit a model to users in a cluster for each cluster and make predictions per cluster

- k-Means for the Netflix Prize

DBSCAN: DENSITY BASED CLUSTERING

DBSCAN CLUSTERING

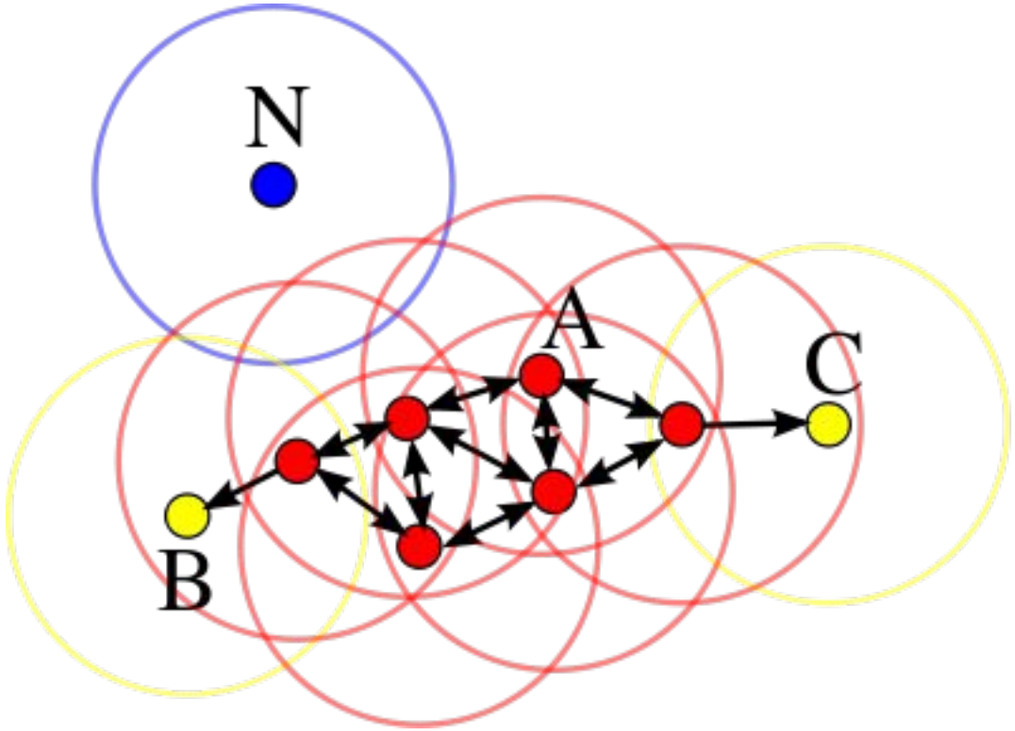
- DBSCAN: Density-based spatial clustering of applications with noise

- Main idea: Group together closely-packed points by identifying
  - Core points
  - Reachable points
  - Outliers (not reachable)

- Two parameters:
  - min_samples
  - ε (eps)

