INTRO TO DATA SCIENCE

SESSION 8: K-MEANS CLUSTERING

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DAT13 SF // April 1, 2015

AGENDA

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

EXERCISES (IF TIME ALLOWS):
II. K-MEANS CLUSTERING IN PYTHON

I. CLUSTER ANALYSIS

SO, WHERE ARE WE ON OUR 2X2?

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

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

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Q: What does categorical mean in this context?

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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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greedy – captures local structure (depends on initial conditions)

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

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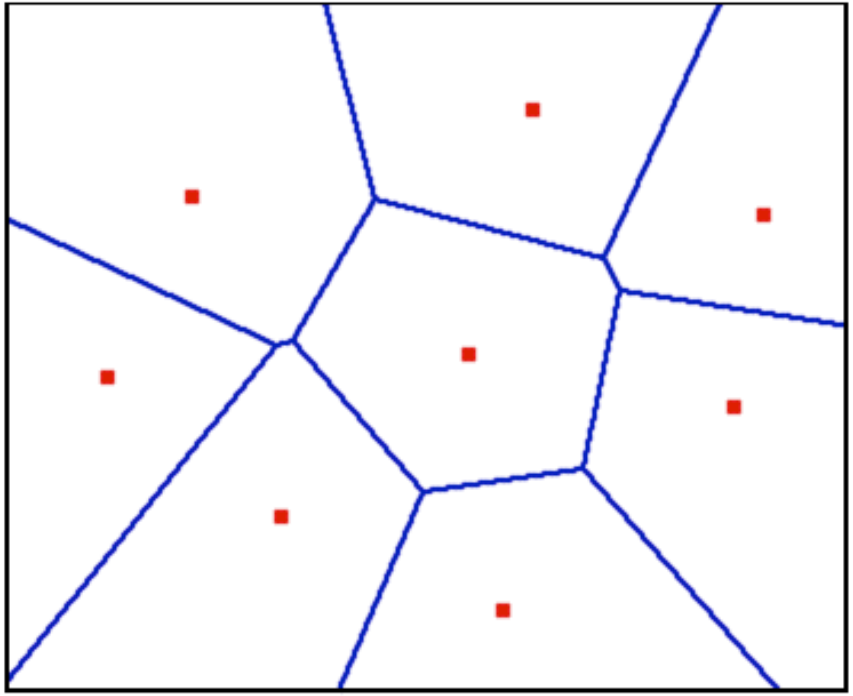
centroid – the mean of the data points in a cluster

→ *requires <u>continuous</u> (vector-like) features*

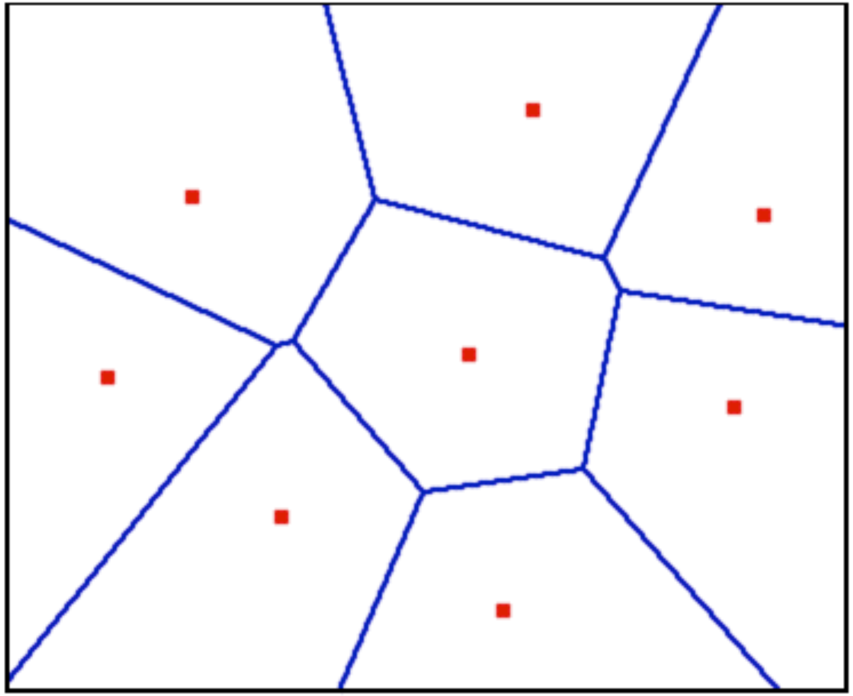
→ *highlights <u>iterative</u> nature of algorithm*

Q: What do these partitions look like?



