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 different goals: **feature discovery, pattern recognition**
- **Clustering** is a common and fundamental example of unsupervised learning

CLUSTERING

CLUSTERING

- **Clustering**: Organization of *unlabeled* data into groups
- **Clustering** algorithms try to find meaningful groups within data
- What is a meaningful group?

CLUSTERING

- **Clustering**: Organization of *unlabeled* data into groups
- **Clustering** algorithms try to find meaningful groups within data
- "Meaningful" group/cluster:
    - Points within a group are similar to each other
    - Points from different groups are dissimilar
- What is similar?

CLUSTERING

- **Clustering**: Organization of *unlabeled* data into groups
- **Clustering** algorithms try to find meaningful groups within data
- "Meaningful" group/cluster:
  - Points within a group are similar to each other
  - Points from different groups are dissimilar
- Similarity:
  - Distance measure, e.g. Euclidean, Manhattan, Cosine, Rogers-Tanimoto, Gower, etc.

CLUSTERING

- To summarize,
  - **Proximity measure:** can be similarity (large if similar) or dissimilarity (small if similar) measure
  - **Criterion function:** to evaluate a clustering
  - **Algorithm to optimize clustering:** for e.g. optimize the criterion

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

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

DELIVERABLE

Answers to the above questions

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWERS

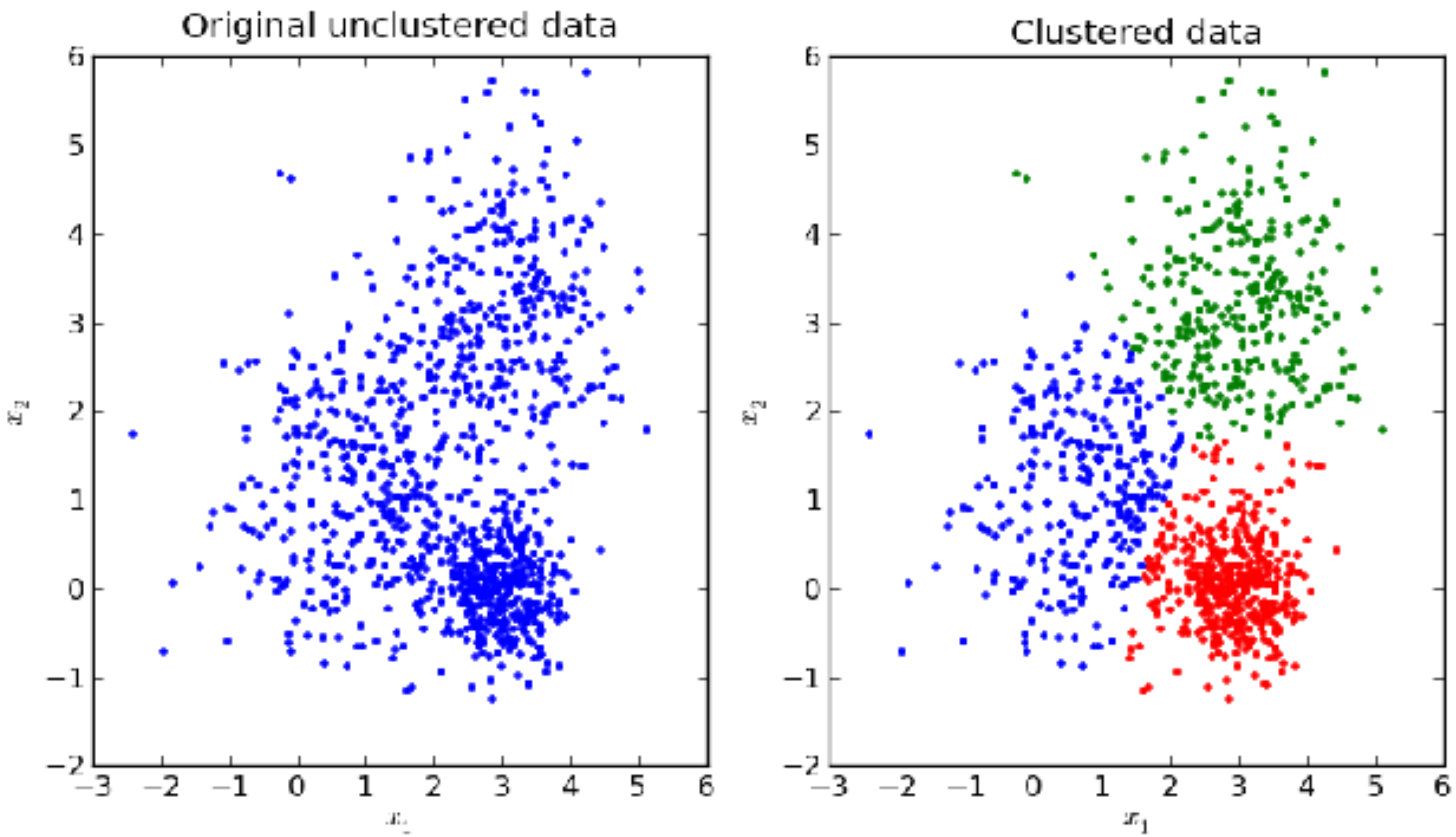
1. Recommendation Systems e.g. Netflix genres
2. Medical Imaging: differentiate tissues
3. Identifying market segments
4. Discover communities in social networks
5. Lots of applications for genomic sequences (homologous sequences, genotypes)
6. Earthquake epicenters
7. Fraud detection

