GENERAL ASSEMBLY

CLUSTERING

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GA DATA SCIENCE

REVIEW

- What kind of supervised learning problems do you know?
- What are their differences?
- Which models did you get to know?
- How did you evaluate your models?
- What kind of optimisations or parameter tuning you were able to do?

LEARNING OBJECTIVES

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

OPENING

UNSUPERVISED LEARNING

UNSUPERVISED LEARNING

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

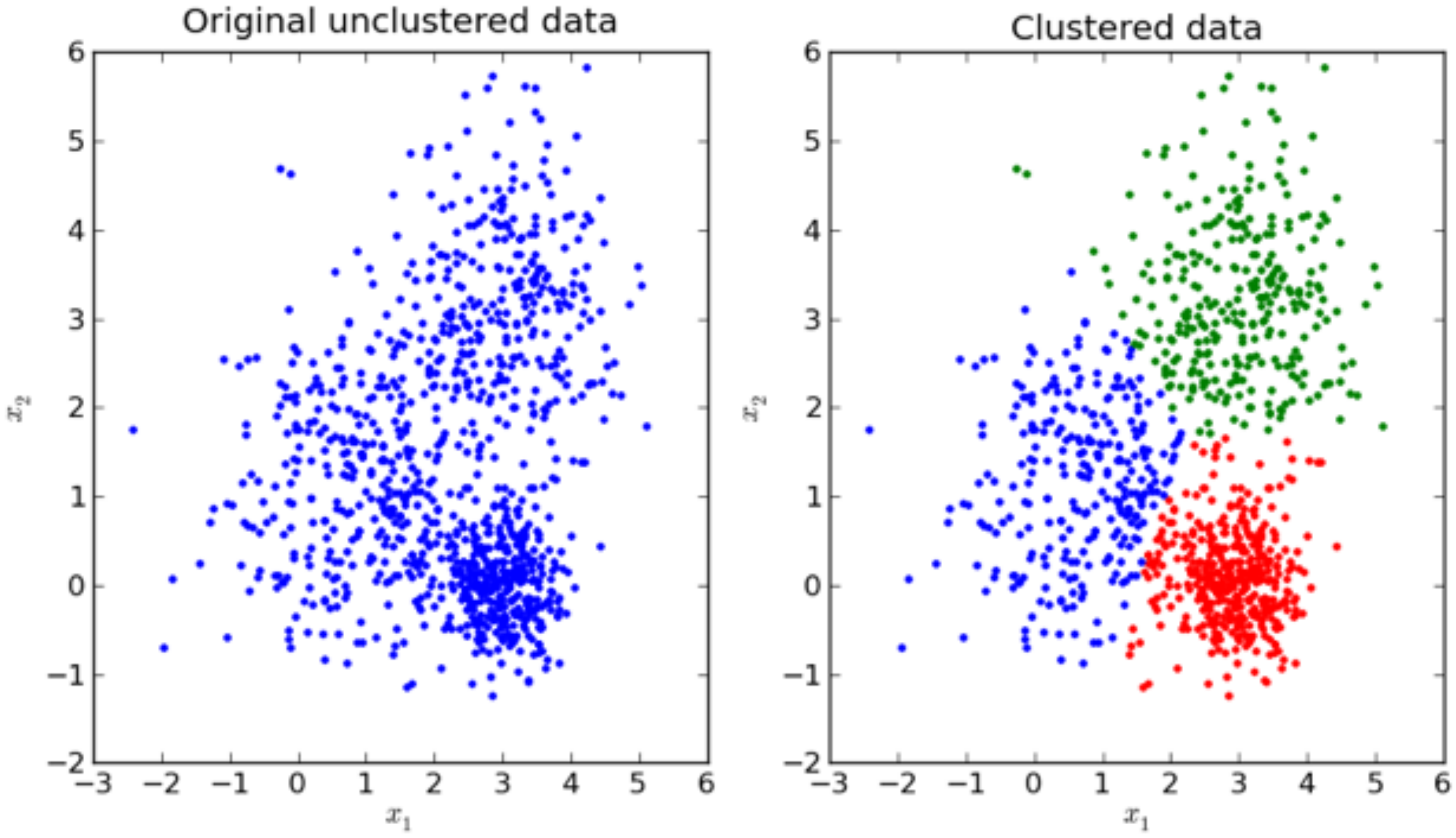
- **Unsupervised learning** has a different goal: **label discovery**

