GENERAL ASSEMBLY

INTRO TO DATA SCIENCE
LECTURE 11: K-MEANS CLUSTERING

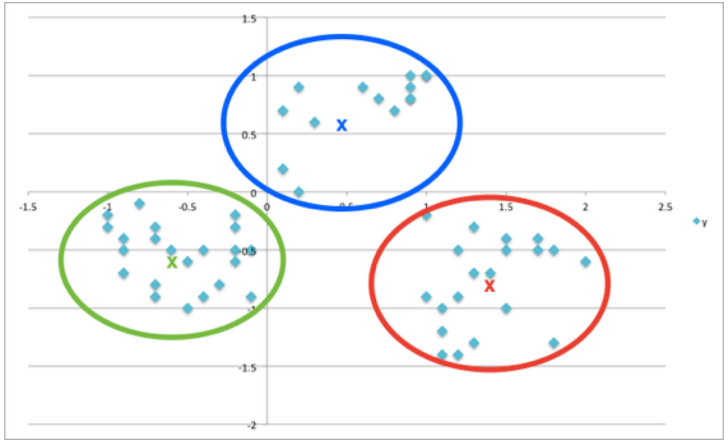
Francesco Mosconi
DAT16 SF // September 2, 2015

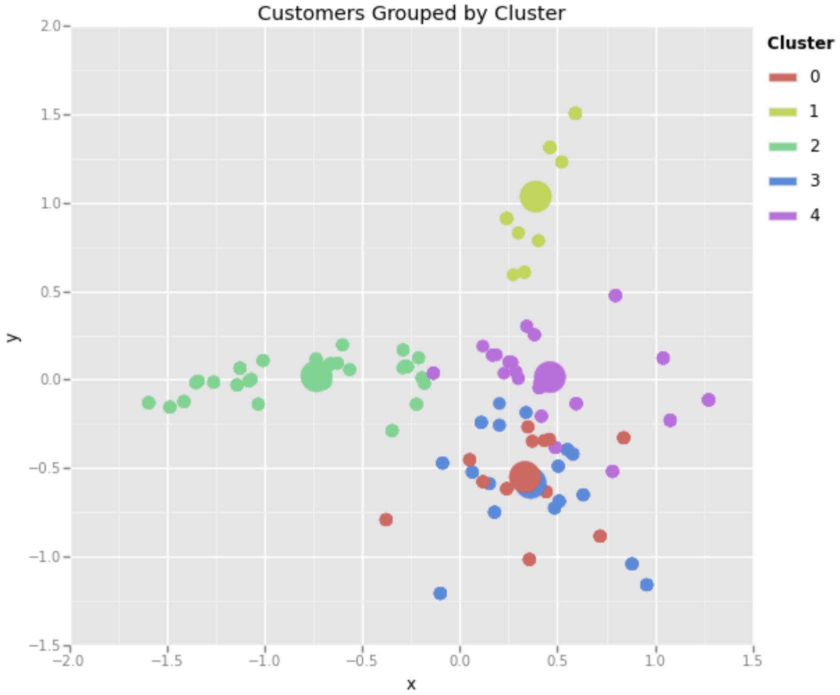
DATA SCIENCE IN THE NEWS

Customer Segmentation in Python

by Greg

August 25, 2015





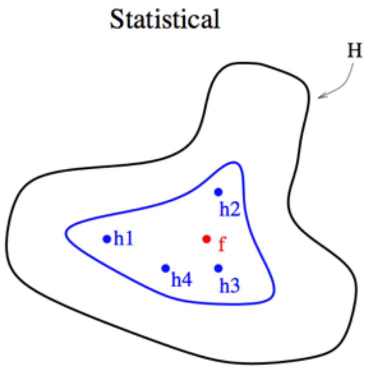
http://blog.yhathq.com/posts/customer-segmentation-using-python.html

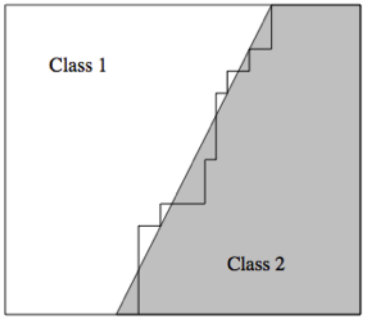
LAST TIME:

I. ENSEMBLE TECHNIQUES
II. PROBLEMS IN CLASSIFICATION
III. BAGGING
IV. BOOSTING
V. RANDOM FORESTS

EXERCISE:

VI. LAB





QUESTIONS?

