GENERAL ASSEMBLY

DATA SCIENCE

SYD DAT 8

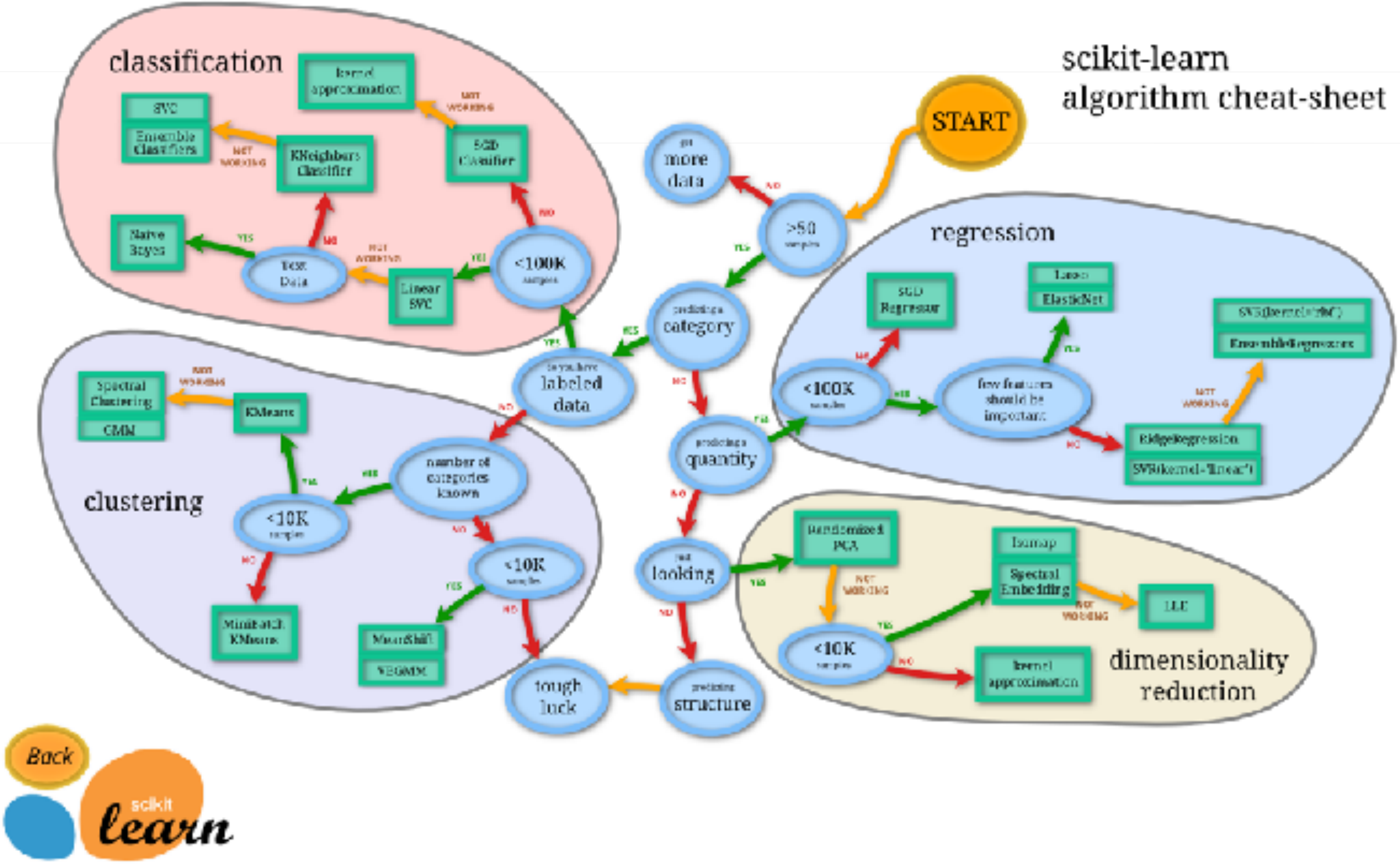
Week 4 - Clustering
Thursday 15th June

AGENDA

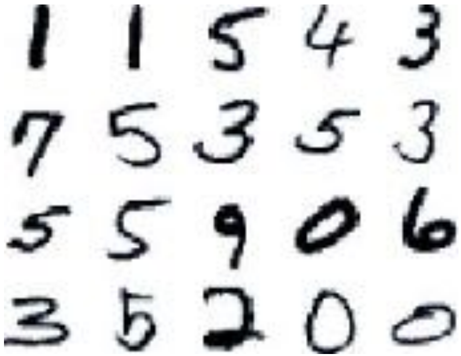
1. Motivation / Review
2. What is Clustering?
3. What is K-Means and how does it work?
4. Lab
5. Discussion

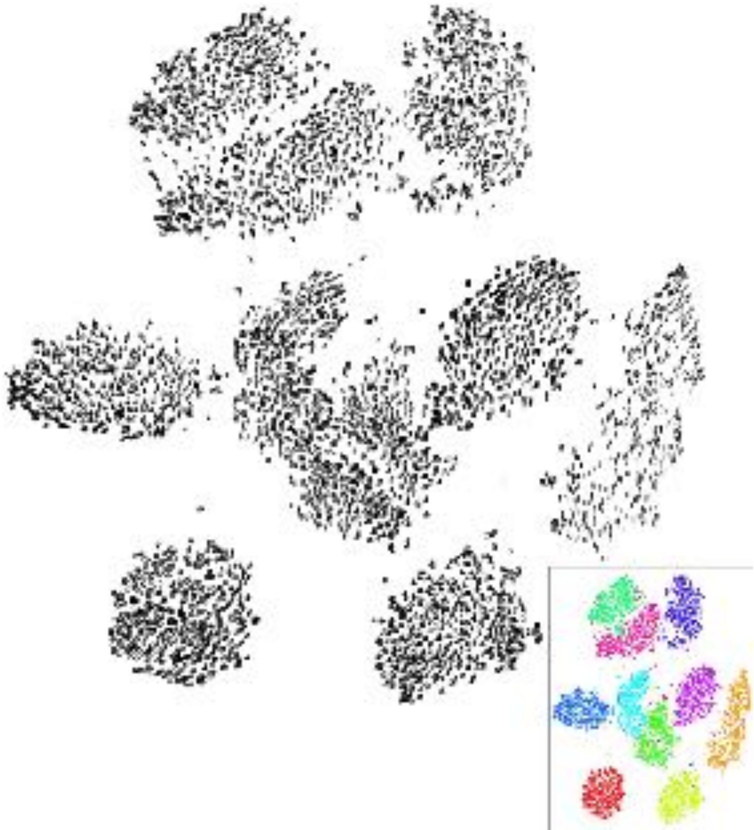
lexer

WHAT IS CLUSTERING AND WHY DO IT?