CLUSTERING ALGORITHMS

CLUSTERING: Types of clustering algorithms

- Clustering algorithms are of several types based on model assumptions:
    - Centroid-based
    - Density-based
    - Hierarchical (connectivity- or linkage-based)
    - Distribution-based

CLUSTERING: Centroids



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

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

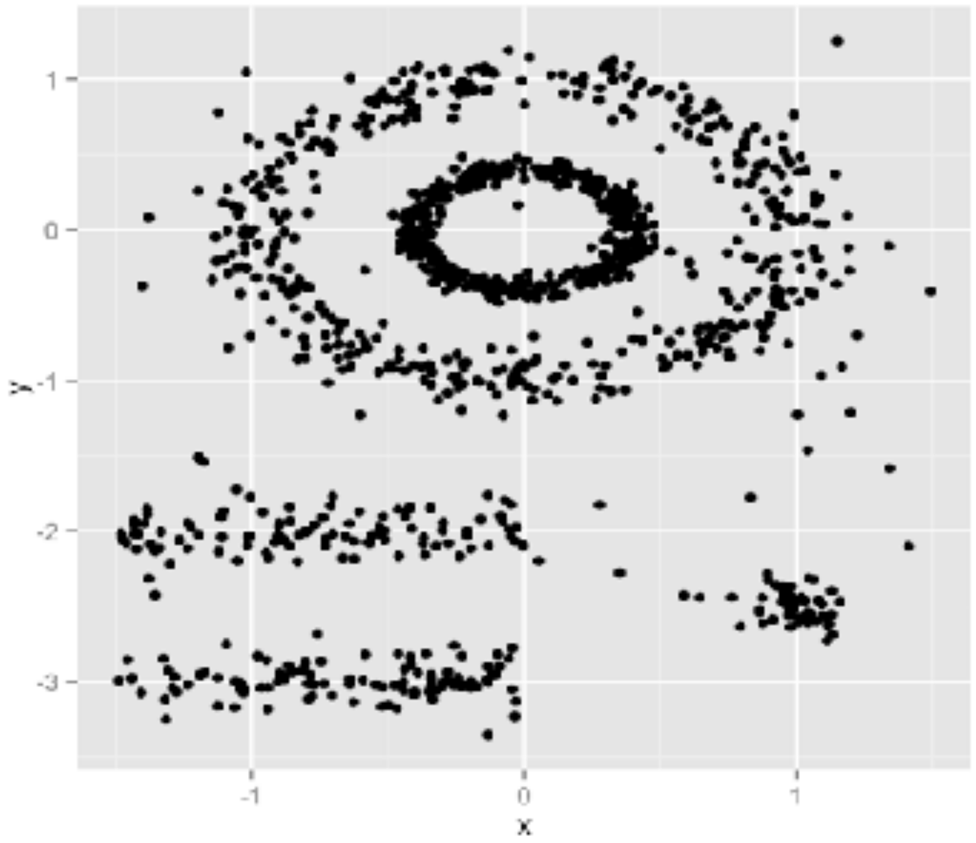
ANSWER THE FOLLOWING QUESTIONS

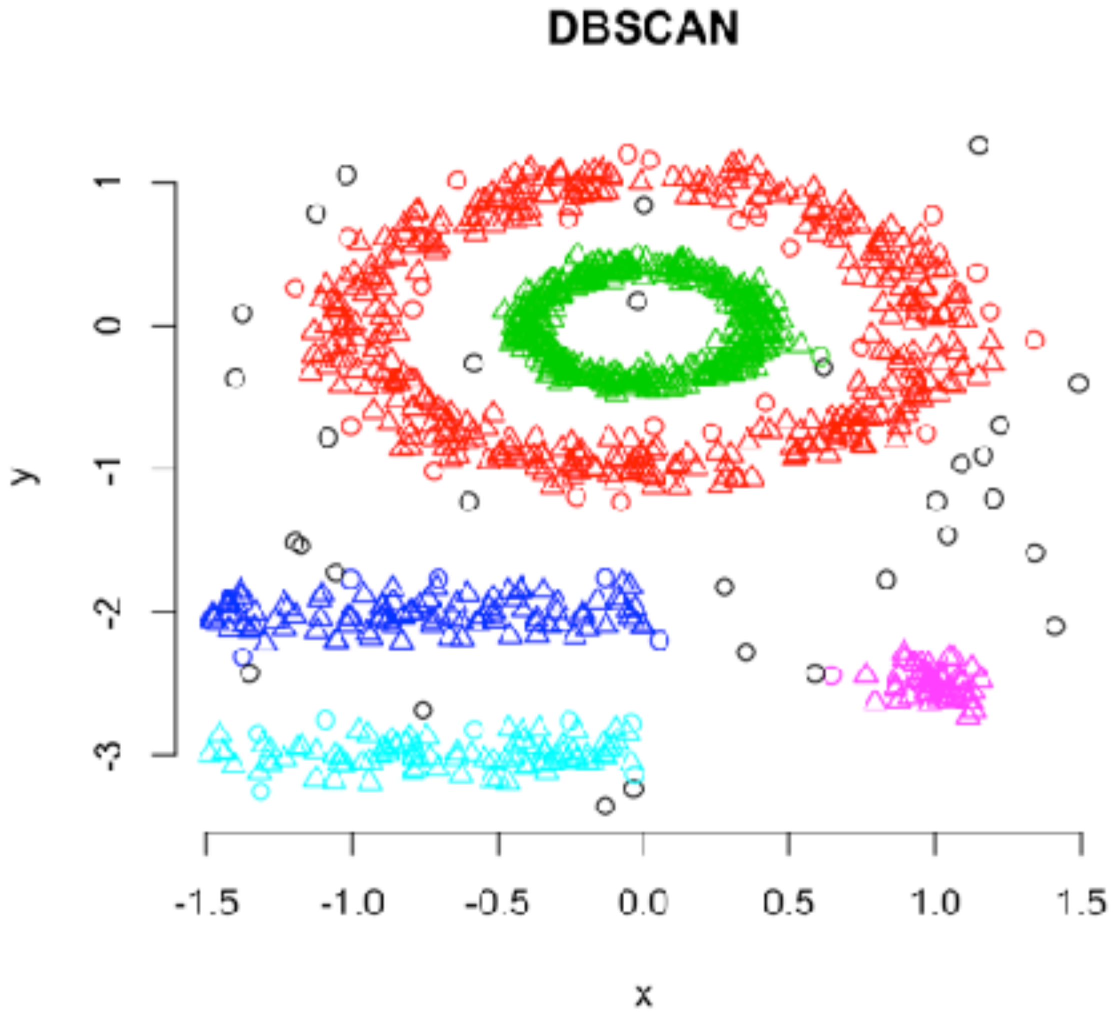
1. Why might data often appear in centered clusters?