WHAT WAS THE MOST INTERESTING THING YOU LEARNT?

WHAT WAS THE HARDEST TO GRASP?

I. CLUSTER ANALYSIS
II. K-MEANS CLUSTERING
III. CLUSTER VALIDATION

EXERCISES:
IV. K-MEANS CLUSTERING IN PYTHON

KEY OBJECTIVES

- UNDERSTAND HOW CLUSTERING TECHNIQUES FIT IN THE GLOBAL ML LANDSCAPE
- UNDERSTAND K-MEANS CLUSTERING AND BE ABLE TO USE IT IN PYTHON

CLUSTER ANALYSIS

SO, WHERE ARE WE ON OUR 2X2?

	Continuous	Categorical
Supervised	???	???
Unsupervised	???	???

	Continuous	***Categorical***
Supervised	*regression*	*classification*
Unsupervised	*dimension reduction*	*clustering*

	Continuous	**Categorical**
Supervised	*regression*	*classification*
Unsupervised	*dimension reduction*	*clustering*

Q: What does categorical mean in this context?

Q: What is a cluster?

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A: A group of similar data points.

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The concept of similarity is central to the definition of a cluster, and therefore to cluster analysis.

In general, greater similarity between points leads to better clustering.

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Clustering provides a layer of abstraction from individual data points.

The goal is to extract and enhance the natural structure of the data (not to impose arbitrary structure!)

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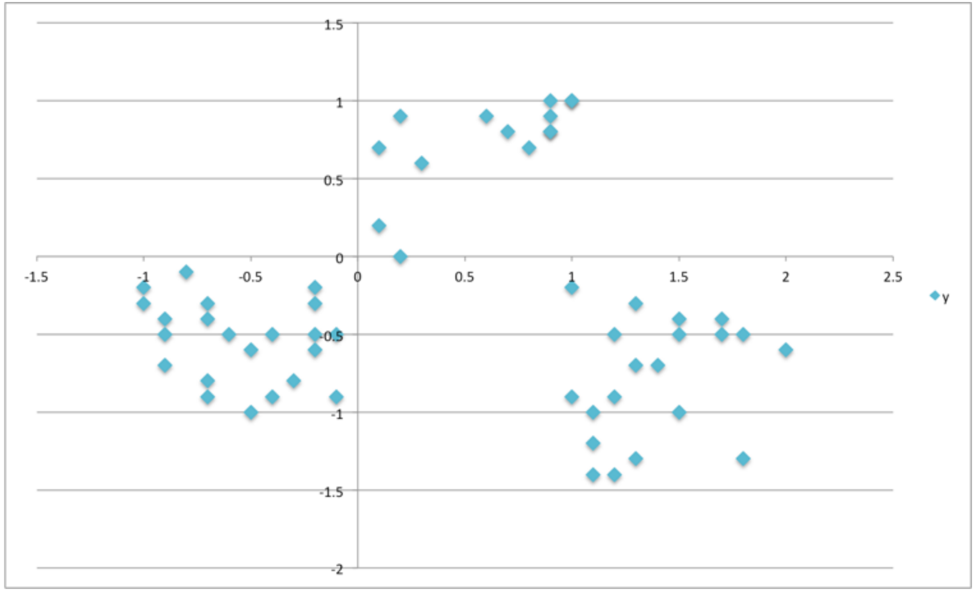
The real purpose of clustering is data exploration, so a solution is anything that contributes to your understanding.

Quick check: how many clusters do you see?



