GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 11: K-MEANS CLUSTERING

I. CLUSTER ANALYSIS

	continuous	*categorical*
supervised	*regression*	*classification*
unsupervised	*dimension reduction*	*clustering*

supervised	*making predictions*
unsupervised	*discovering patterns*

supervised	*labeled examples*
unsupervised	*no labeled examples*

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.

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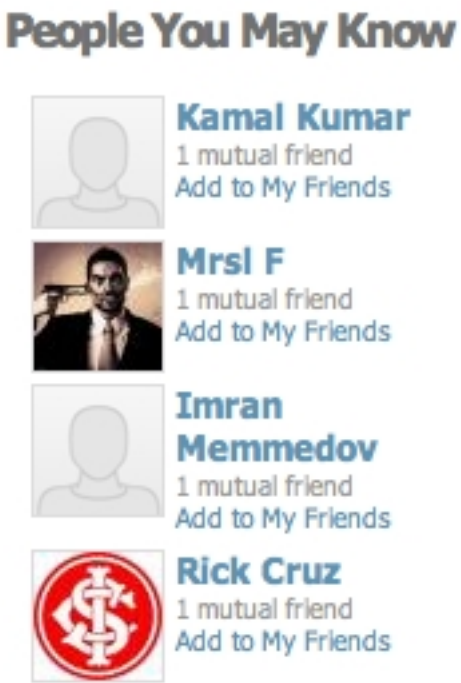
Clustering provides a layer of abstraction from individual data points.

The goal is to extract and enhance the natural structure of the data (not to impose arbitrary structure!)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Priority Inbox: Unsupervised Learning

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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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greedy – captures local structure

partition – 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

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

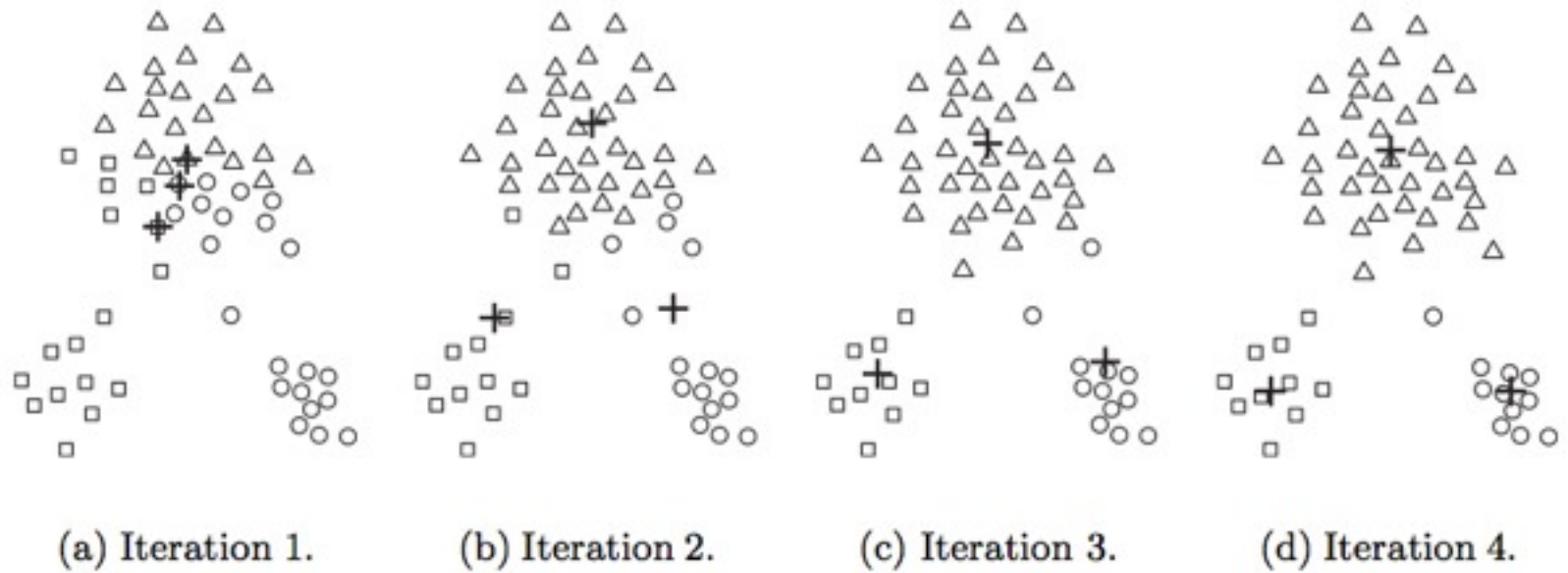

Figure 8.3. Using the K-means algorithm to find three clusters in sample data.

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

K-means is algorithmically pretty efficient (time & space complexity is linear in number of records).