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

EXERCISE

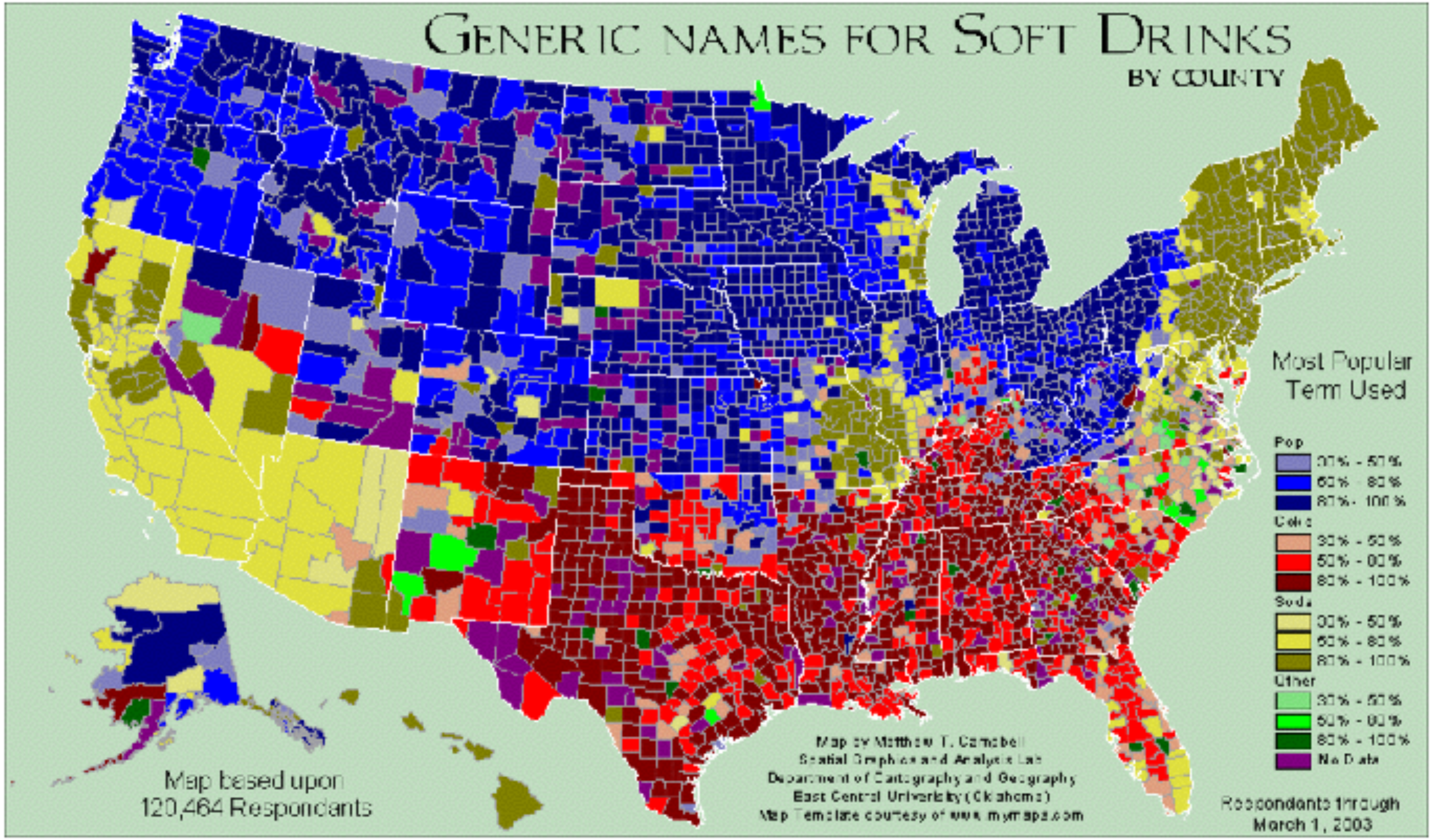
ANSWER THE FOLLOWING QUESTIONS

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

DELIVERABLE