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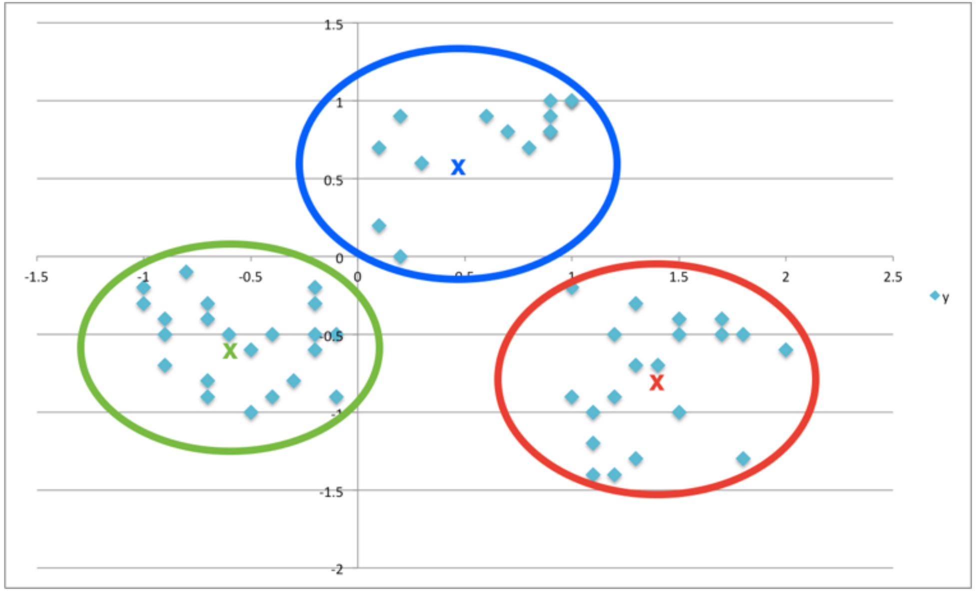

K-MEANS CLUSTERING

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greedy *– captures local structure (depends on initial conditions)*

partition *– performs complete clustering (each point belongs to exactly one cluster)*

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A: Each point is assigned to the cluster with the nearest centroid.

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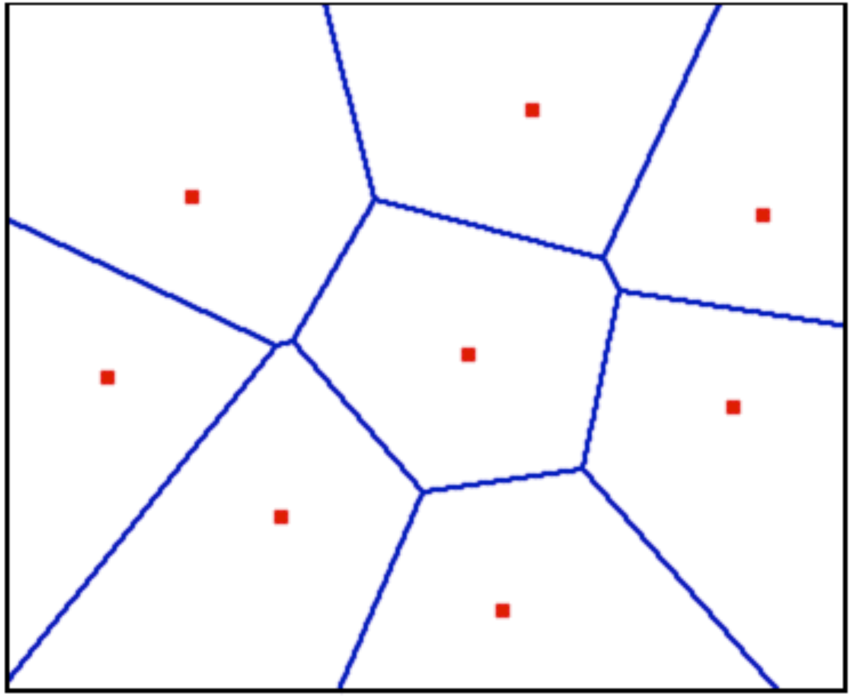
centroid *– the mean of the data points in a cluster*
-> requires continuous (vector-like) features
-> highlights iterative nature of algorithm

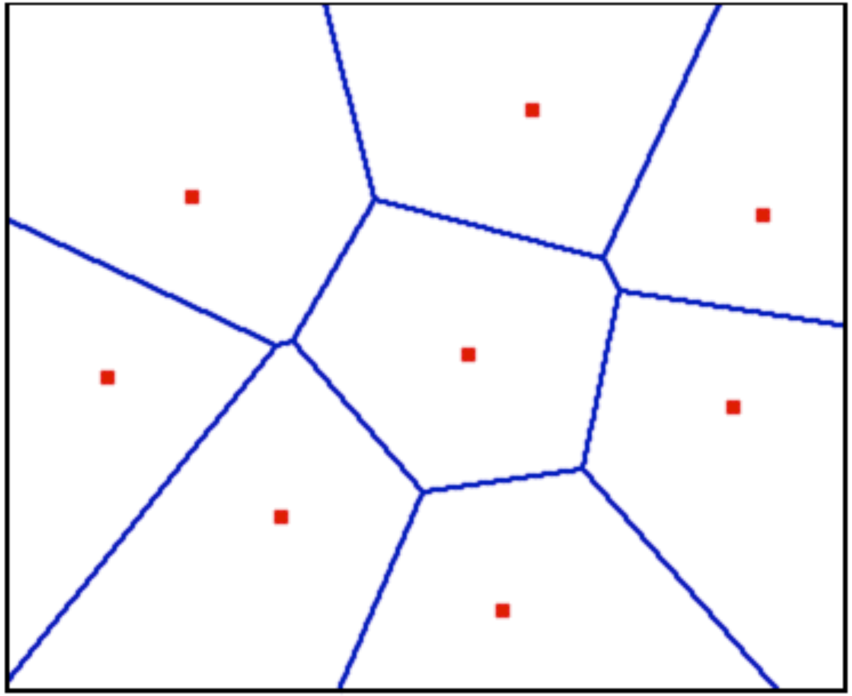
Q: What do these partitions look like?