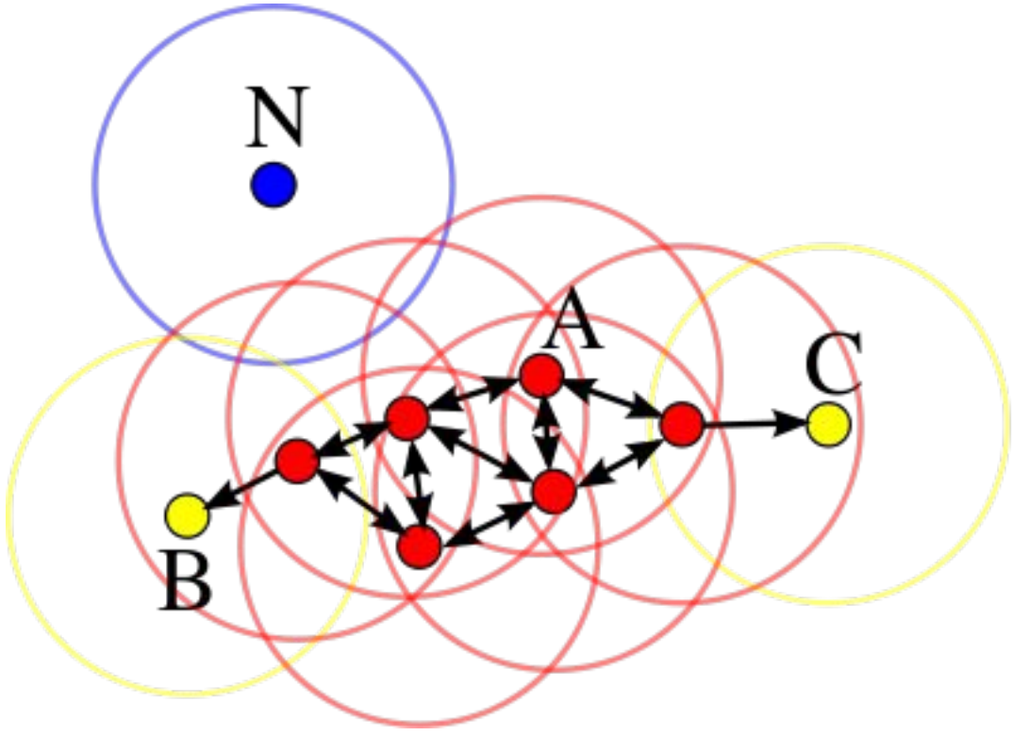
DBSCAN CLUSTERING

- Core points: at least **min_samples** points within **eps** of the core point
  - Such points are *directly reachable* from the core point
- Reachable: point *q* is reachable from *p* if there is a path of core points from *p* to *q*
- Outlier: not reachable



DBSCAN CLUSTERING

- Each cluster is a collection of connected points reachable by ε (or less)



CLUSTERING: Density-Based

Advantages:

- Finds non linearly separable (arbitrarily-shaped) clusters
- No need to assume a fixed number of clusters
- Robust to outliers

CLUSTERING: Density-Based

Disadvantages:

- Sensitivity to Euclidean distance measure problems
  - “Curse of dimensionality”
- Doesn’t work well when clusters are of varying densities

