GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 7: K-MEANS CLUSTERING

LAST TIME:

LOGISTIC REGRESSION

- CONCEPTS
- GENERALIZING THE LINEAR MODEL
- INTERPRETING RESULTS

QUESTIONS?

I. CLUSTER ANALYSIS
II. K-MEANS CLUSTERING
III. INTERPRETING RESULTS

EXERCISES:
II. K-MEANS CLUSTERING IN R

I. CLUSTER ANALYSIS

	continuous	*categorical*
supervised	???	???
unsupervised	???	???

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

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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.

II. K-MEANS CLUSTERING

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A: A **greedy** *learner that* **partitions** *a data set into k clusters.*

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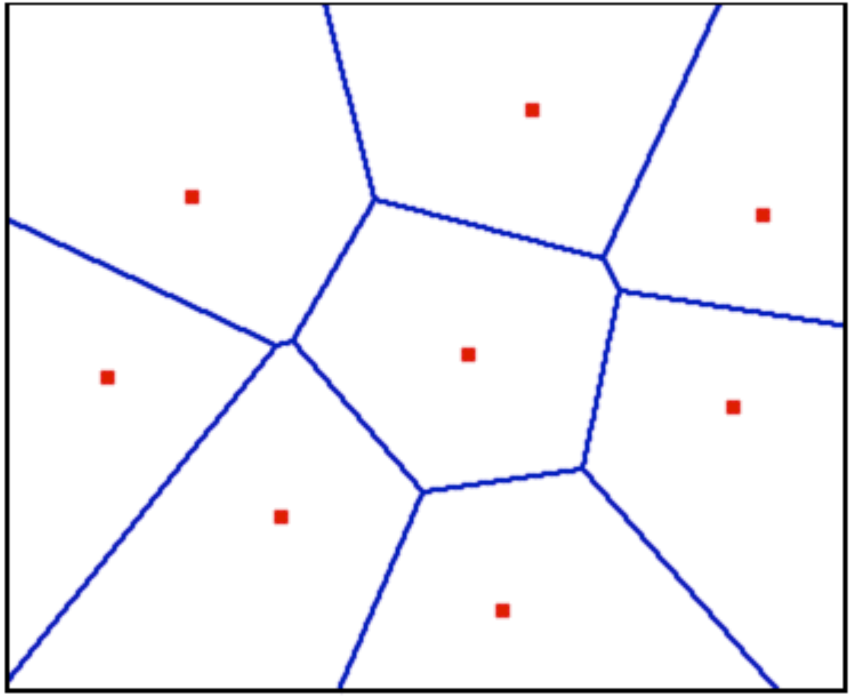
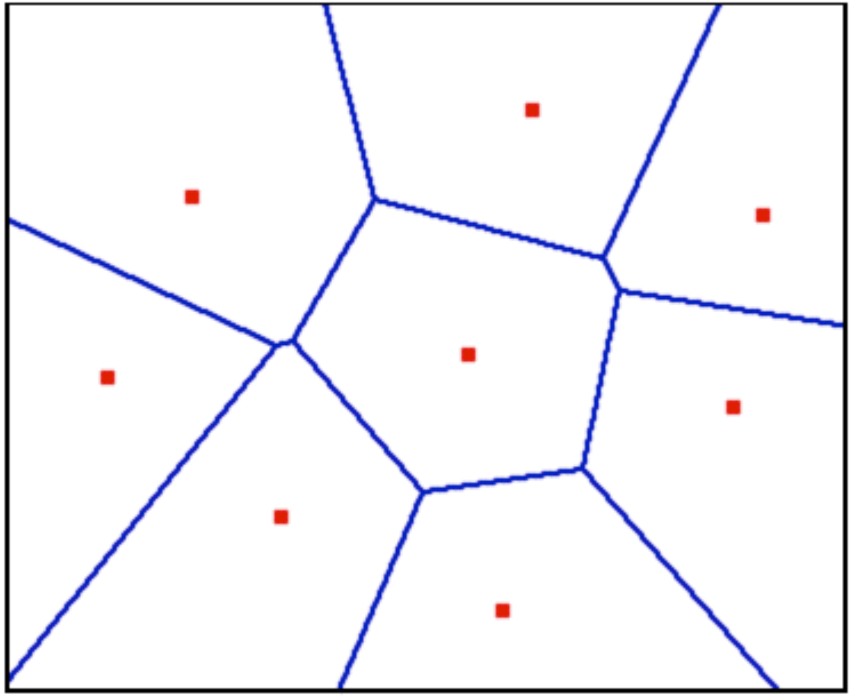
A: Each point is assigned to the cluster with the nearest **centroid**.