CENTROIDS & PARTITIONS



source: http://www.dma.fi.upm.es/mabellanas/tfcs/fvd/images/voronoi.gif

CENTROIDS & PARTITIONS



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NOTE

These partitions are sometimes called Voronoi cells, and these maps Voronoi diagrams.

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This means that the same data can yield very different clustering results depending on the scale and the units used.

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Therefore it’s important to think about your data representation before applying a clustering algorithm.

These graphs show two different representations of the same data:

SCALE DEPENDENCE

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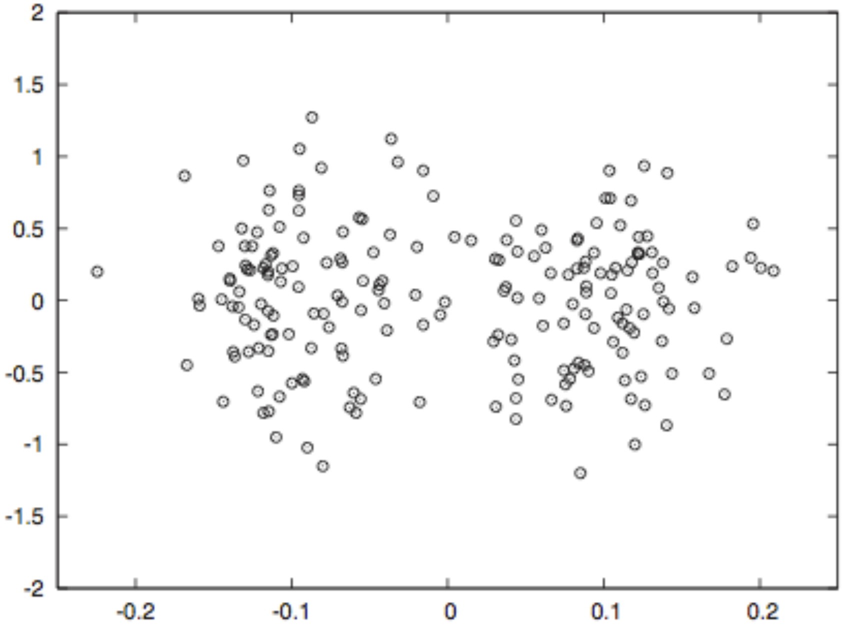
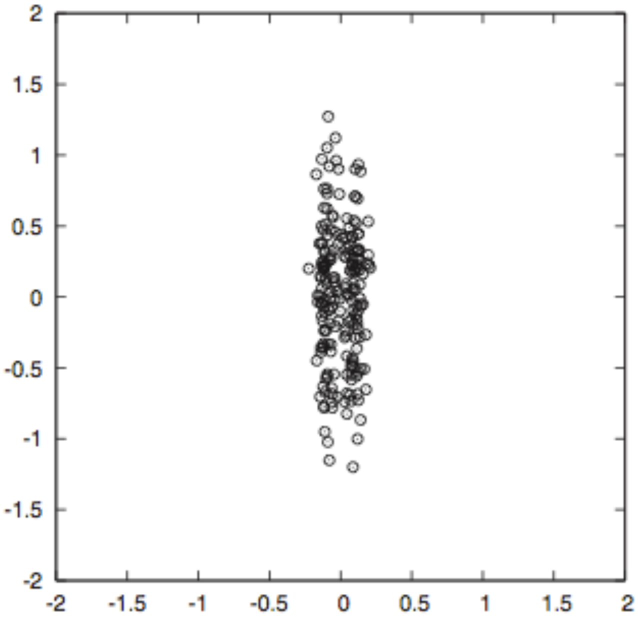