- Awesome Demo

ACTIVITY: KNOWLEDGE CHECK

ANSWER THE FOLLOWING QUESTIONS

1. How does DBSCAN differ from k-means?

DELIVERABLE

Answers to the above questions

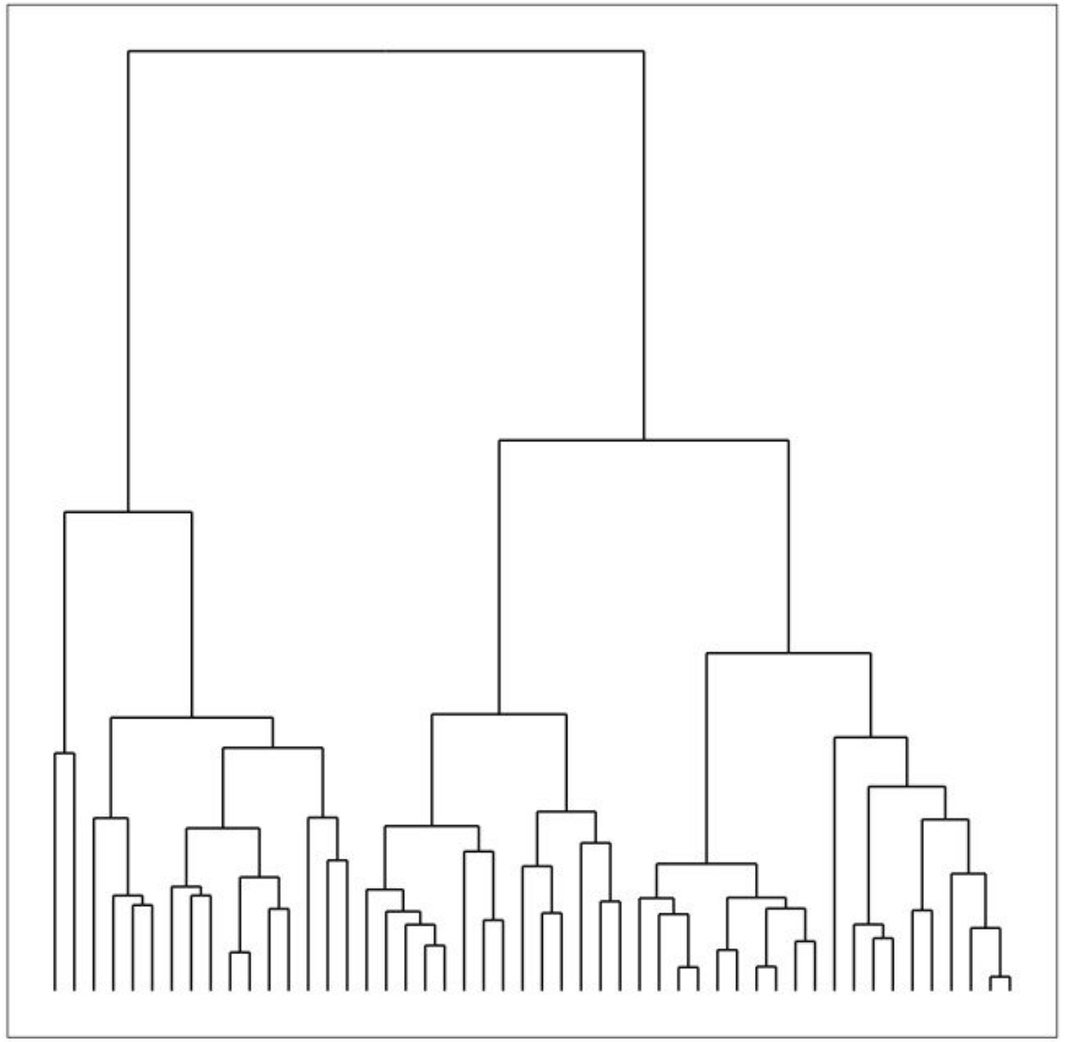
HIERARCHICAL CLUSTERING

CLUSTERING: Hierarchical

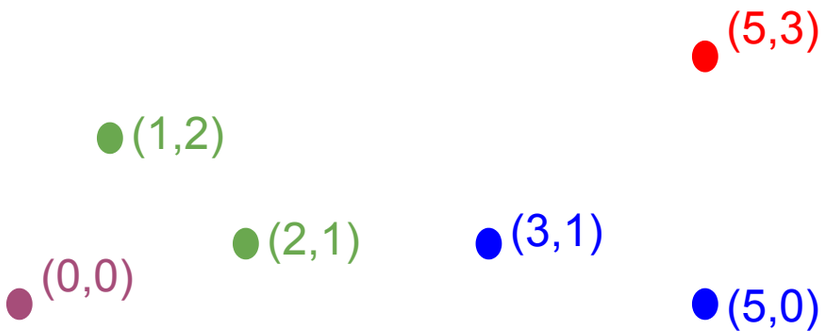
- Build hierarchies of clusters
  - Based on classification trees (next lesson)

<u>Benefits:</u>

- No fixed number of clusters
- Dendrogram displays multiple granularities of clustering
- Multiple distance metric options
- Captures non-spherical clusters