scikit-learn
algorithm cheat-sheet
START
classification
regression
clustering
dimensionality reduction
>50 samples
get more data
predicting a category
do you have labeled data
predicting a quantity
just looking
predicting structure
tough luck
<100K samples
SGD Classifier
kernel approximation
Linear SVC
Text Data
Naive Bayes
KNeighbors Classifier
SVC
Ensemble Classifiers
number of categories known
<10K samples
KMeans
Spectral Clustering
GMM
MiniBatch KMeans
MeanShift
VBGMM
SGD Regressor
Lasso
ElasticNet
few features should be important
RidgeRegression
SVR(kernel='linear')
SVR(kernel='rbf')
EnsembleRegressors
Randomized PCA
Isomap
Spectral Embedding
LLE
kernel approximation
YES
NO
NOT WORKING
Back
scikit learn

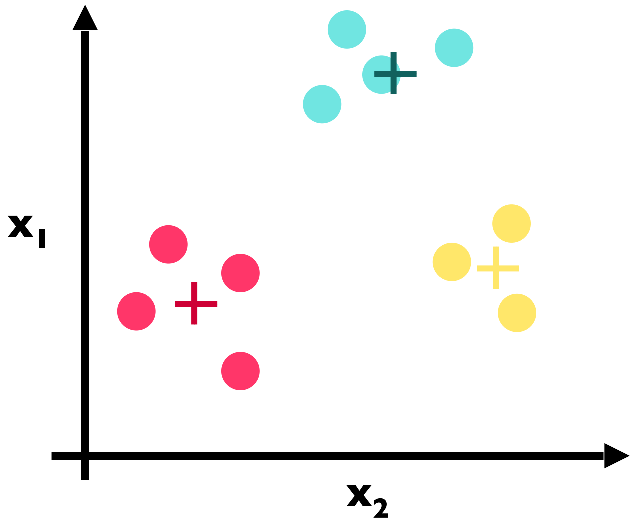
MNIST





Olivetti Faces

- What is a Cluster?
- Why would we do this?
- What is K-Means?



Recall unsupervised learning is when we are trying to find interesting patterns or groups in our data. We don't have a variable we are trying to predict (a Y value).

Clustering aims to discover subgroups in our data where the points are similar to each other. So we have a collection of groups and all points belonging to the same group are similar. Points in different groups are different to each other.

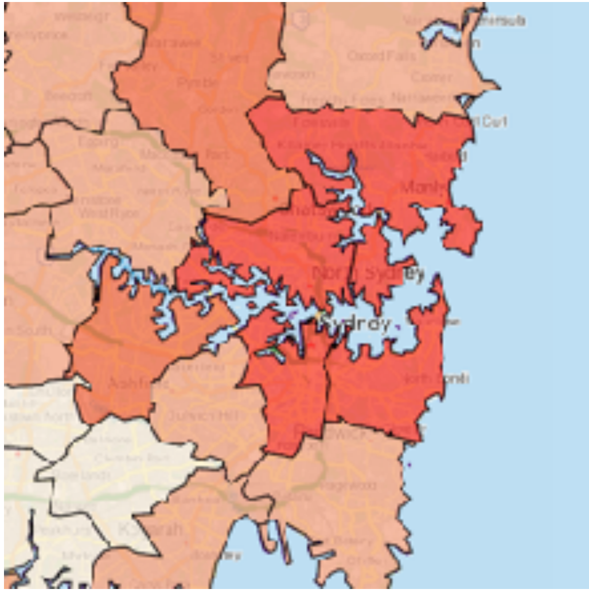
We have to decide what variables we will construct the groups on. What makes them different (or similar)?

To enhance our understanding of a dataset by dividing the data into groups.

Clustering provides a layer of abstraction from individual data points.

The goal is to extract and enhance the natural structure of the data

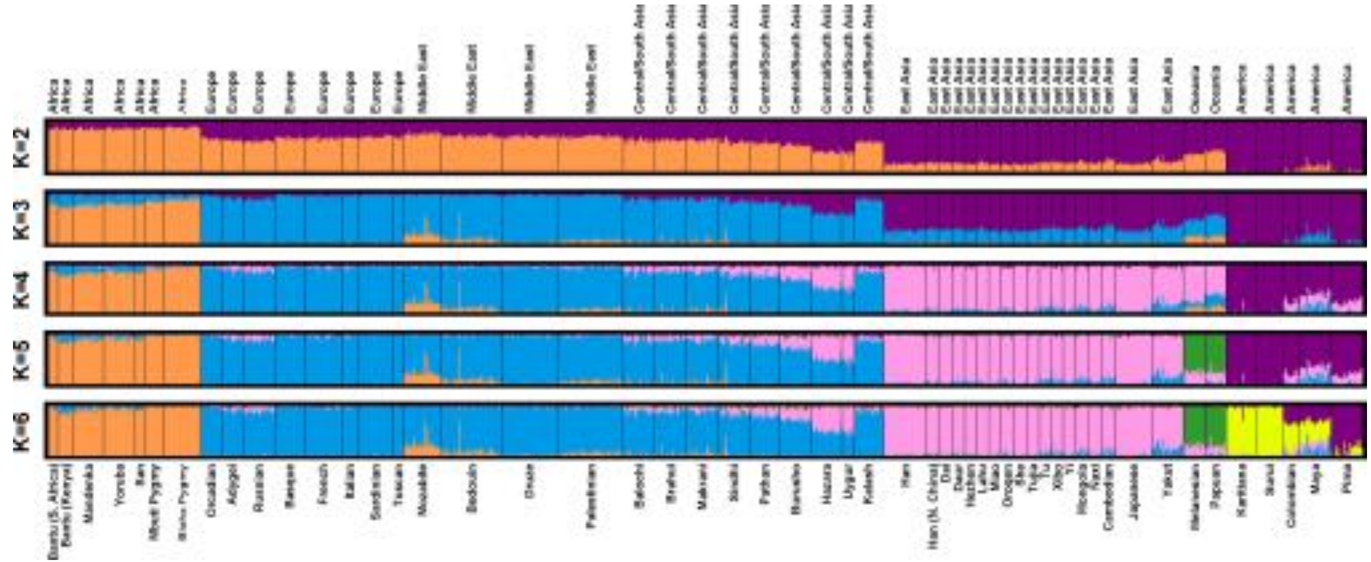
Marketing teams might want to group customers into like groups as a way of summarising the data



WHY WOULD WE CLUSTER DATA?

Financial groups may want to group transactions into like groups as a way to find unusual payments

Genetics data can be clustered to identify ancestry



HOW DO WE CLUSTER DATA?