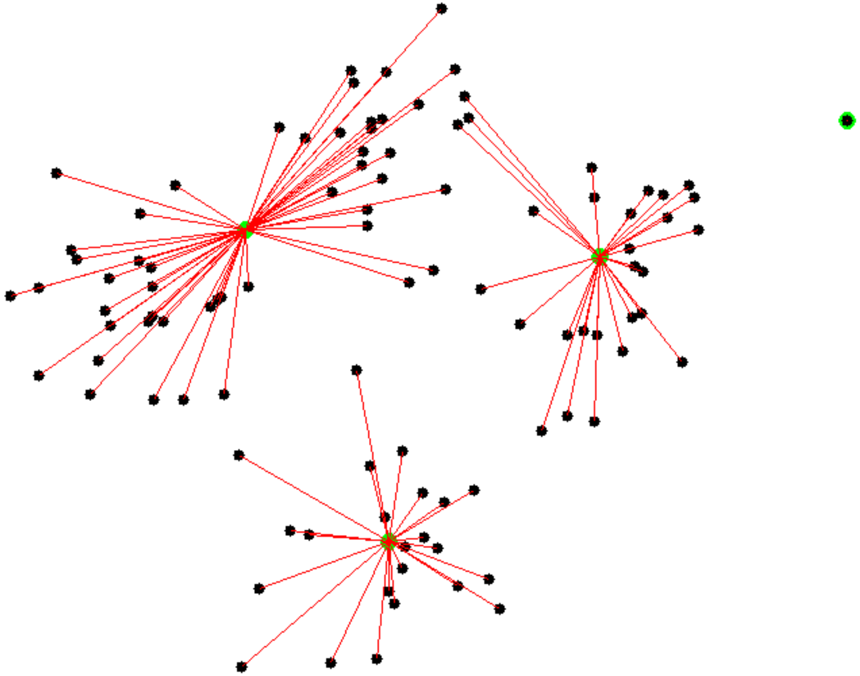
source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

THE BASIC K-MEANS ALGORITHM

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*



http://shabal.in/visuals/kmeans/2.html

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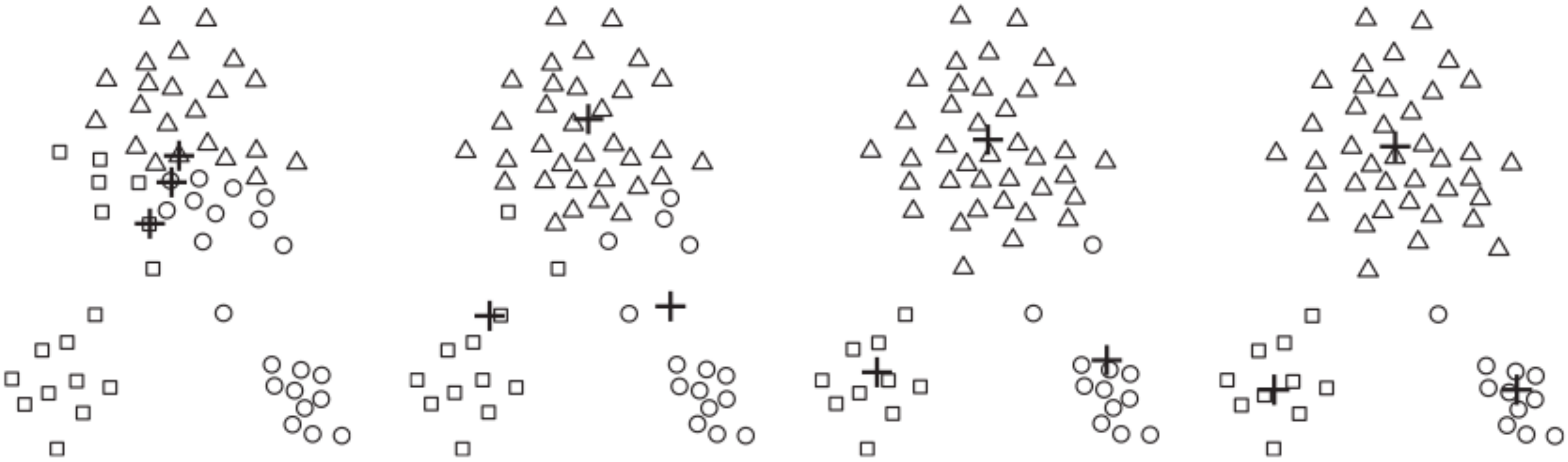

(a) Iteration 1. (b) Iteration 2. (c) Iteration 3. (d) Iteration 4.