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

CENTROIDS & PARTITIONS



NOTE

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

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

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

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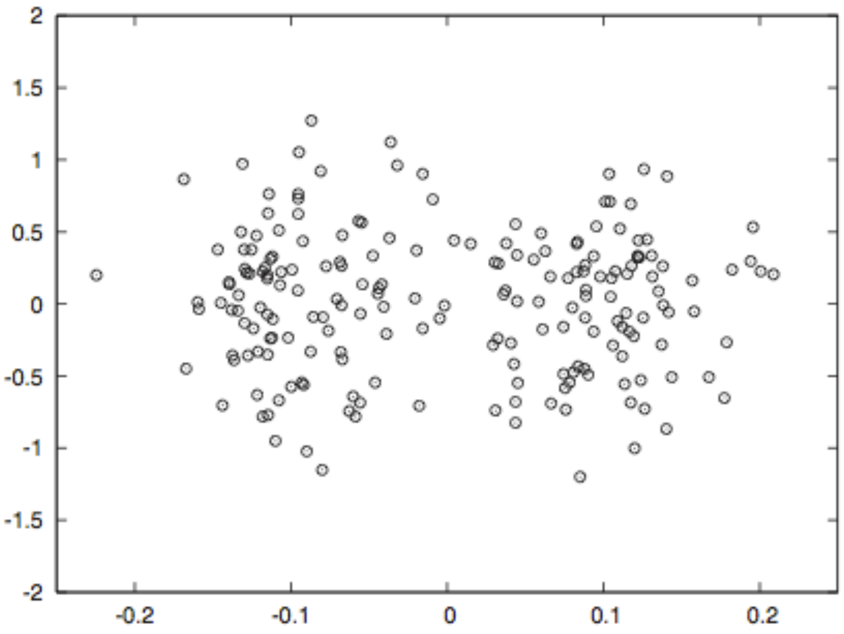