1) Choose k initial centroids (note that k is an input)

2) For each point:
   - find distance to each centroid
   - assign point to nearest centroid

3) Recalculate centroid positions

4) Repeat steps 2-3 until stopping criteria met

There are several options:

- randomly (but may yield divergent behavior)
- perform alternative clustering task, use resulting centroids as initial k-means centroids
- start with global centroid, choose point at max distance, repeat (but might select outlier)

The similarity criterion is determined by the measure we choose.

In the case of k-means clustering, the similarity metric is the **Euclidian distance:**

$$d(x_1, x_2) = \sqrt{\sum_{i=1}^{N} (x_{1i} - x_{2i})^2}$$

Q: How do we re-compute the positions of the centres at each iteration of the algorithm?

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A: By calculating the centroid (i.e., the geometric centre)

STEP 4 - CONVERGENCE

We iterate until some stopping criteria are met; in general, suitable convergence is achieved in a small number of steps.

Stopping criteria can be based on the centroids (eg, if positions change by no more than ε) or on the points (eg, if no more than x% change clusters between iterations).

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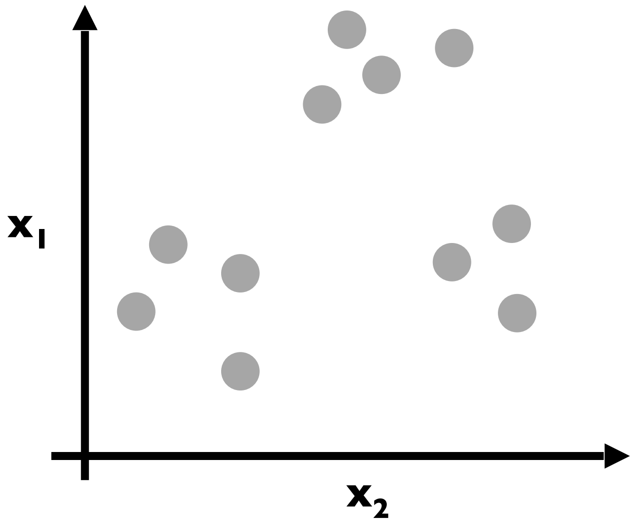

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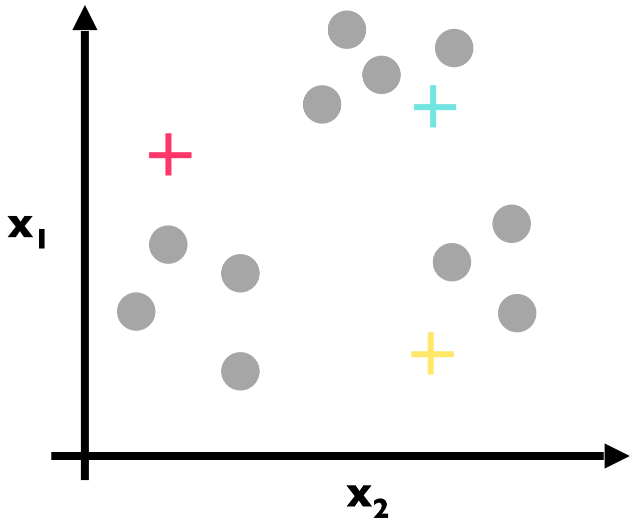

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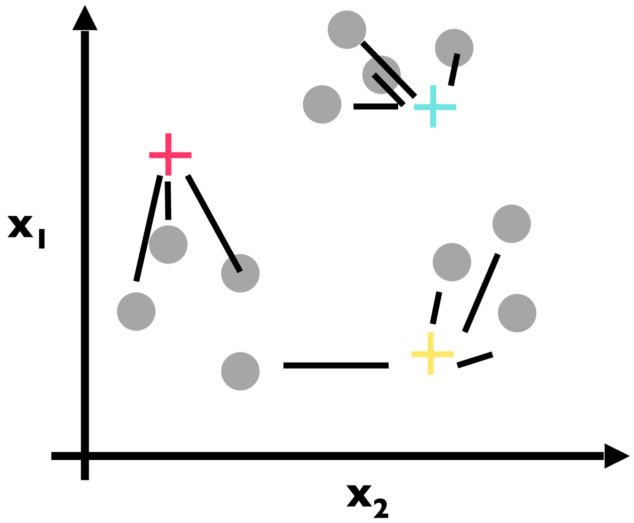
4) Repeat steps 2-3 until stopping criteria met



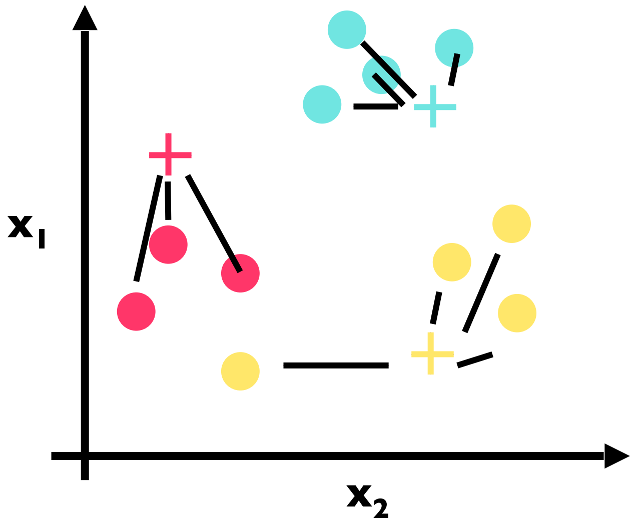
1) Choose k initial centroids

2) For each point:

- find distance to each centroid
- **assign point to nearest centroid**

3) Recalculate centroid positions

4) Repeat steps 2-3 until stopping criteria met



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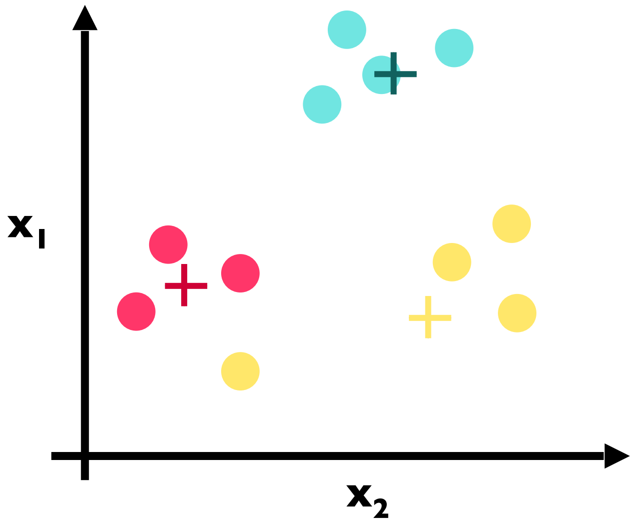