Figure 8.3. Using the K-means algorithm to find three clusters in sample data.

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

STRENGTHS & WEAKNESSES

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Difficulties can sometimes be overcome by increasing the value of k and combining subclusters in a post-processing step.

STEP 1 – CHOOSING INITIAL CENTROIDS

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- start with global centroid, choose point at max distance, repeat (but might select outlier)

STEP 2 – SIMILARITY MEASURES

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NOTE

Technically, by defining a similarity measure we are mapping our observations into a metric space.

A similarity measure must satisfy certain general conditions:

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$$d(x, y) \geq 0$$

$$d(x, y) = 0 \iff x = y$$

$$d(x, y) = d(y, x)$$

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NOTE

Another useful property is smoothness.

There are a number of different similarity measures to choose from, and in general the right choice depends on the problem.

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We can express different semantics about our data through the choice of metric.

Ex: One popular metric for text mining problems (or any problem with sparse binary data) is the Jaccard coefficient,

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|}$$

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$$J(A,B) = \frac{|A \cap B|}{|A \cup B|}$$

Applying this metric to a problem expresses the sparse nature of the data, and makes a variety of text mining techniques accessible.

The matrix whose entries D_{ij} contain the values d(x, y) for all x and y is called the distance matrix.

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For this reason, it's really the choice of metric that determines the definition of a cluster.

Q: How do we recompute the positions of the centroids at each iteration of the algorithm?

STEP 3 – OBJECTIVE FUNCTION

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A: By optimizing an objective function that tells us how "good" the clustering is.

The iterative part of the algorithm (recomputing centroids and reassigning points to clusters) explicitly tries to minimize this objective function.

STEP 3 – OBJECTIVE FUNCTION

Ex: Using the Euclidean distance measure, one typical objective function is the sum of squared errors from each point x to its centroid ci:

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} d(x, c_i)^2$$

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Given two clusterings, we will prefer the one with the lower SSE since this means the centroids have converged to better locations (a better local optimum).

STEP 4 – CONVERGENCE

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

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Recall that, in general, different runs of the algorithm will converge to different local optima (centroid configurations).

STEP 4 – CONVERGENCE

quick check:

alone: find 3 business-related problems where you could apply clustering

with the person next to you: discuss which of these are suitable for k-means and why

CLUSTER VALIDATION

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.

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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.

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

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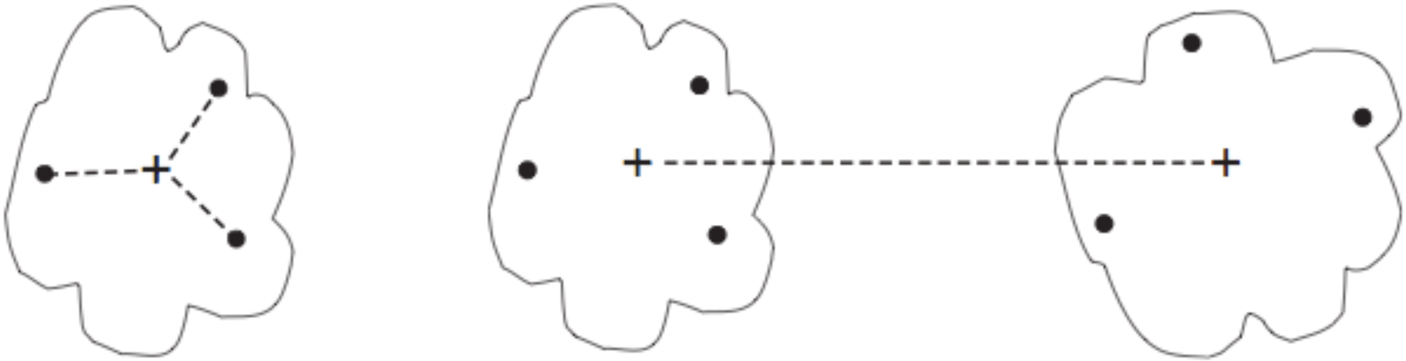
Separation measures clustering effectiveness between clusters.