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

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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 $\mathbb{R}^n$, the typical choice is the **Euclidean distance***:*

$$d(x, y) = \sqrt{\sum (x_i - y_i)^2}$$

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

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?

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

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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.

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.

III. CLUSTER VALIDATION

supervised	*test out your predictions*
unsupervised	*...*

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.*

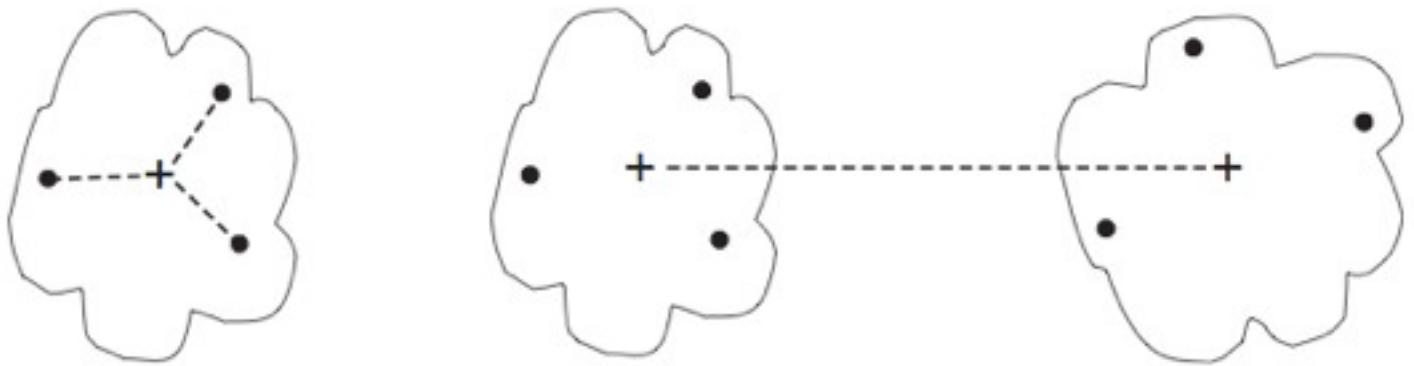
$$\hat{C}(C_i) = \sum_{x \in C_i} d(x, c_i)$$

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.*

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



(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.

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?

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 for different values of k.

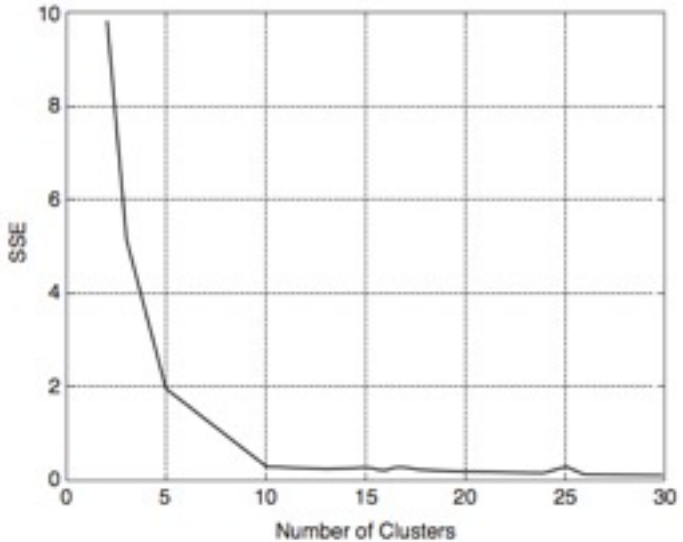

Figure 8.32. SSE versus number of clusters for the data of Figure 8.29.

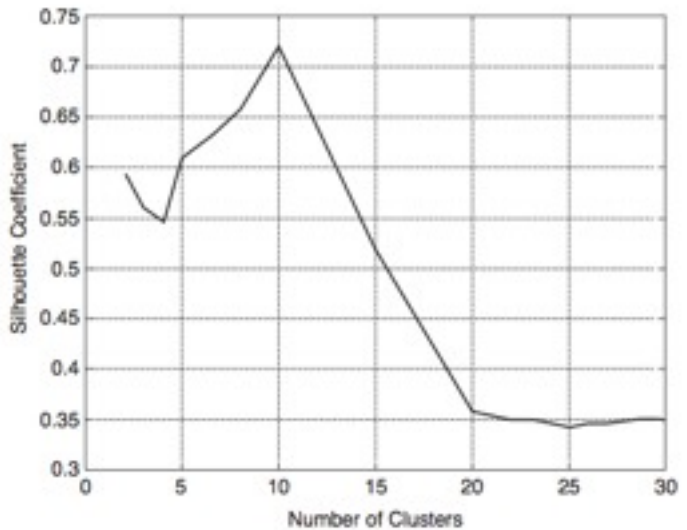

Figure 8.33. Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

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

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

EX: K-MEANS CLUSTERING