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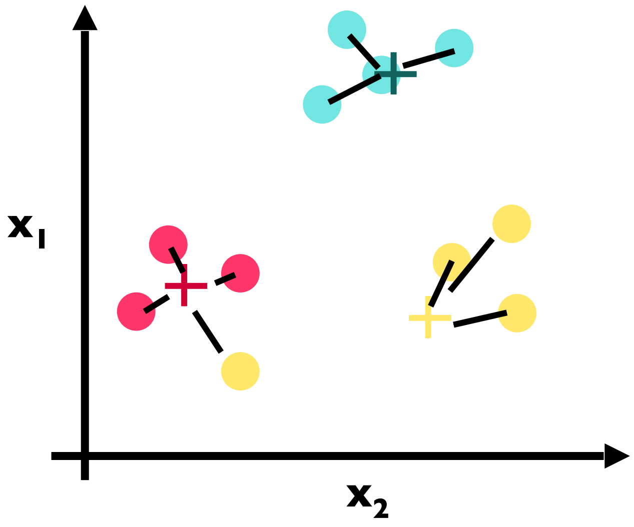

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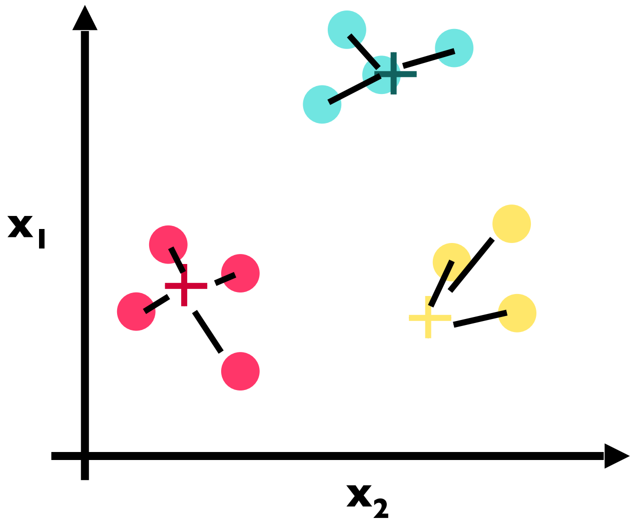

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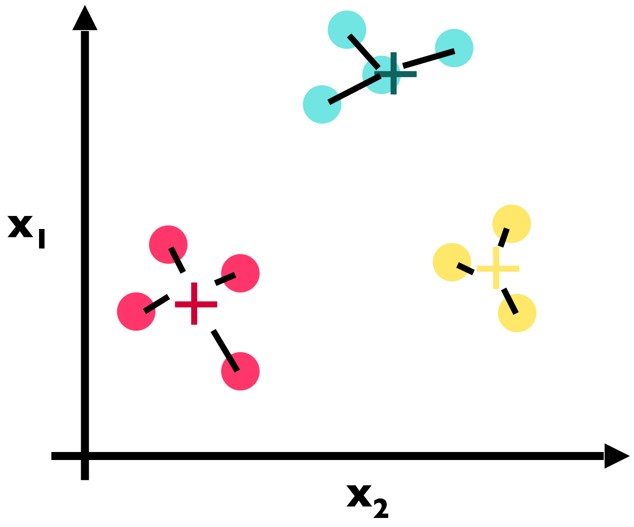

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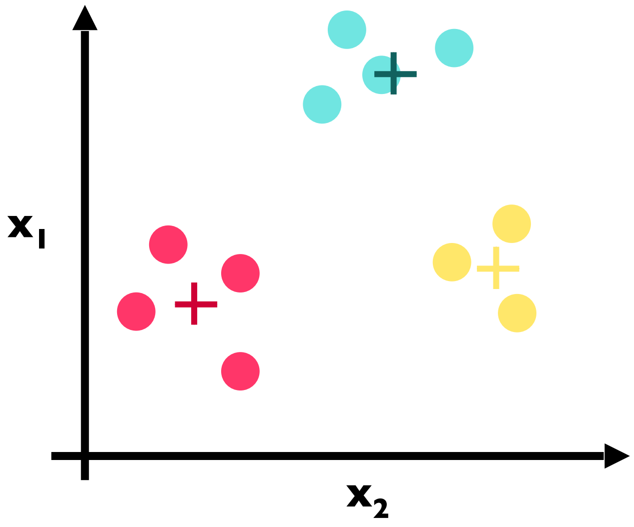

KMEANS WEB DEMO

http://shabal.in/visuals/kmeans/6.html

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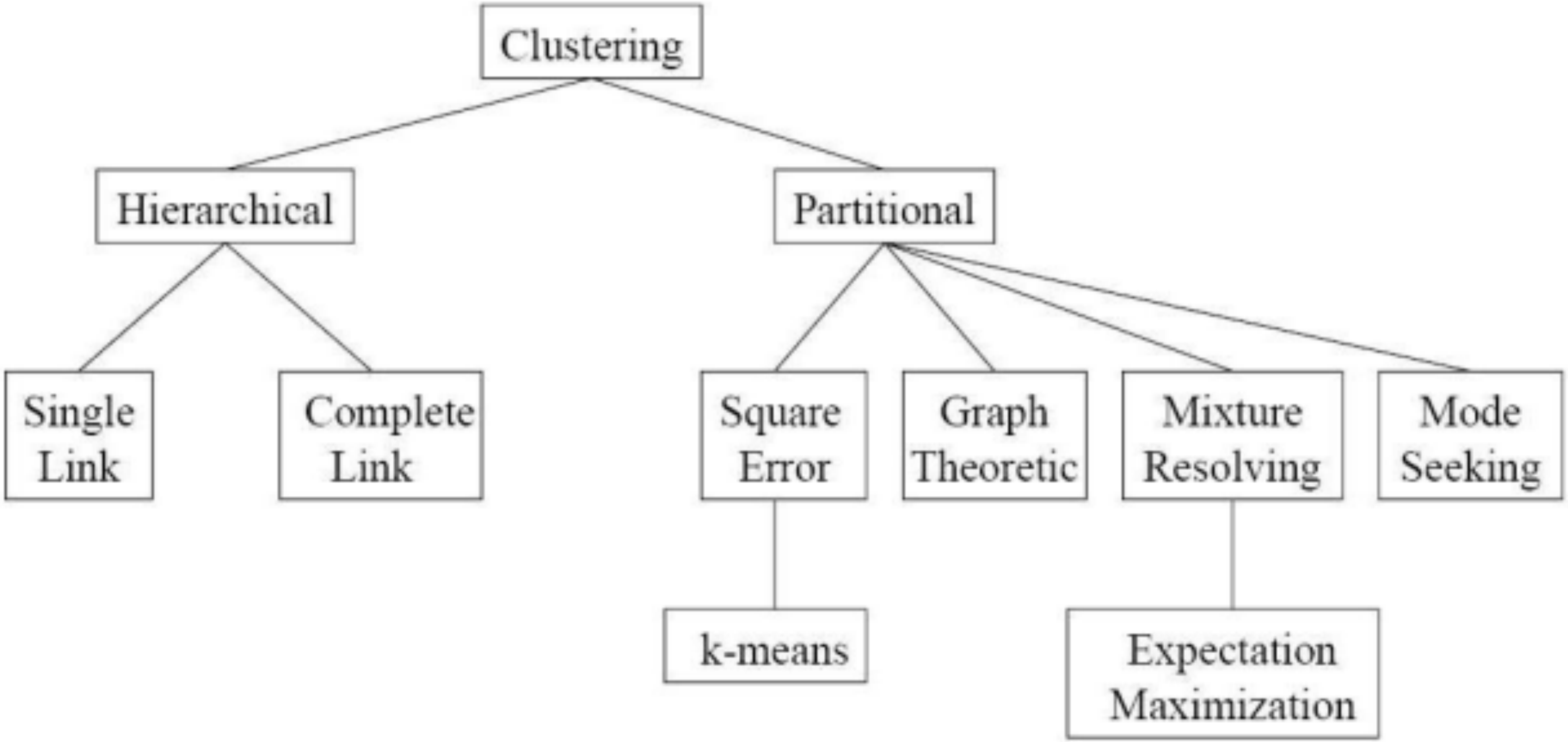
Other good demos:

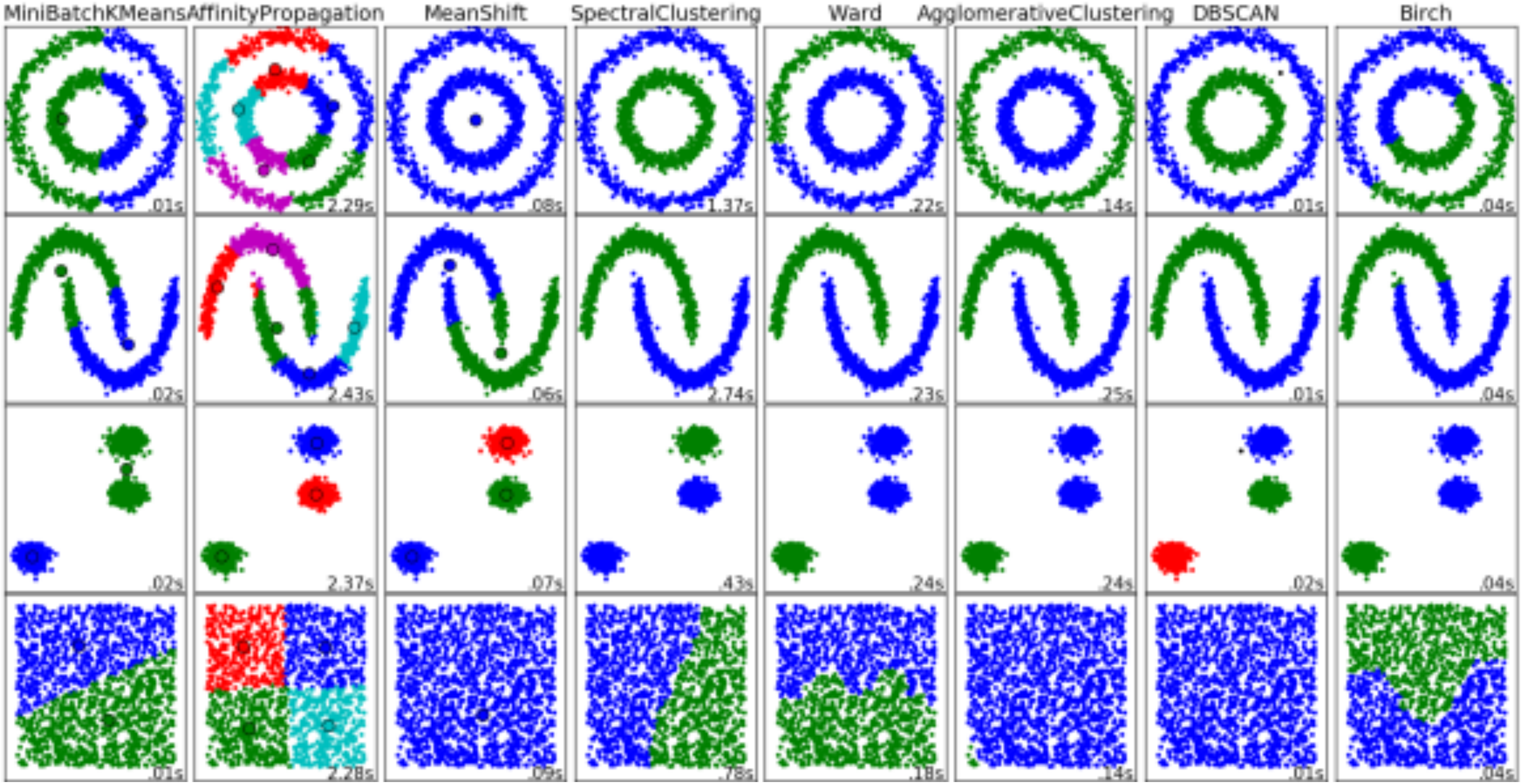
https://www.youtube.com/watch?v=mtkWR8sx0NA
https://www.youtube.com/watch?v=_aWzGGNrcic (especially from minute 4:22)
http://www.onmyphd.com/?p=k-means.clustering

DATA SCIENCE PART TIME COURSE

OTHER CLUSTERING ALGORITHMS


Clustering
Hierarchical
Partitional
Single Link
Complete Link
Square Error
Graph Theoretic
Mixture Resolving
Mode Seeking
k-means
Expectation Maximization