Answers to the above questions

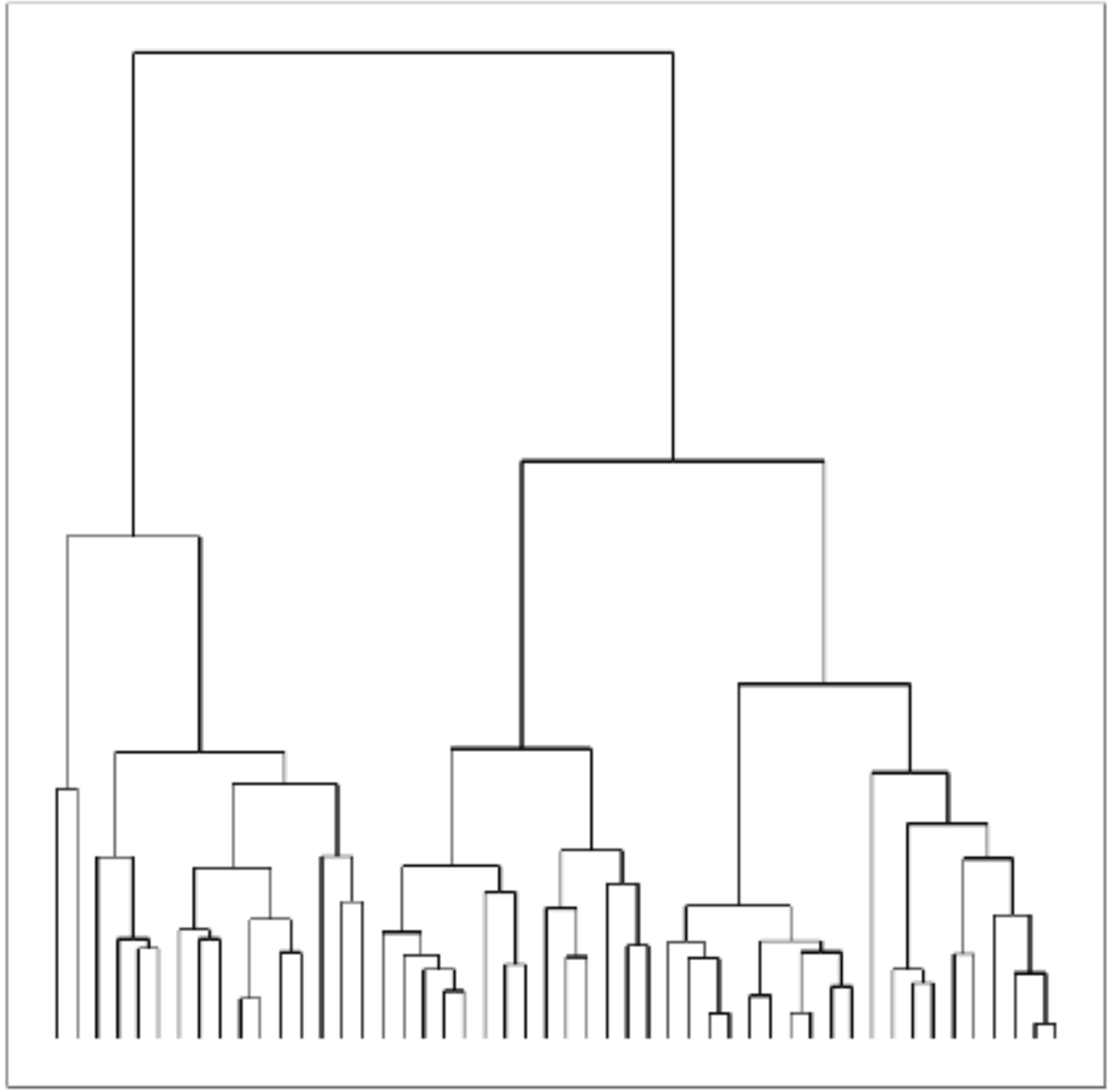
ACTIVITY: KNOWLEDGE CHECK



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

CLUSTERING: Hierarchical