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

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

CLUSTERING

CLUSTERING: Centroids



Source: http://pypr.sourceforge.net/kmeans.html#k-means-example

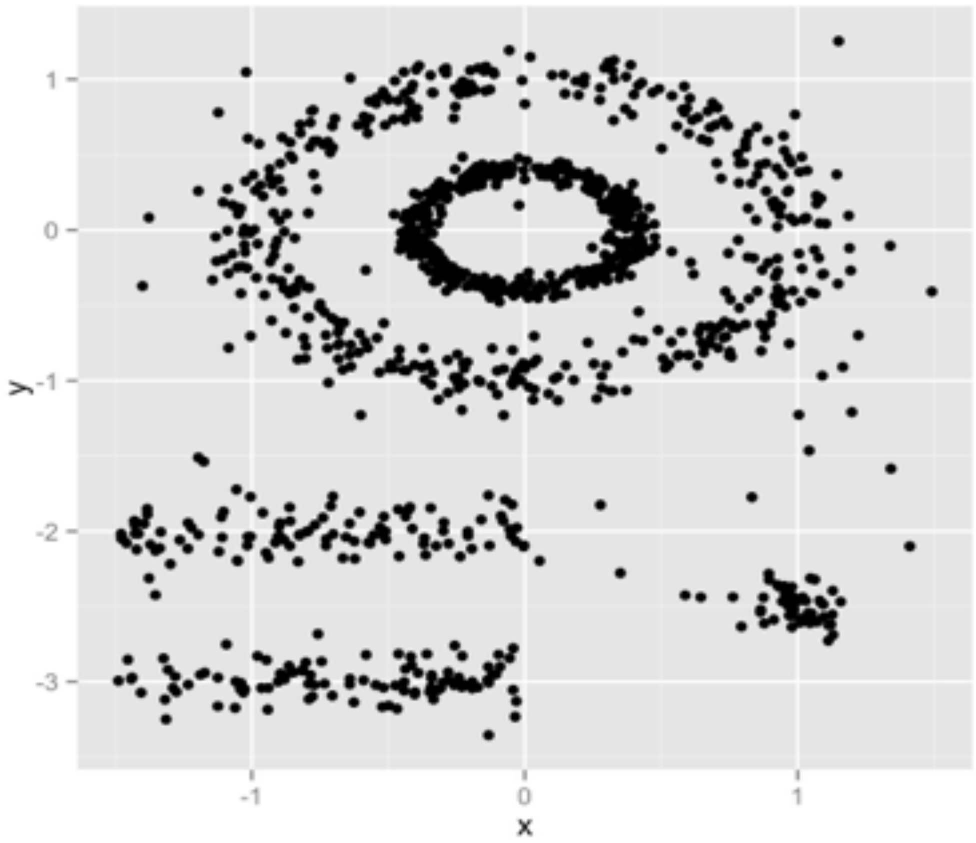
ACTIVITY: KNOWLEDGE CHECK

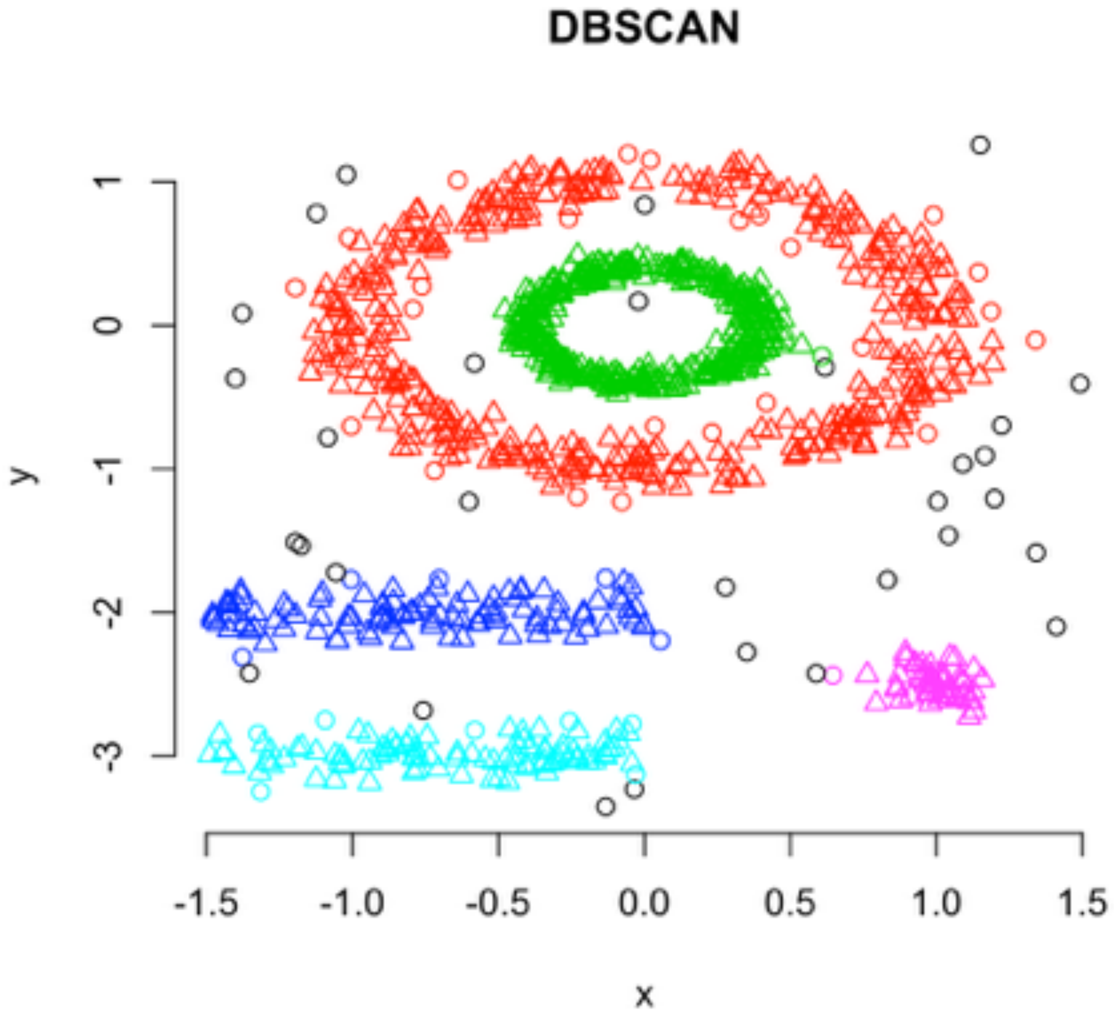
EXERCISE

ANSWER THE FOLLOWING QUESTIONS