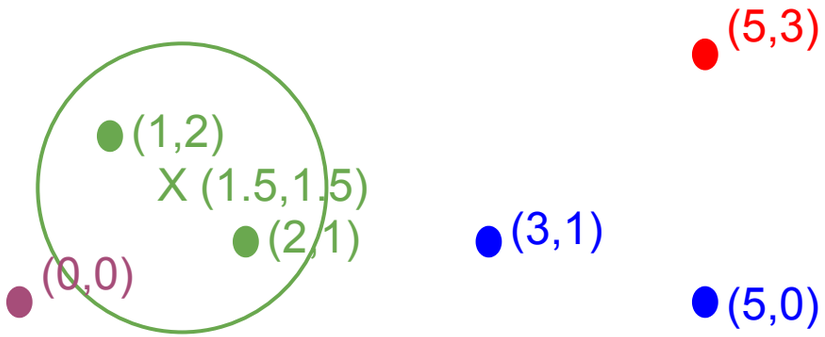


HIERARCHICAL CLUSTERING



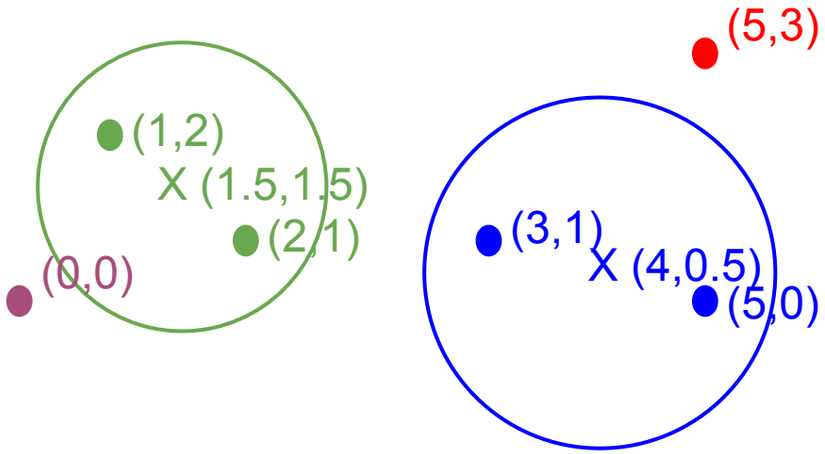
Dendrogram

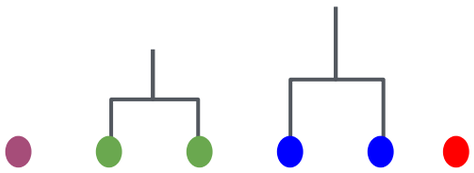
HIERARCHICAL CLUSTERING



Dendrogram

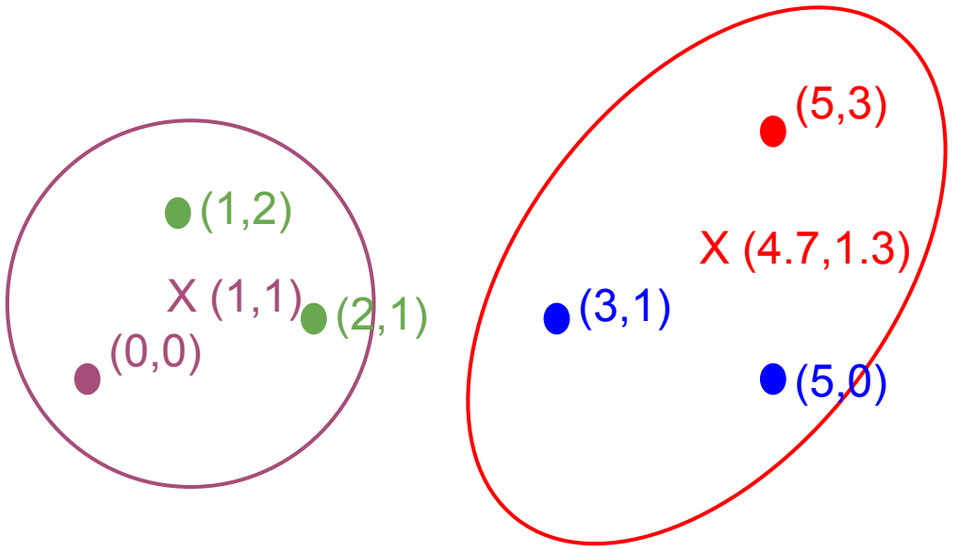
HIERARCHICAL CLUSTERING