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



(a) Cohesion. (b) Separation.

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

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

We can turn these values into overall measures of clustering validity by taking a weighted sum over clusters:

$$\hat{V}_{total} = \sum_{1}^{K} w_i \hat{V}(C_i)$$

Here V can be cohesion, separation, or some function of both.

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Here V can be cohesion, separation, or some function of both.

The weights can all be set to 1 (best for k-means), or proportional to the cluster masses (the number of points they contain).

Cluster validation measures can be used to identify clusters that should be split or merged, or to identify individual points with disproportionate effect on the overall clustering.

SILHOUETTE COEFFICIENT

One useful measure than 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

$b_i = min_j(b_{ij})$

SILHOUETTE COEFFICIENT

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.

SILHOUETTE COEFFICIENT

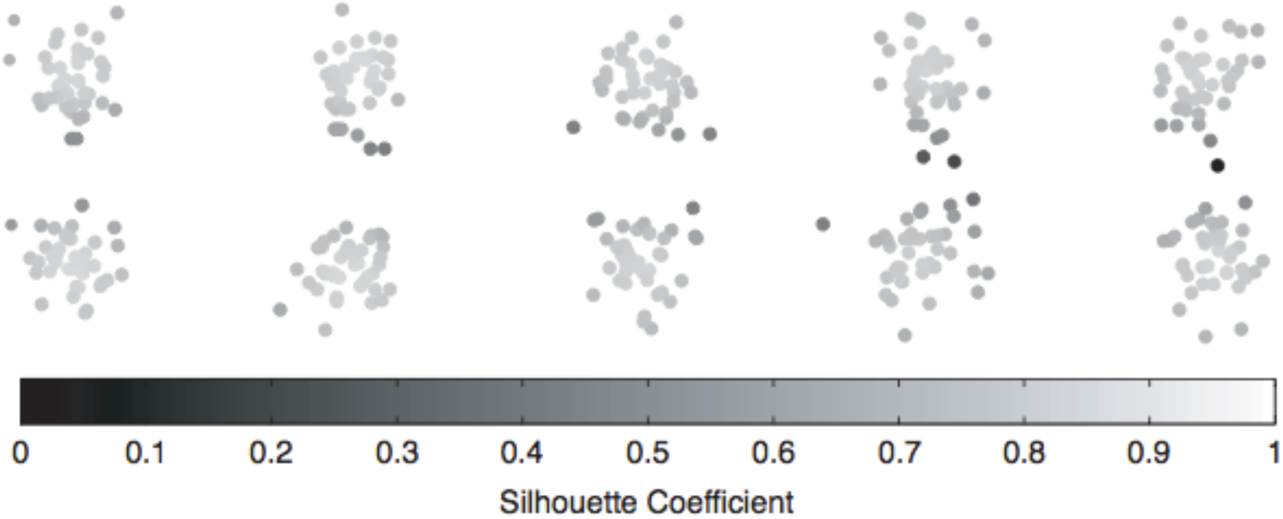

Figure 8.29. Silhouette coefficients for points in ten clusters.

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

SILHOUETTE COEFFICIENT

The silhouette coefficient for the cluster Ci is given by the average silhouette coefficient across all points in Ci:

$$SC(C_i) = \frac{1}{m_i} \sum_{x \in C_i} SC_i$$

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NOTE

This gives a summary measure of the overall clustering quality.

An alternative validation scheme is given by comparing the similarity matrix with an idealized (0/1) similarity matrix that represents the same clustering configuration.