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?



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



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

NOTE

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

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

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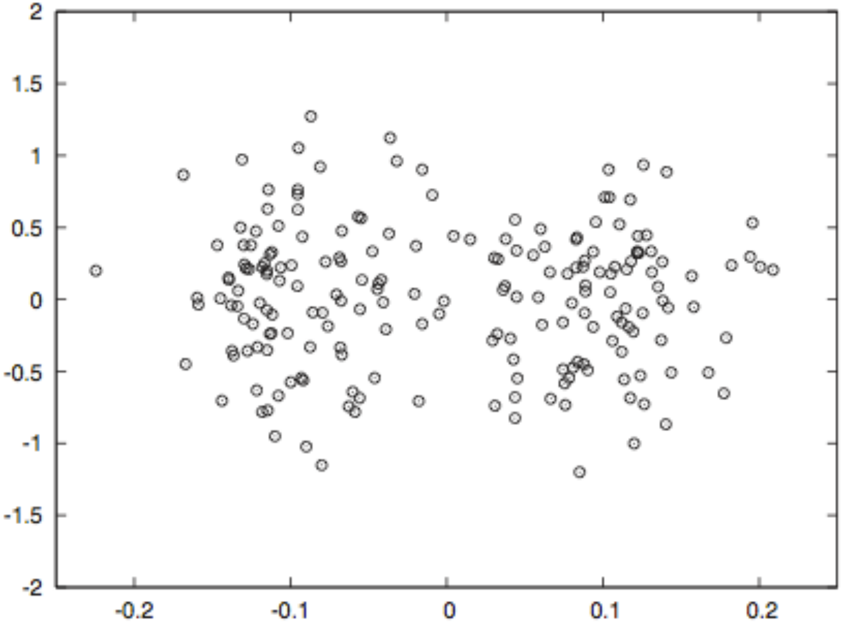
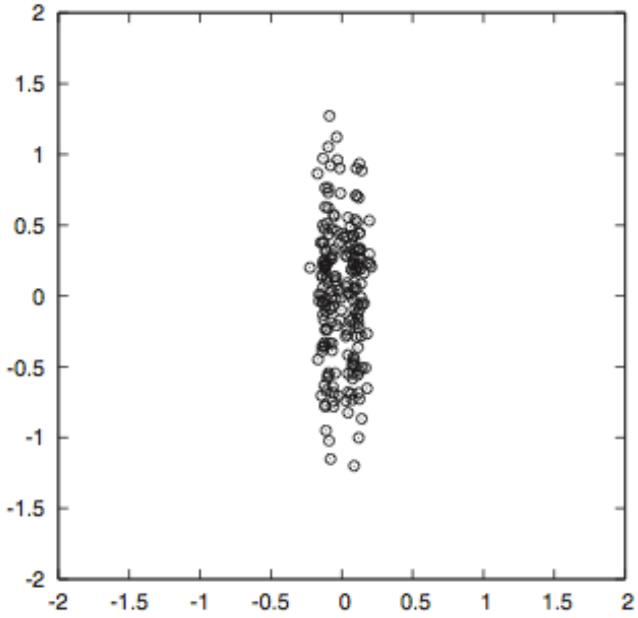