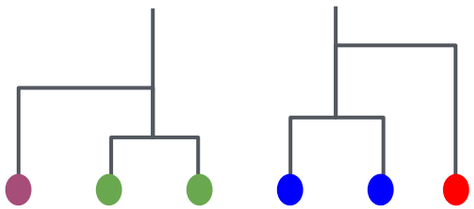




Dendrogram

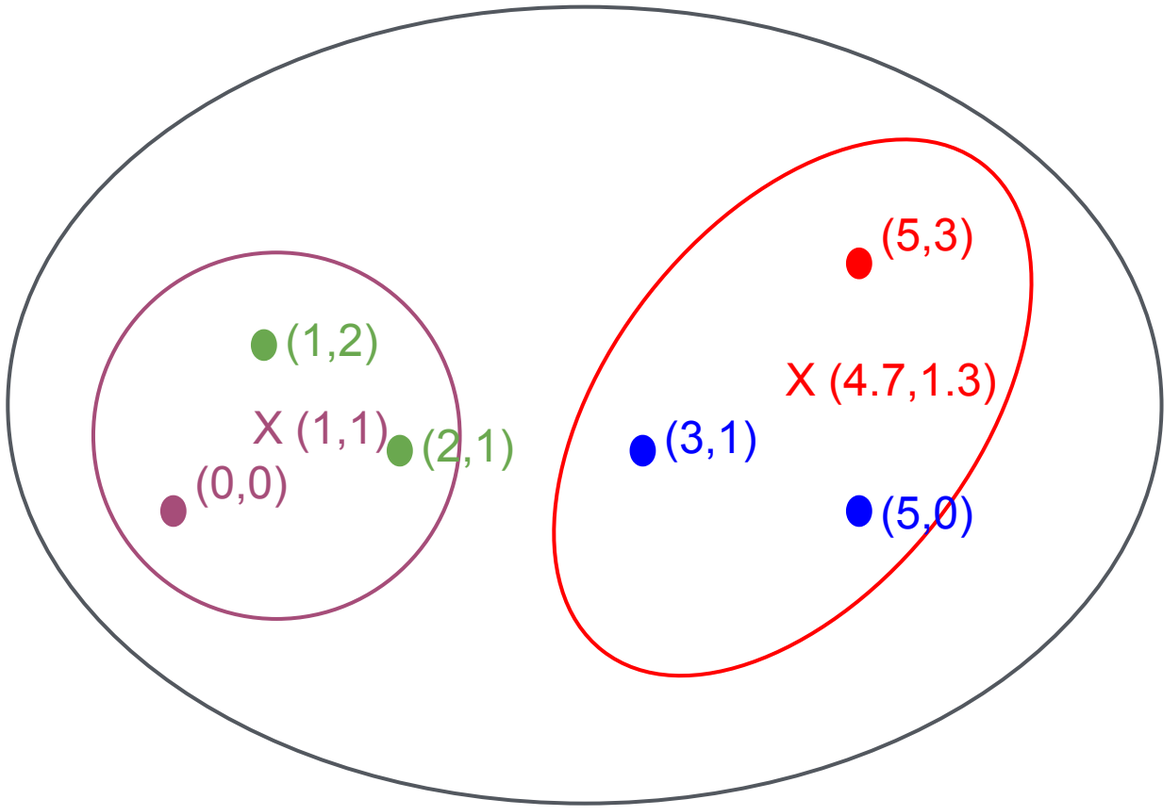
HIERARCHICAL CLUSTERING

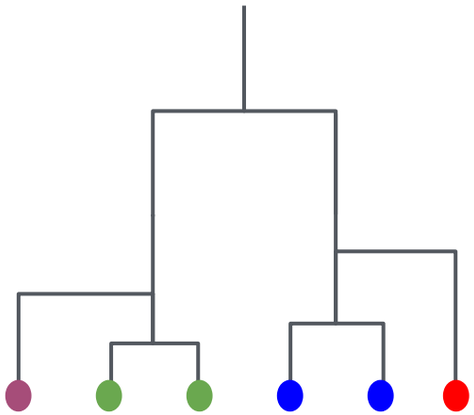




Dendrogram

HIERARCHICAL CLUSTERING





Dendrogram

HIERARCHICAL CLUSTERING