1. Why might data often appear in centred clusters?

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

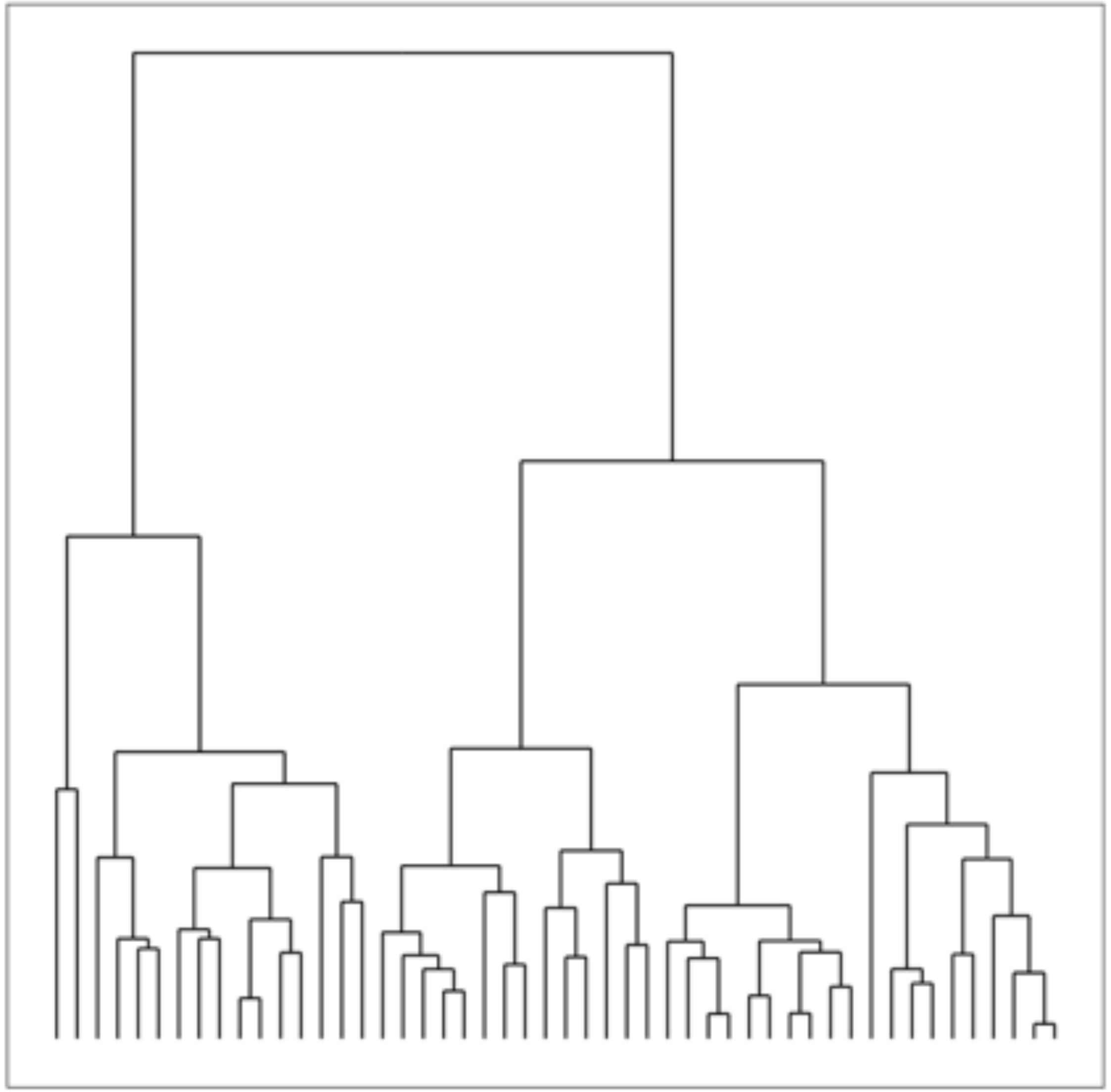
EXERCISE

ANSWER THE FOLLOWING QUESTIONS

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

CLUSTERING: Hierarchical

- Build hierarchies that form clusters
- Based on a tree like structure