VARIETY OF CLUSTERING OPTIONS



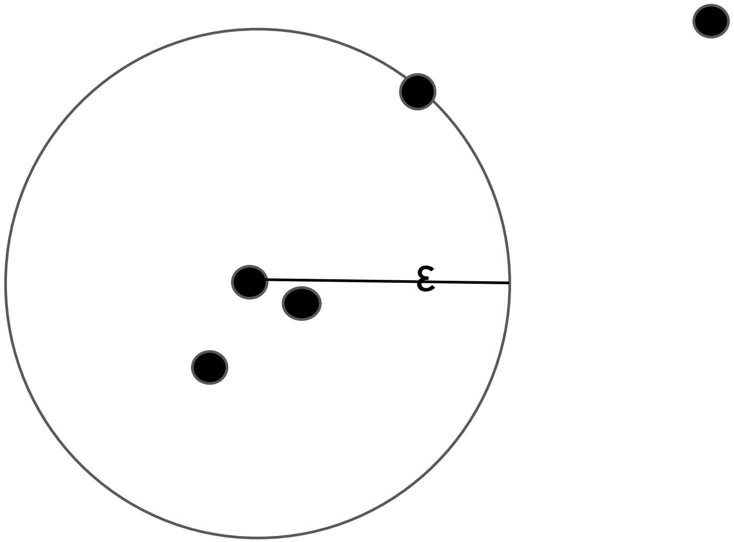
Density-Based Spatial Clustering of Applications with Noise (DBSCAN)

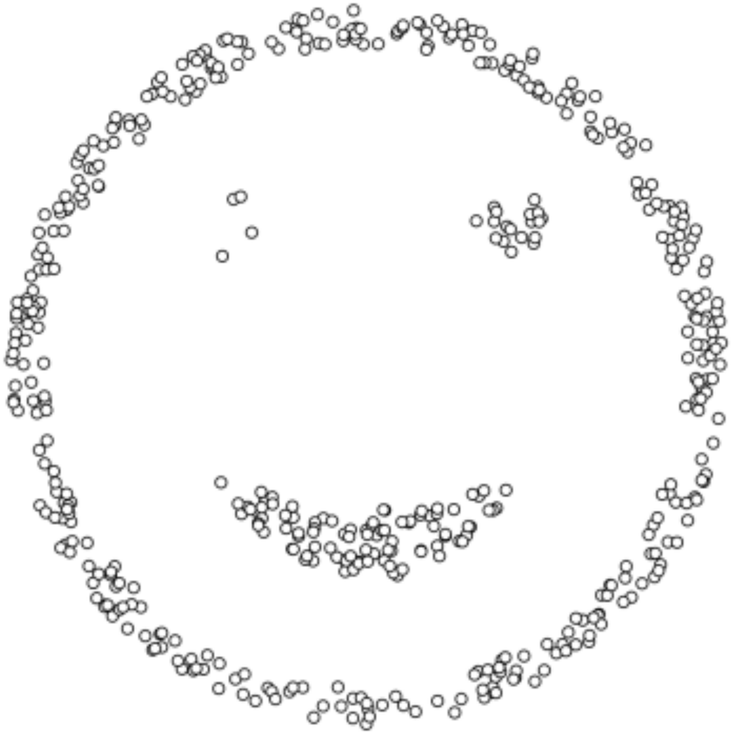
Criteria

- **ε (or Epsilon)** is the radius
- **minPoints** (number of points within the ε-Neighborhood required for classification)

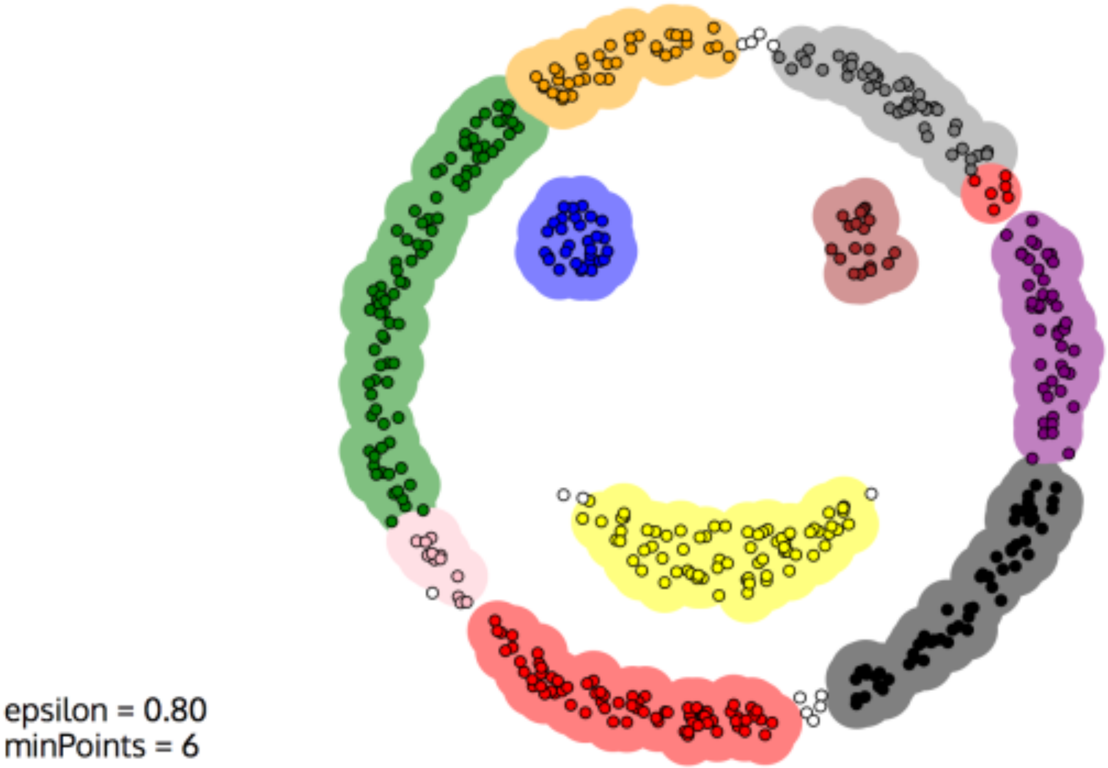
Note

- DBSCAN iterates through every point
- Core object (point meeting the criteria)
- Outlier (outside the radius)