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



ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

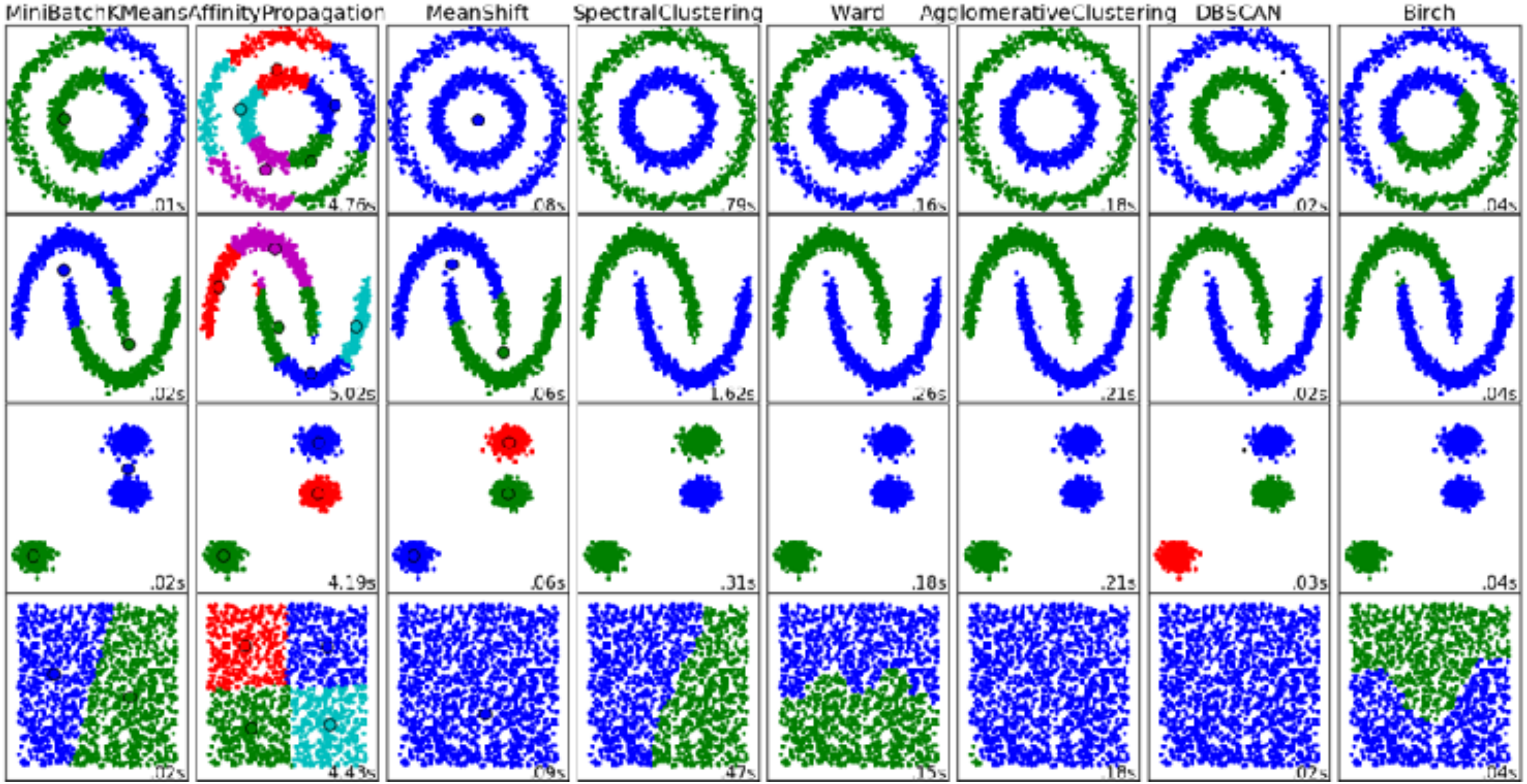
1. How is unsupervised learning different from classification?