ACTIVITY: KNOWLEDGE CHECK

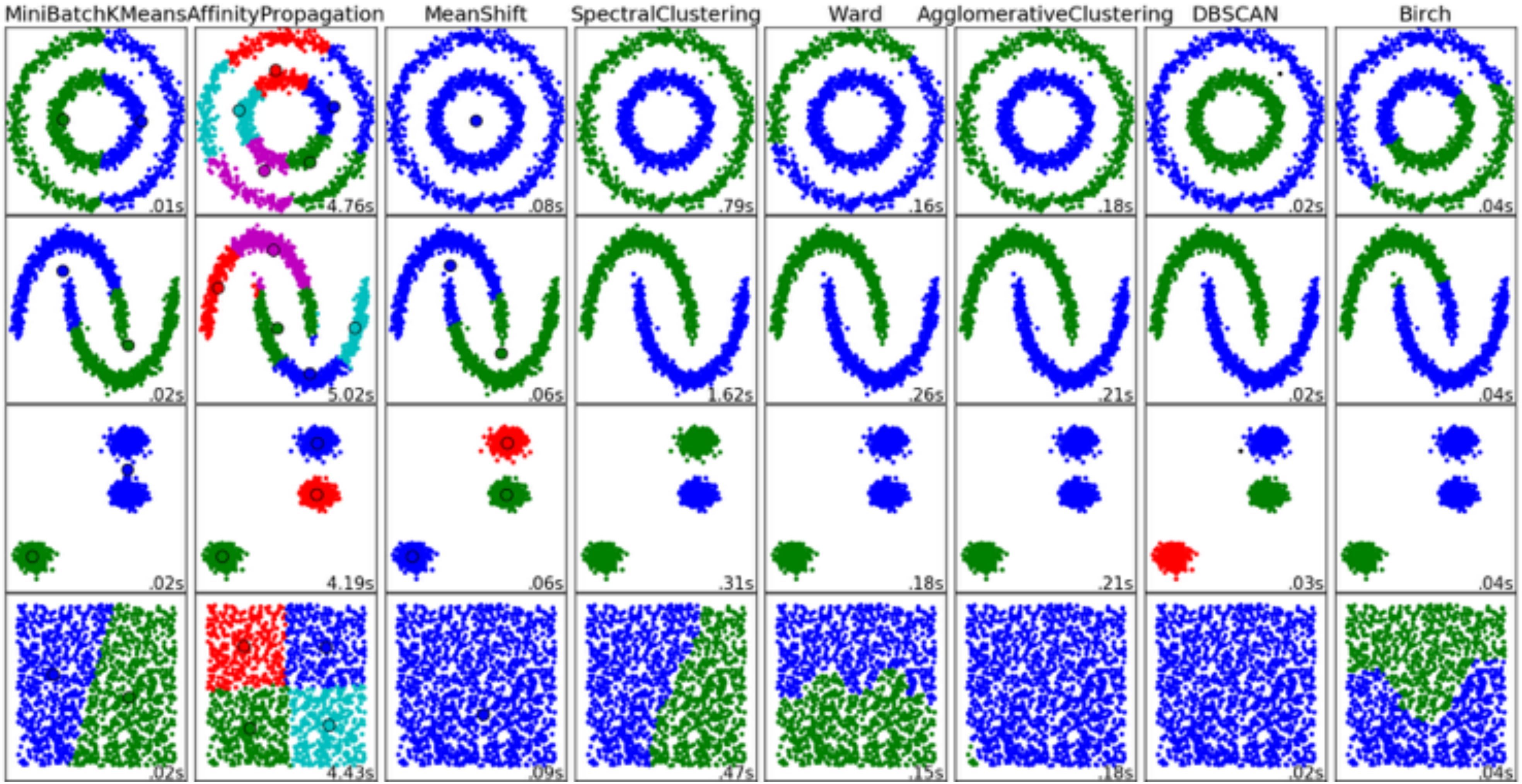
EXERCISE

ANSWER THE FOLLOWING QUESTIONS

1. Why might data often appear in hierarchical clusters?
2. How is unsupervised learning different from classification?

CLUSTERING

- There are many clustering algorithms



ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

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

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 epicentres
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

- k-Means seeks to minimise the sum of squares about the means
- Precisely, find k subsets $S_1, \ldots, S_k$ of the data with means $\mu_1, \ldots, \mu_k$ that minimises:

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

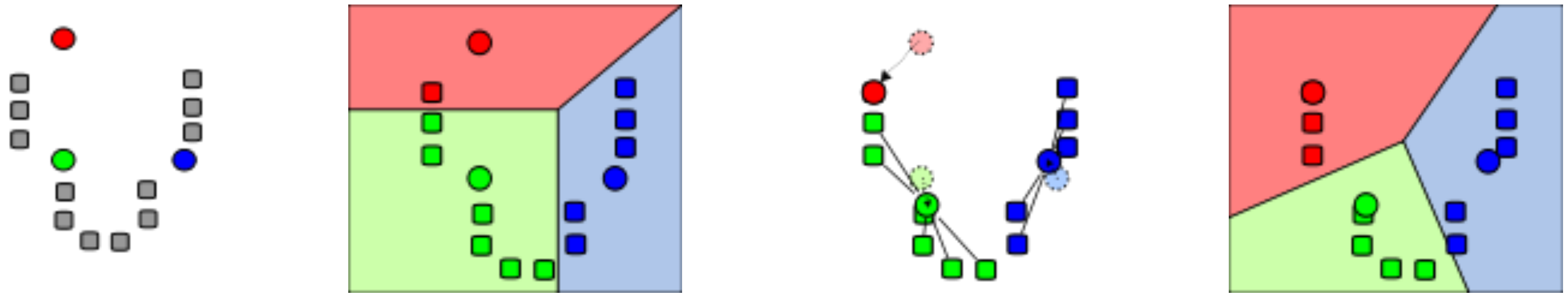
K-MEANS CLUSTERING

- 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?

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

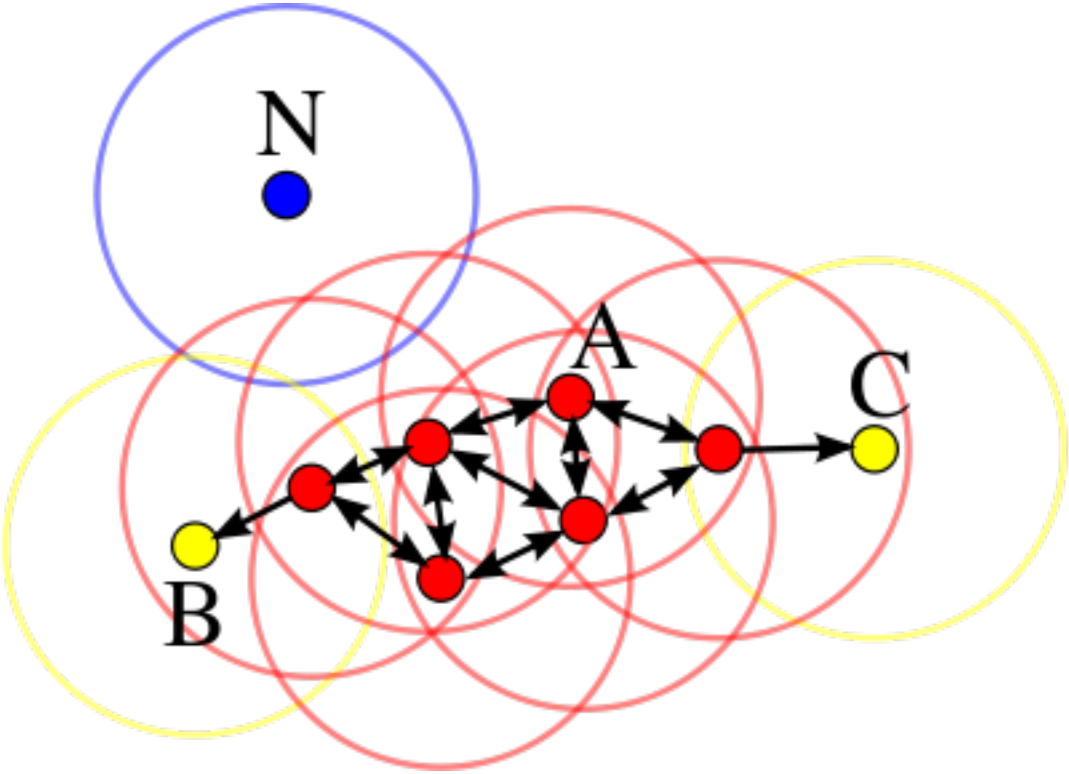
- DBSCAN: Density-based spatial clustering of applications with noise (1996)