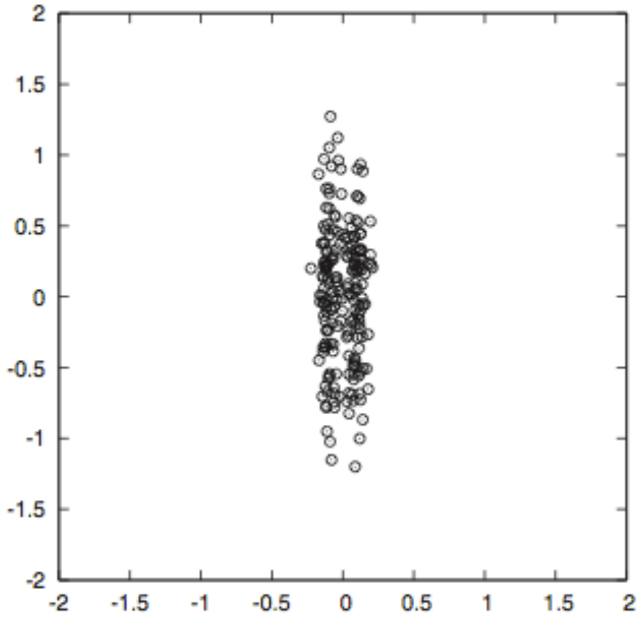

source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

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*

THE BASIC K-MEANS ALGORITHM

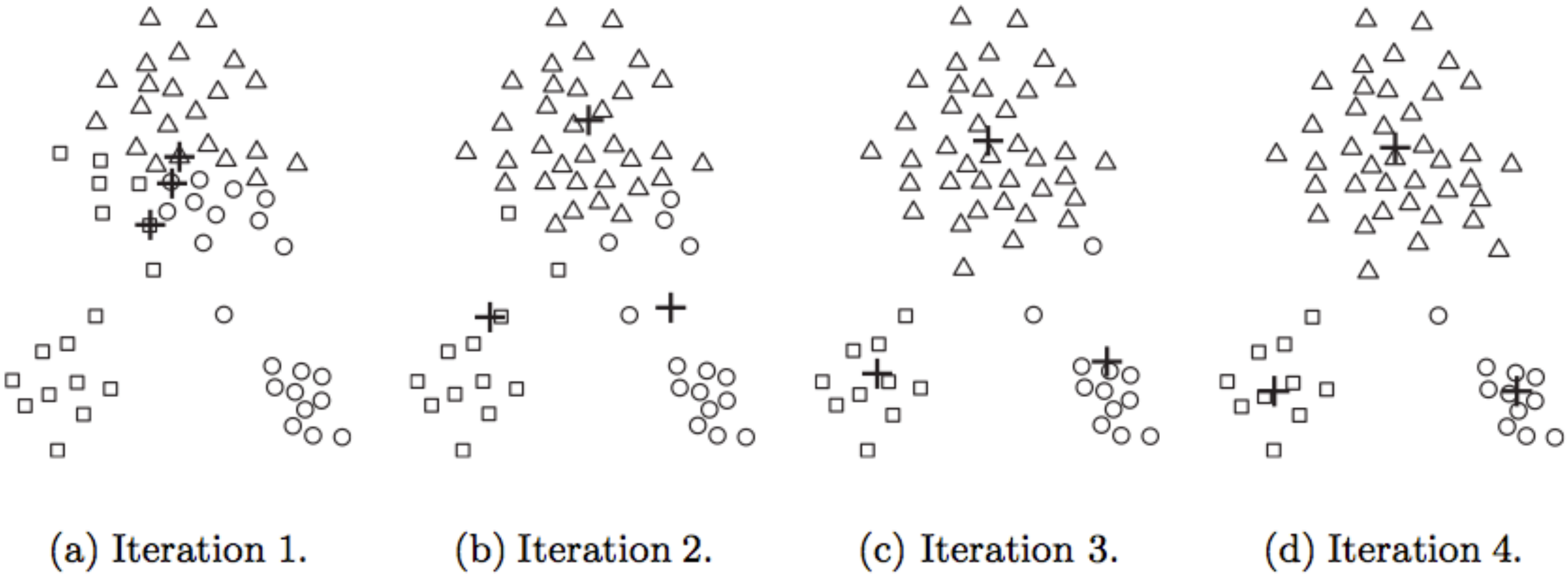

Figure 8.3. Using the K-means algorithm to find three clusters in sample data.

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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STEP 1 – CHOOSING INITIAL CENTROIDS

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- randomly (but may yield divergent behavior)

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

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

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

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

(symmetry)

$$d(x, y) + d(y, z) \geq d(x, z)$$

(triangle inequality)

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.

STEP 3 – OBJECTIVE FUNCTION

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).

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).

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.*

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

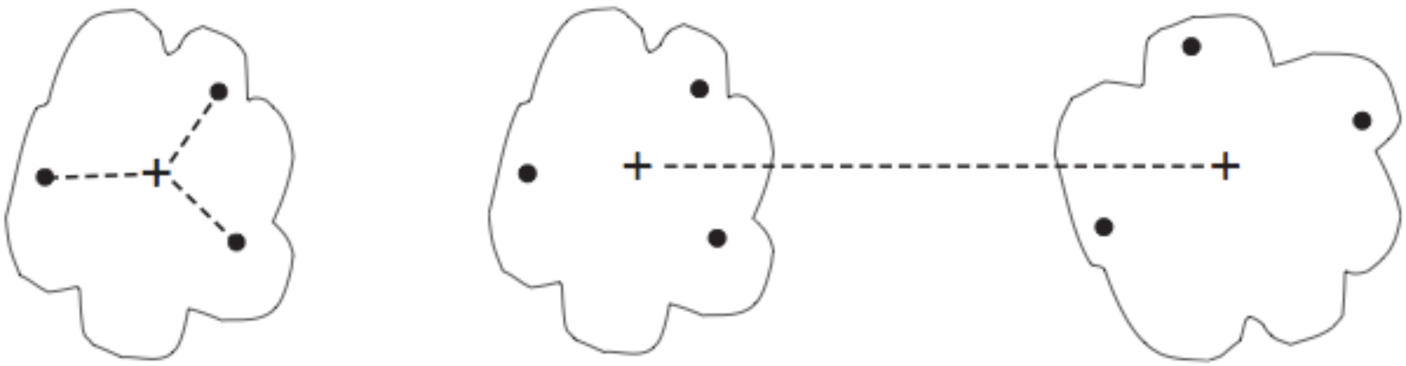
Cohesion *measures clustering effectiveness within a cluster.*

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

Separation *measures clustering effectiveness between clusters.*

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

CLUSTER VALIDATION



(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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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 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 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