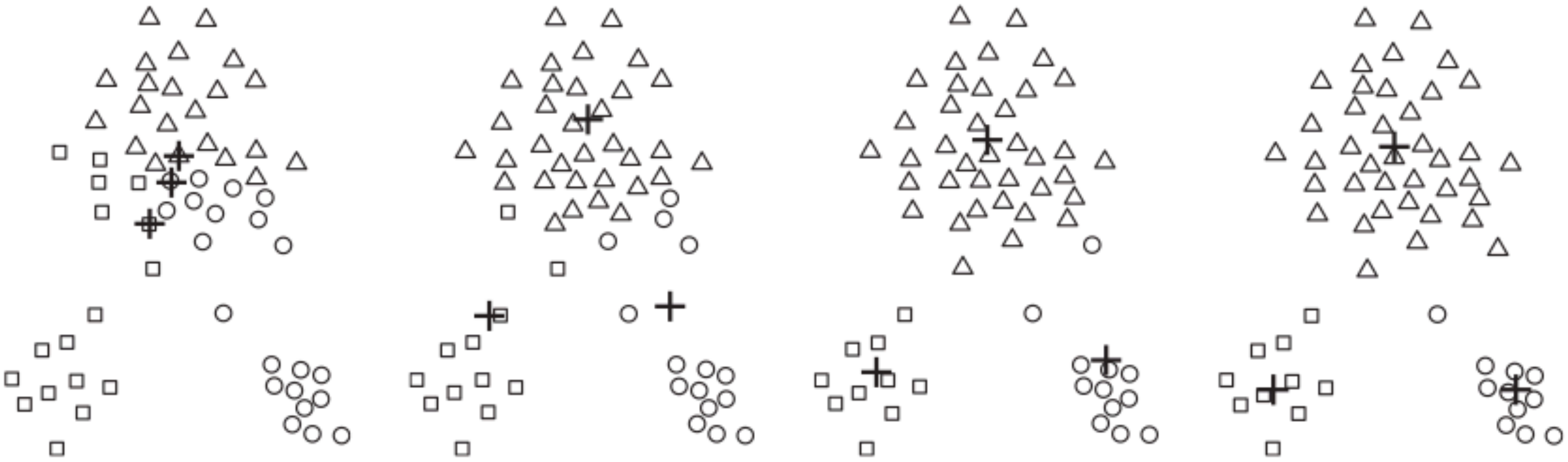
source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

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*

THE BASIC K-MEANS ALGORITHM



(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

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

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- *perform alternative clustering task, use resulting centroids as initial k-means centroids*

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A: 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)*

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The "nearness" criterion is determined by the similarity/distance measure we discussed earlier.

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This measure makes quantitative inference possible.

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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For data that takes values in R^n, the typical choice is the **Euclidean distance***:*

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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.

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

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

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The iterative part of the algorithm (recomputing centroids and reassigning points to clusters) explicitly tries to minimize this 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 c_i:*

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

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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).

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

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Stopping criteria can be based on the centroids (eg, if positions change by no more than ε), the points (eg, if no more than $x\%$ change clusters between iterations), or time (eg, stop after 8 hours).

III. 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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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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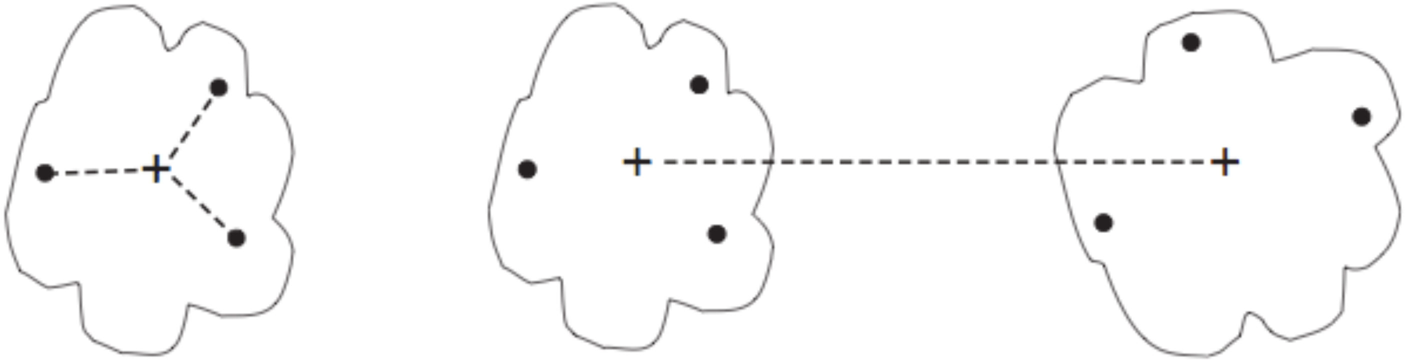
Separation *measures clustering effectiveness between clusters.*

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



(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

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.

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
$b_i = min_j(b_{ij})$

The silhouette coefficient can be 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.