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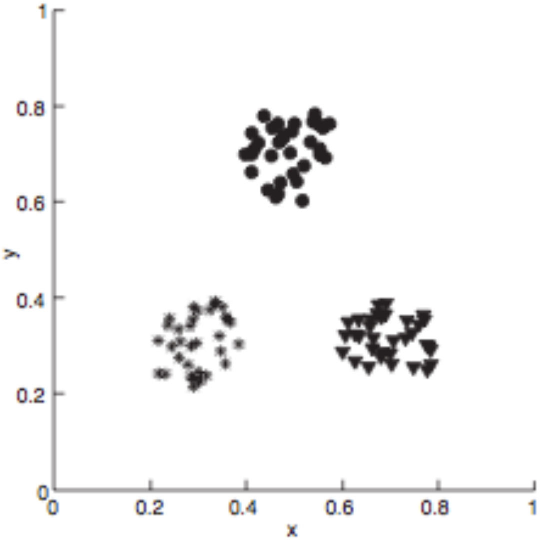
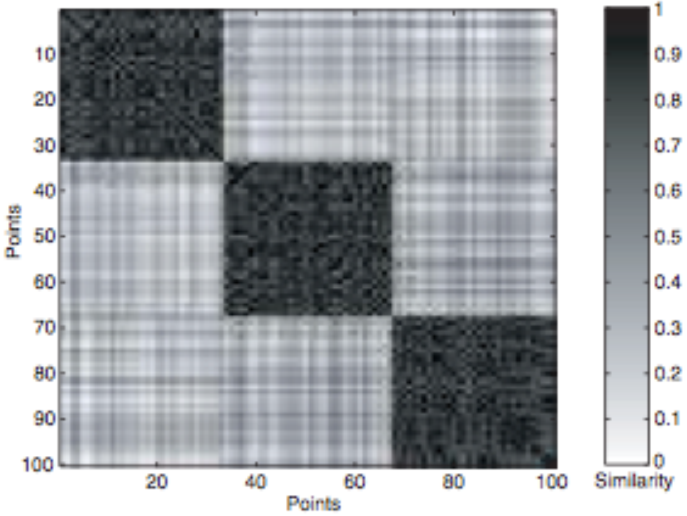
This can be done either graphically or using correlations.



(a) Well-separated clusters.



(b) Similarity matrix sorted by K-means cluster labels.

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

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

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Q: How would you do this?

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Q: How would you do this?
A: By computing the overall SSE or SC for different values of k.

CLUSTER VALIDATION

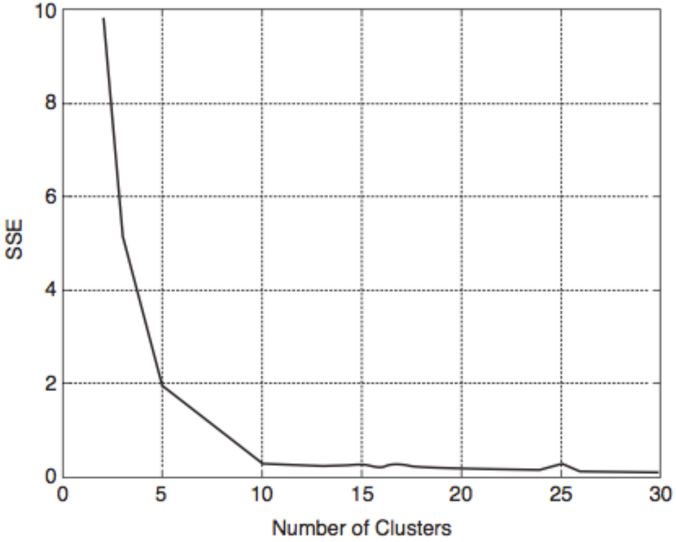

Figure 8.32. SSE versus number of clusters for the data of Figure 8.29.

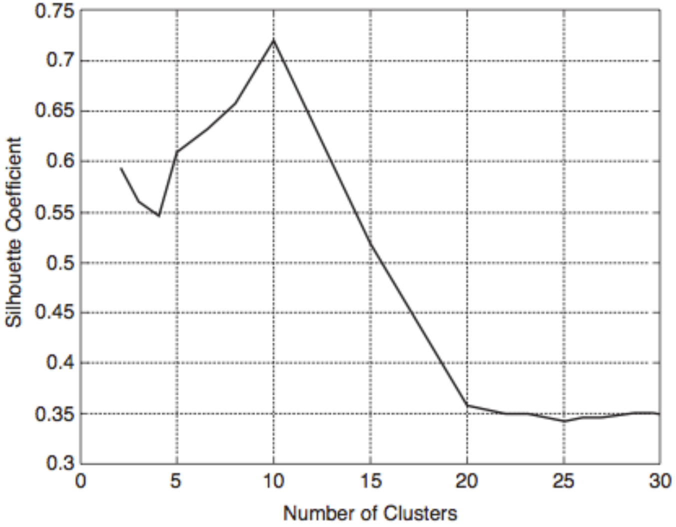

Figure 8.33. Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

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

Q: How can you determine your level of confidence in these validation metrics?

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A: Statistically; eg, by computing frequency distributions for these metrics (over several runs of the algorithm) and determining statistical significance.

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

quick check:

what is the silhouette coefficient?
(in your own words)

EX: K-MEANS CLUSTERING