We'll discuss hierarchical models more once we cover decision trees

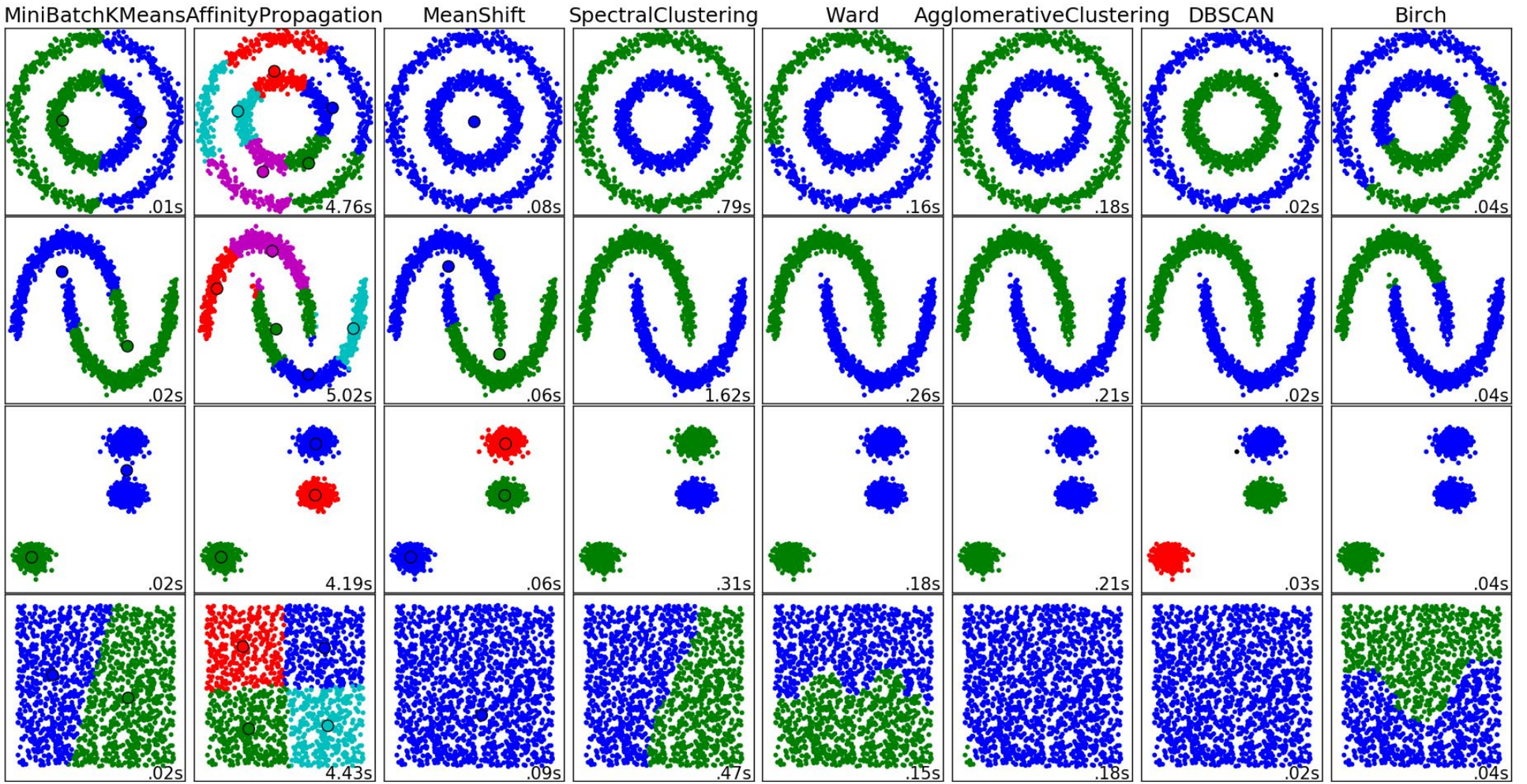
- For now we can fit with sklearn

```
from sklearn.cluster import AgglomerativeClustering
est = AgglomerativeClustering(n_clusters=4)
est.fit(X)
labels = est.labels_
```