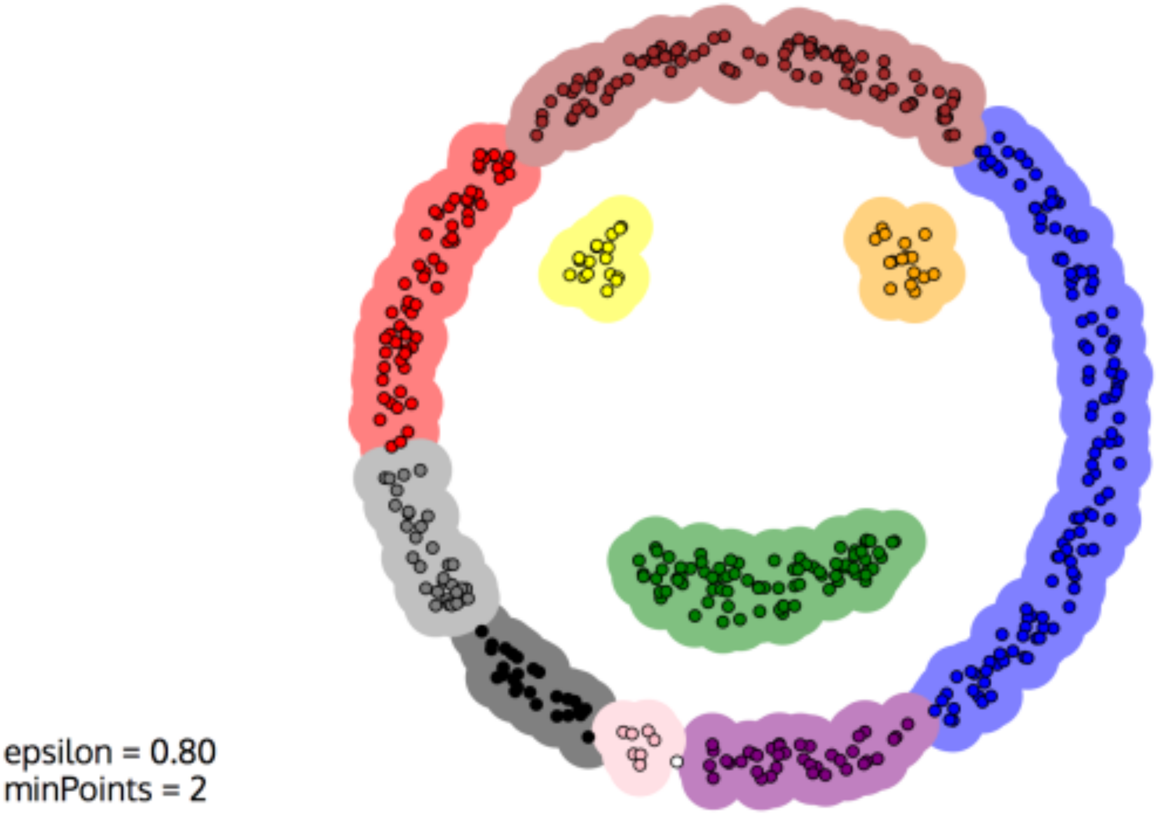




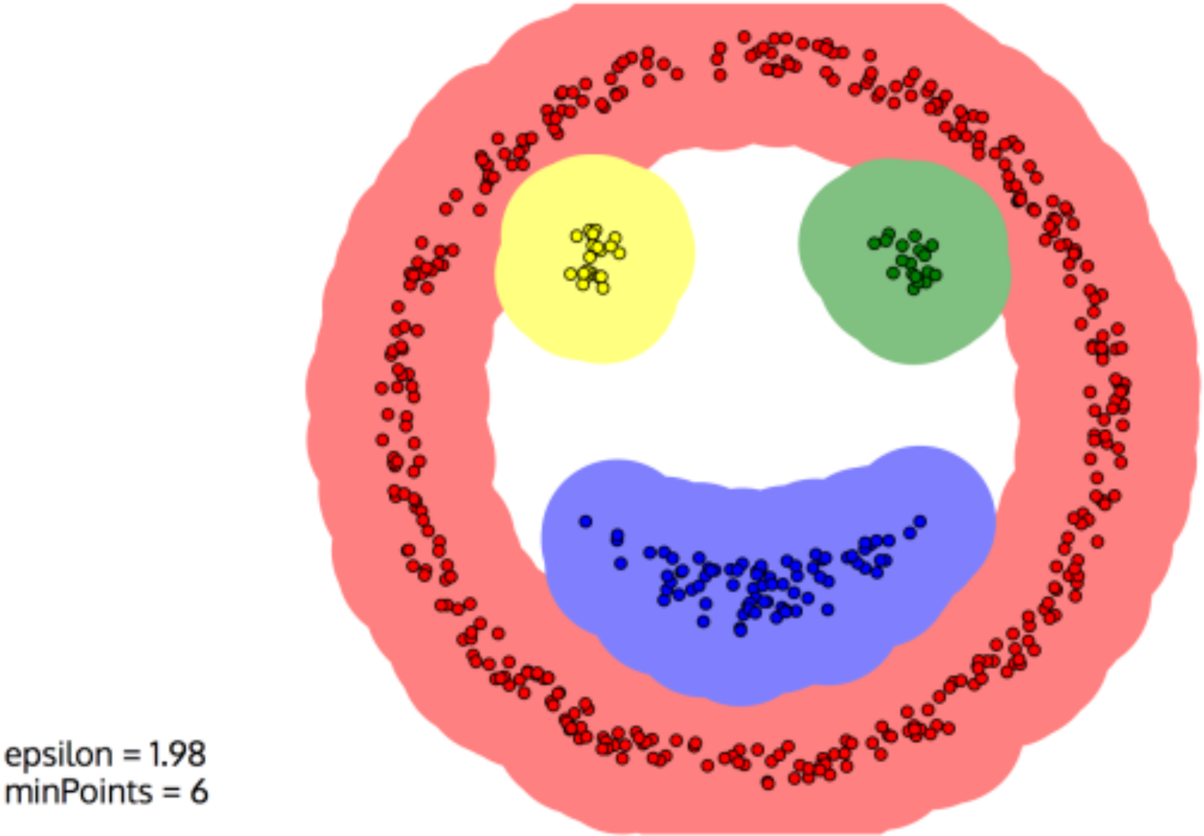
11 Clusters
Patchy



10 Clusters
Less Patchy



4 Clusters
Lion King



https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

Pros

Recovers more complex cluster shapes
Finds the number of clusters
Automatically find outliers

Cons

Requires a distance function
Not as scalable as K-means
Calculating connected components can be difficult

HOW DO WE KNOW OUR CLUSTERS ARE ANY GOOD?

In general, k-means will converge to a solution and return a partition of k clusters, even if no natural clusters exist in the data.

We will look at two validation metrics useful for partitional clustering, **cohesion** and **separation**.