DELIVERABLE

Answers to the above questions

CLUSTERING

- There are many clustering algorithms



K-MEANS: CENTRIOD 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

- 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:

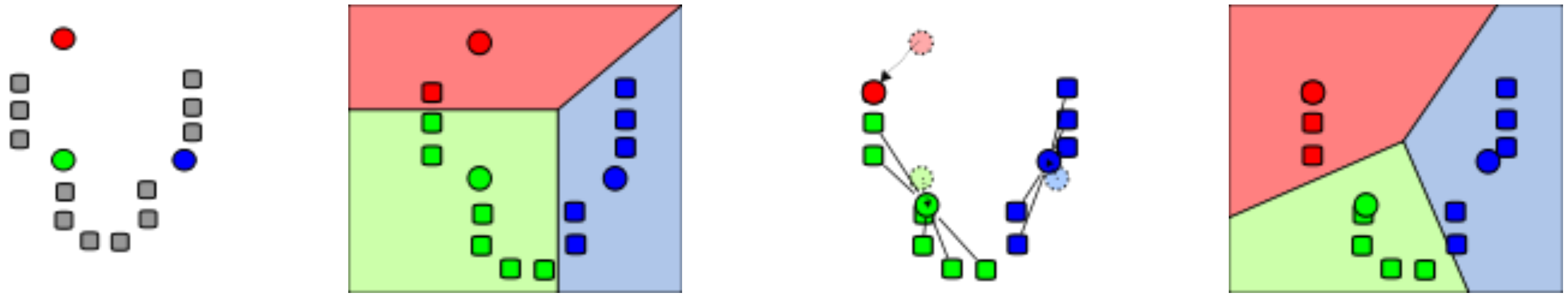
$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \left\| \mathbf{x} - \boldsymbol{\mu}_i \right\|^2$$

K-MEANS CLUSTERING

- 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

- from sklearn.cluster import KMeans
- est = KMeans(n_clusters=3)
- est.fit(X)
- labels = est.labels_

Let’s try it out!

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

1. How do we assign meaning to the clusters we find?
2. Do clusters always have meaning?

DELIVERABLE

Answers to the above questions

K-MEANS CLUSTERING

- Assumptions are important! k-Means assumes:
    - k is the correct number of clusters
    - the data is isotropically distributed (circular/spherical distribution)
    - the variance is the same for each variable
    - clusters are roughly the same size

Nice counterexamples / cases where assumptions are not met:

- http://varianceexplained.org/r/kmeans-free-lunch/
- Scikit-Learn Examples

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

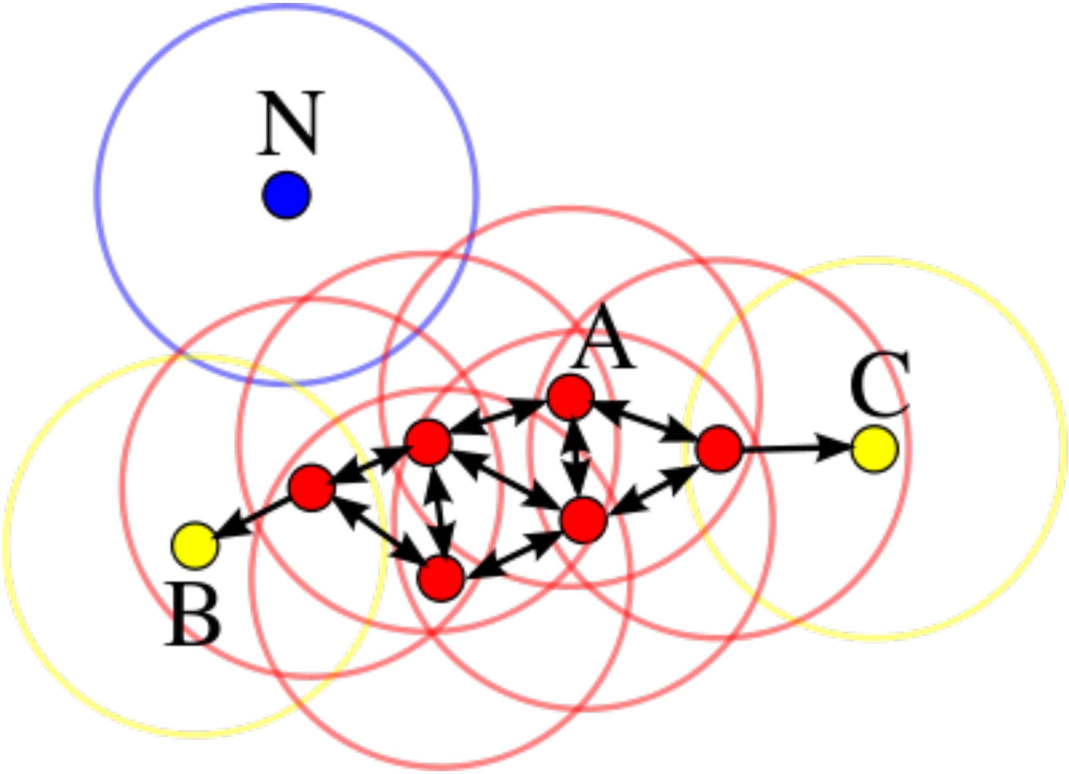
- DBSCAN: Density-based spatial clustering of applications with noise (1996)