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

- Two parameters:
  - min_samples
  - eps

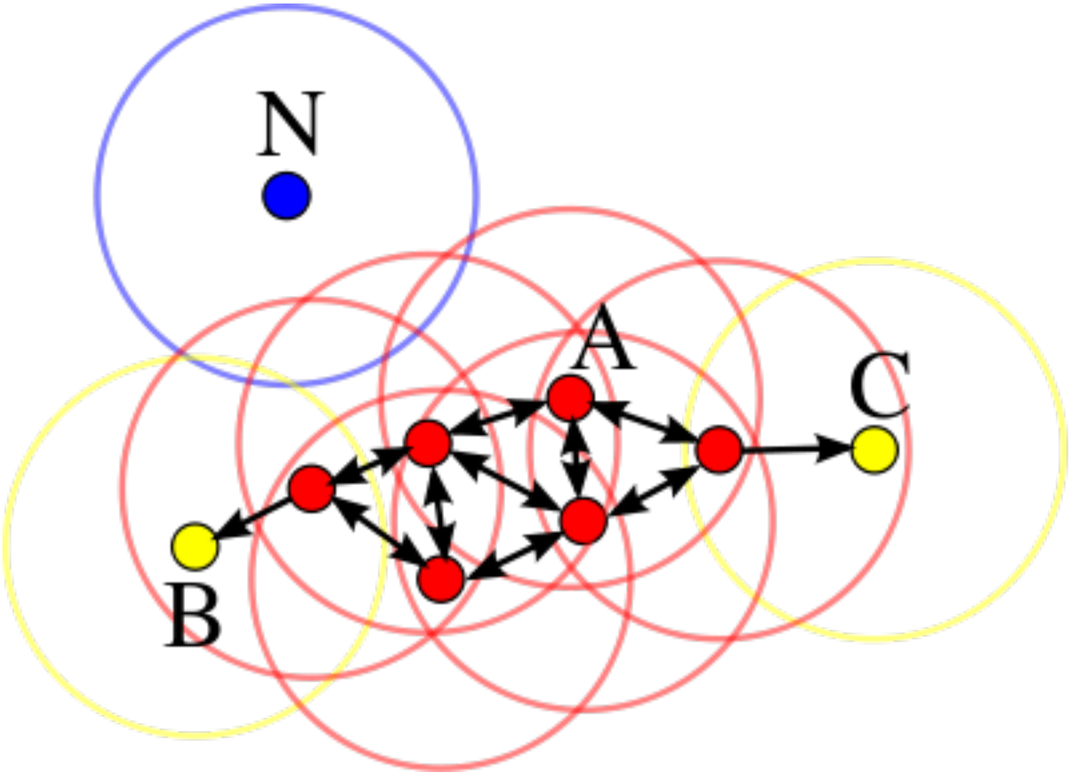
DBSCAN CLUSTERING

- 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

ACTIVITY: KNOWLEDGE CHECK

EXERCISE

ANSWER THE FOLLOWING QUESTIONS

1. How does DBSCAN differ from k-means?

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: CLUSTERING USERS

EXERCISE

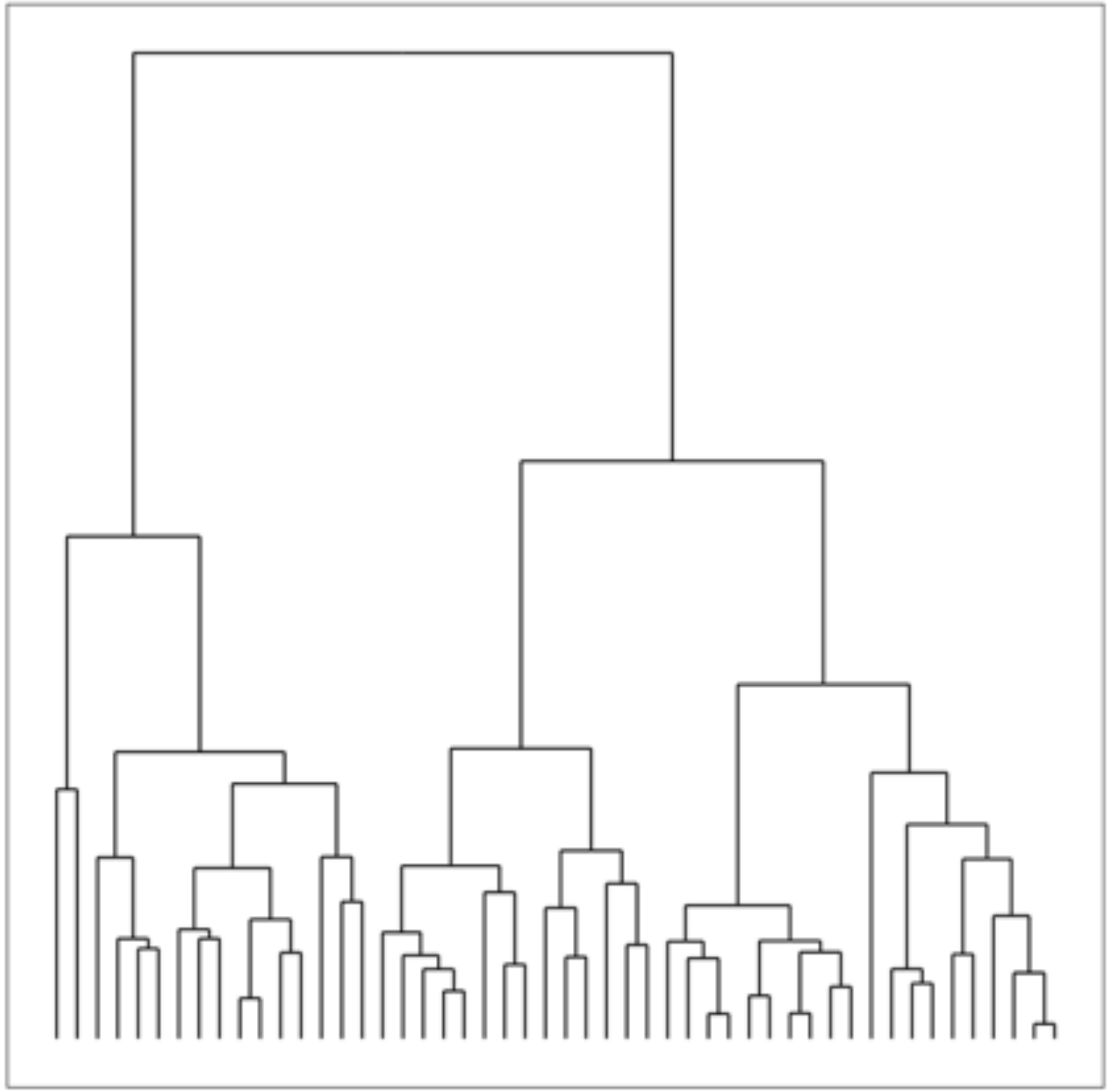
ANSWER THE FOLLOWING QUESTIONS

1. How does DBSCAN differ from k-means?

HIERARCHICAL CLUSTERING

CLUSTERING: Hierarchical

- Build hierarchies that form clusters
- Based on a tree-like structure
- Starts at the bottom with individual clusters
- The most similar data points are combined into a single cluster
- Continue in an agglomerative procedure



HIERARCHICAL CLUSTERING

We can fit the model 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)

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
- 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

COURSE

BEFORE NEXT CLASS

UPCOMING

- Final Project part 4 submission on Wednesday