Cohesion measures clustering effectiveness within a cluster.

$$\hat{C}(C_i) = \sum_{x \in C_i} d(x, c_i)$$

Separation measures clustering effectiveness between clusters.

$$\hat{S}(C_i, C_j) = d(c_i, c_j)$$

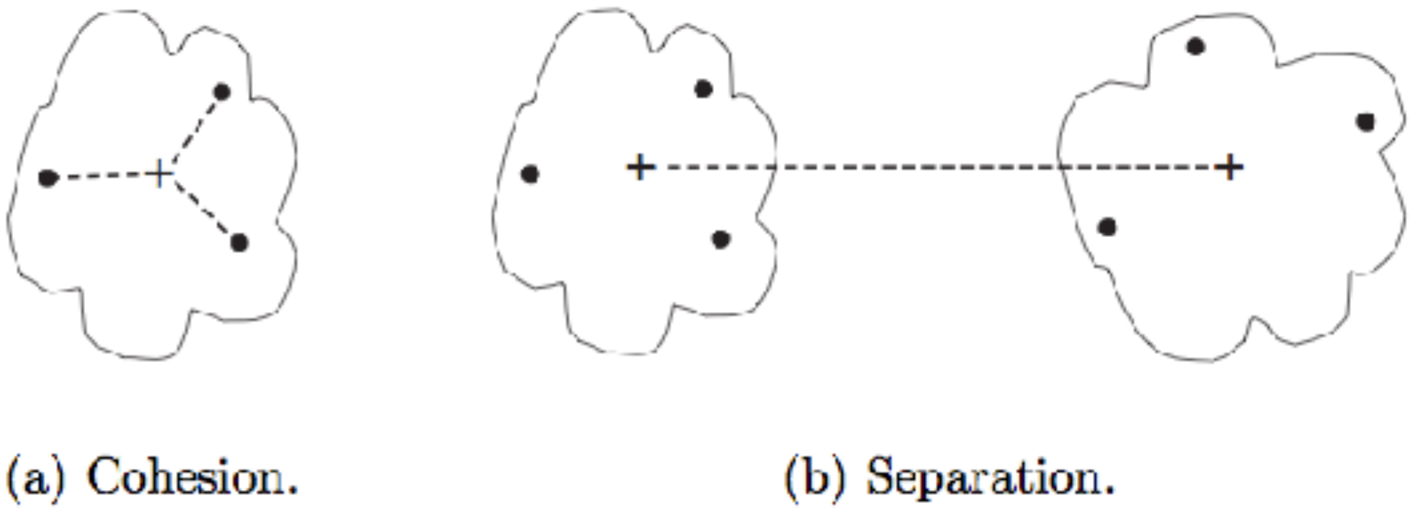


Figure 8.28. Prototype-based view of cluster cohesion and separation.

source: http://www-users.cs.umn.edu/~kumar/dmbook/ch8.pdf

A useful measure that combines the ideas of cohesion and separation is the silhouette coefficient. For point x_i, this is given by:

$$SC_i = \frac{b_i - a_i}{max(a_i, b_i)}$$

such that:

a_i = average in-cluster distance to x_i

b_{ij} = average between-cluster distance to x_i

$b_i = min_j(b_{ij})$

The silhouette coefficient can take values between -1 and 1.

In general, we want separation to be high and cohesion to be low. This corresponds to a value of SC close to +1.

A negative silhouette coefficient means the cluster radius is larger than the space between clusters, and thus clusters overlap

One useful application of cluster validation is to determine the best number of clusters for your dataset.

Q: How would you do this?

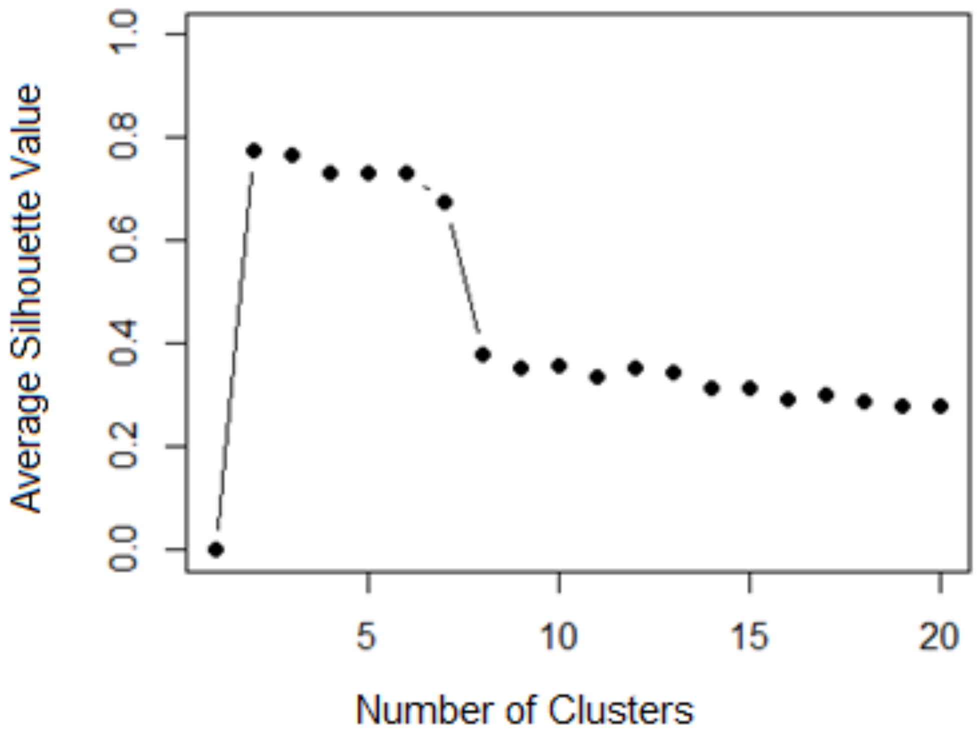
One useful application of cluster validation is to determine the best number of clusters for your dataset.

Q: How would you do this?

A: By computing the Silhouette Coefficient for different values of k.

Ultimately, cluster validation and clustering in general are suggestive techniques that rely on human interpretation to be meaningful.

Art


Average Silhouette Value
0.0
0.2
0.4
0.6
0.8
1.0
5
10
15
20
Number of Clusters

Strengths:

K-means is a popular algorithm because of its computational efficiency and simple and intuitive nature.

Weaknesses:

However, K-means is highly scale dependent, and is not suitable for data with widely varying shapes and densities.

LAB

SYNCHING YOUR FORK WITH THE COURSE REPO

1. re-name your labs with lab_name.<yourname>.ipynb (to prevent a conflict)
2. cd <path to the root of your SYD_DAT_6 local repo>
3. commit your changes ahead of sync
    - git status
    - git add .
    - git commit -m "descriptive label for the commit"
    - git status
4. download new material from official course repo (upstream) and merge it
    - git checkout master (ensures you are in the master branch)
    - git fetch upstream
    - git merge upstream/master

HOMEWORK

Read the following

- Chapter 10.3 of Introduction to Statistical Learning - Clustering Methods in Introduction to Statistical Learning (15 pages)
- Pre Reading:
  - http://www.slideshare.net/MrChrisJohnson/algorithmic-music-recommendations-at-spotify
  - http://techblog.netflix.com/2012/04/netflix-recommendations-beyond-5-stars.html