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

- Two parameters:
    - min_samples
    - eps

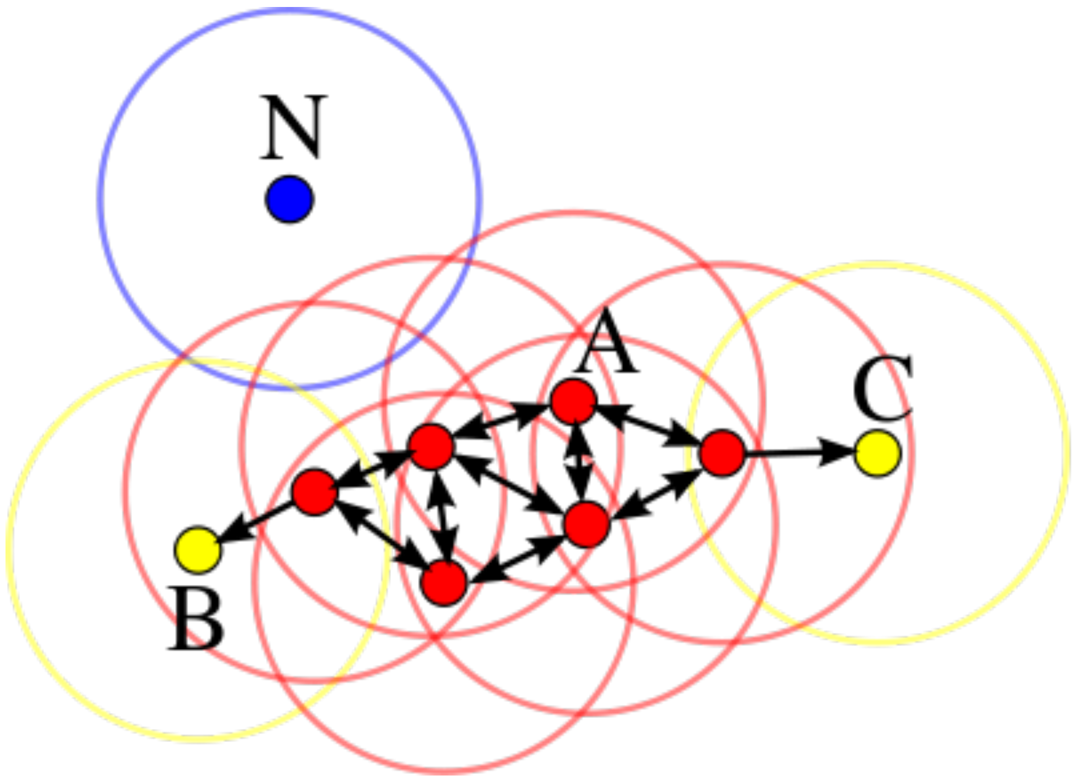
DBSCAN CLUSTERING

- 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

- A cluster is a collection of connected core and reachable points



CLUSTERING: Density-Based

- Another example: Page 6
- Awesome Demo

DBSCAN CLUSTERING

- from sklearn.cluster import DBSCAN
- est = DBSCAN(eps=0.5, min_samples=10)
- est.fit(X)
- labels = est.labels_

Let’s try it out!

DBSCAN CLUSTERING

- DBSCAN advantages:
  - Can find arbitrarily-shaped clusters
  - Don't have to specify number of clusters
  - Robust to outliers
- DBSCAN disadvantages:
  - Doesn't work well when clusters are of varying densities
    - hard to chose parameters that work for all clusters
  - Can be hard to chose correct parameters regardless