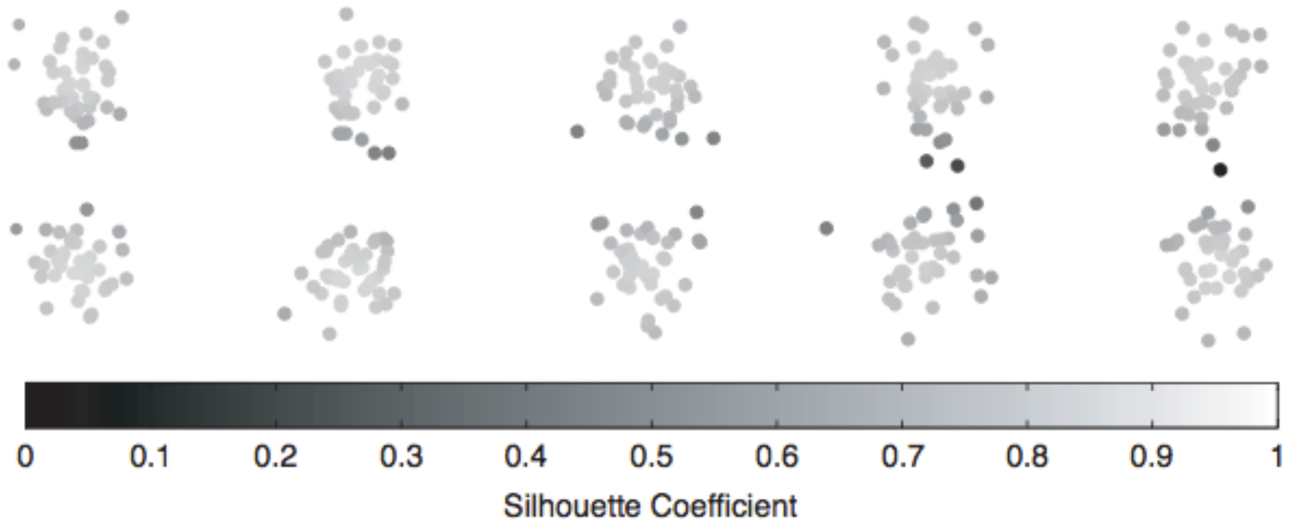


Figure 8.29. Silhouette coefficients for points in ten clusters.

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

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

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NOTE

This gives a summary measure of the overall clustering quality.

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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 overall SSE or SC for different values of k.

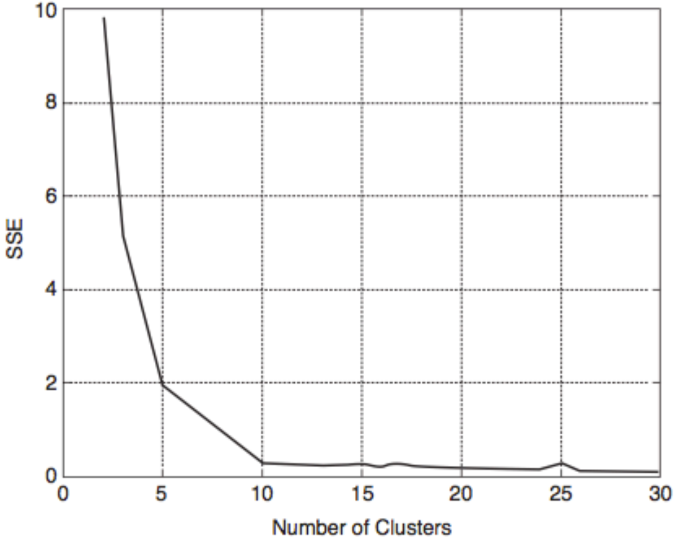

Figure 8.32. SSE versus number of clusters for the data of Figure 8.29.

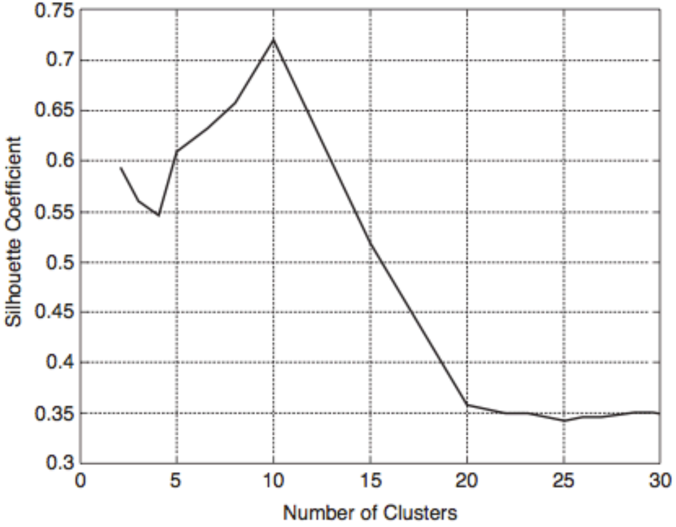

Figure 8.33. Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

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

EX: K-MEANS CLUSTERING