We'll try it out in the starter-code

CLUSTERING OVERVIEW

- There are many clustering algorithms



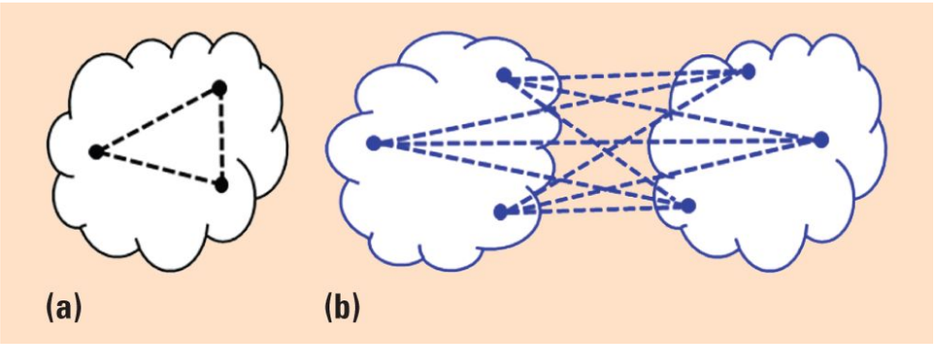
GUIDED PRACTICE

CLUSTERING METRICS

CLUSTERING METRICS

- As usual we need a metric to evaluate model fit

- For clustering we use a metric called the Silhouette Coefficient



  - **a** is the mean distance between a sample and all other points in the cluster
  - **b** is the mean distance between a sample and all other points in the *nearest* cluster

- The Silhouette Coefficient is: $$\frac{b - a}{\max(a, b)}$$

- Ranges between 1 and -1
- Average over all points to judge the cluster algorithm

CLUSTERING METRICS

```
from sklearn import metrics
from sklearn.cluster import KMeans
kmeans_model = KMeans(n_clusters=3, random_state=1).fit(X)
labels = kmeans_model.labels_
metrics.silhouette_score(X, labels, metric='euclidean')
```

CLUSTERING METRICS

- There are a number of other metrics based on:
  - Mutual Information
  - Homogeneity
  - Adjusted Rand Index (when you know the labels on the training data)

INDEPENDENT PRACTICE

CLUSTERING, CLASSIFICATION, AND REGRESSION

ACTIVITY: KNOWLEDGE CHECK

ANSWER THE FOLLOWING QUESTIONS

1. How might we combine clustering and classification?

DELIVERABLE

Answers to the above questions

CLUSTERING, CLASSIFICATION, AND REGRESSION

- We can use clustering to discover new features and then use those features for either classification or regression
- For classification, we could use e.g. k-NN to classify new points into the discovered clusters (i.e. unsupervised prediction)
- For regression, we could use a dummy variable for the clusters as a variable in our regression

ACTIVITY: CLUSTERING + CLASSIFICATION

EXERCISE

1. Using the starter code, perform a k-means clustering on the flight delay data
2. Use the clustering to create a classifier

DELIVERABLE

A completed notebook

CONCLUSION

TOPIC REVIEW

REVIEW AND NEXT STEPS

- Clustering is used to discover features, e.g. segment users or assign labels (such as species)

- Clustering may be the goal (user marketing) or a step in a data science pipeline

BEFORE NEXT CLASS

BEFORE NEXT CLASS

UPCOMING

- Unit Project 4 and Project Proposal - Due Thurs!

LESSON

Q & A

LESSON

EXIT TICKET

DON’T FORGET TO FILL OUT YOUR EXIT TICKET