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

1. How does DBSCAN differ from k-means?

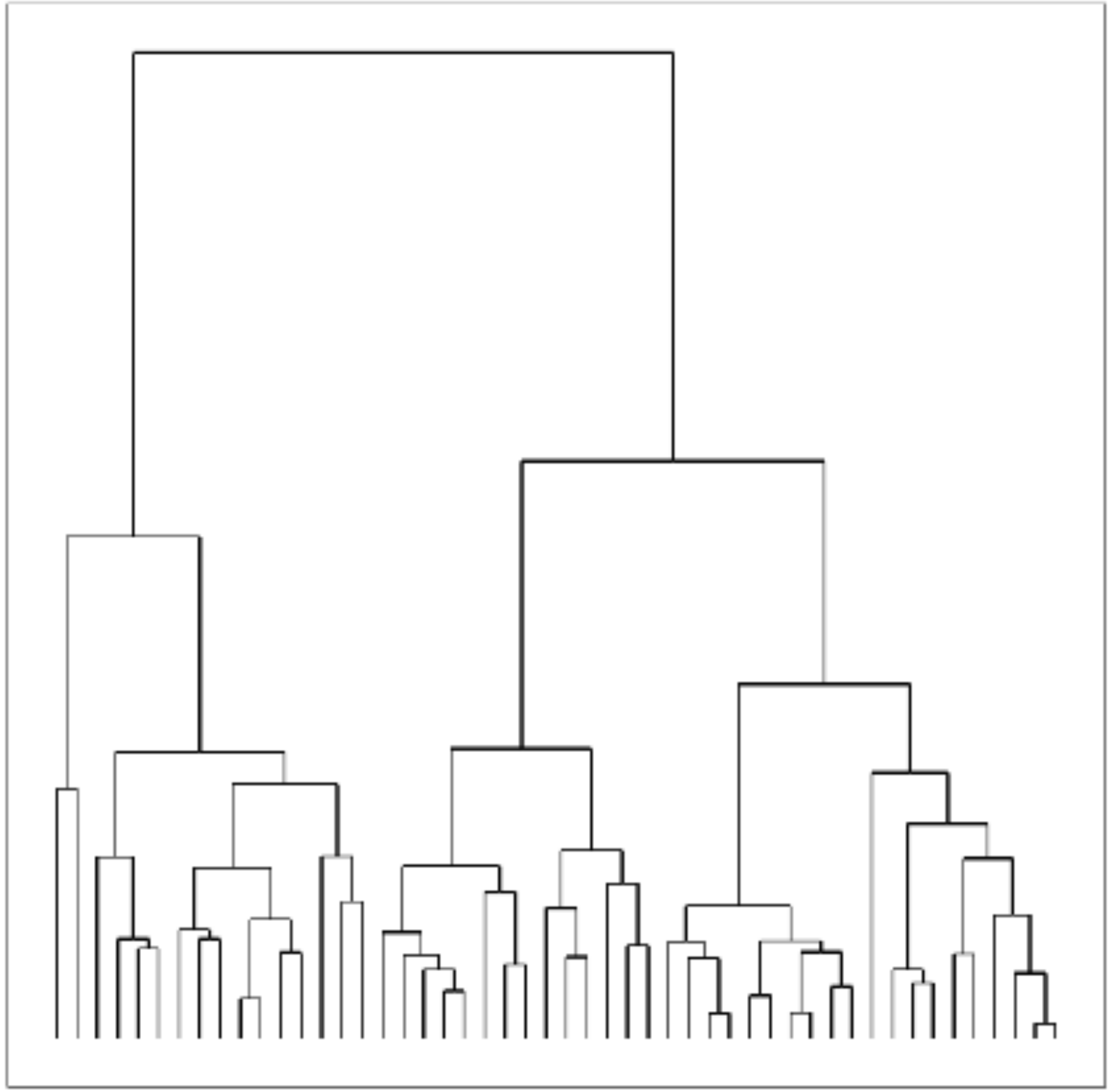
DELIVERABLE

Answers to the above questions

HIERARCHICAL CLUSTERING

CLUSTERING: Hierarchical

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



HIERARCHICAL CLUSTERING

We'll discuss the details once we cover decision trees. For now we can black box the model and fit with sklearn

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

Let's try it out!

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)

CLUSTERING, CLASSIFICATION, AND REGRESSION

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

1. How might we combine clustering and regression or 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
- For regression, we could use a dummy variable for the clusters as a variable in our regression

ACTIVITY: CLUSTERING + REGRESSION

EXERCISE

EXERCISE

1. Follow along as we do an example of clustering with regression.

DELIVERABLE

A completed notebook

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
- Additional reading:
  - https://docs.scipy.org/doc/scipy/reference/spatial.distance.html
  - https://github.com/nicodv/kmodes
  - http://www.mit.edu/~9.54/fall14/slides/Class13.pdf

BEFORE NEXT CLASS

UPCOMING

- Final Project part 2
    - Due Date: Dec 11th
- Unit Project part 4
    - Due Date: Dec 11th

LESSON

Q & A

LESSON

EXIT TICKET

DON’T FORGET TO FILL OUT YOUR EXIT TICKET