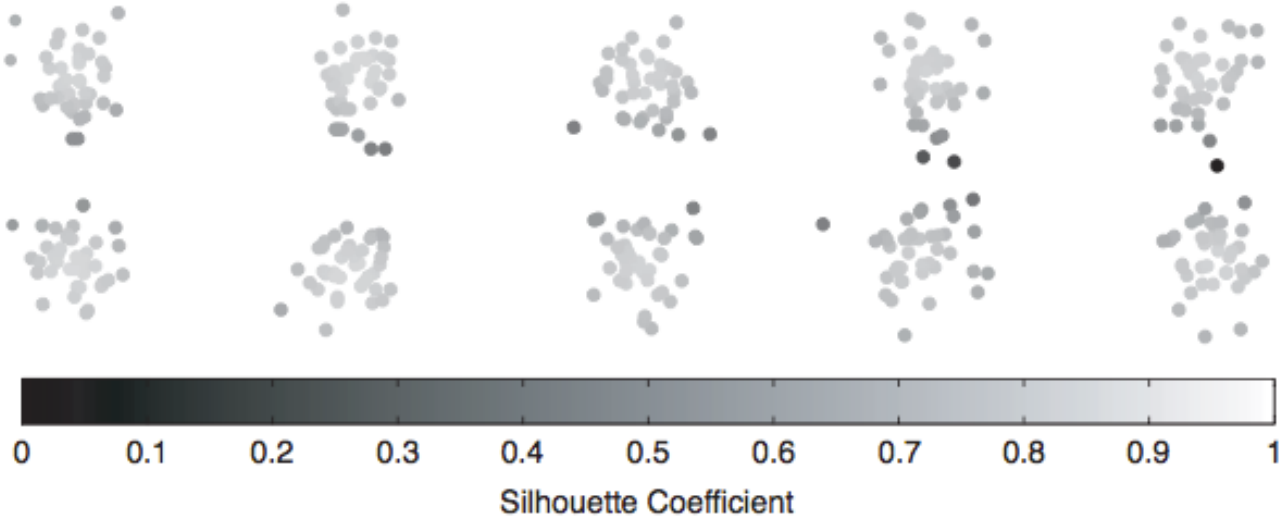

Figure 8.29. Silhouette coefficients for points in ten clusters.

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

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

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

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NOTE

This gives a summary measure of the overall clustering quality.

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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

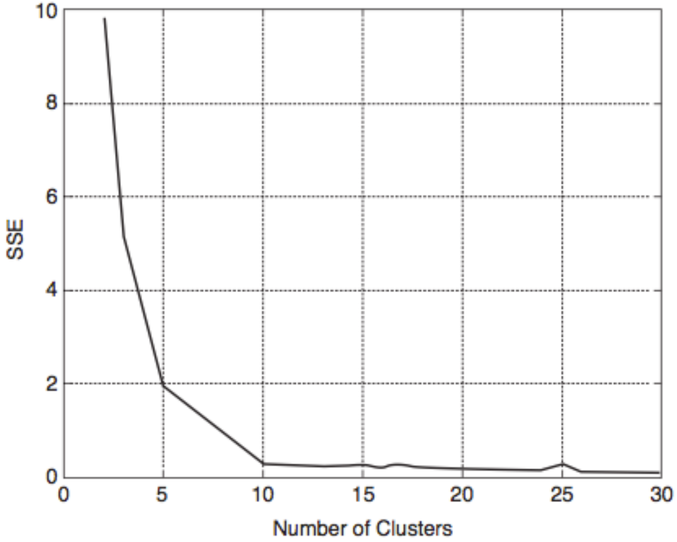

Figure 8.32. SSE versus number of clusters for the data of Figure 8.29.

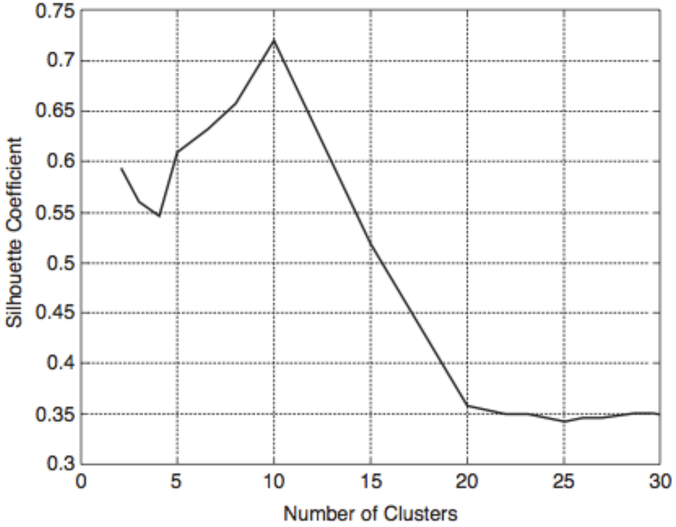

Figure 8.33. Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

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

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

EX: K-MEANS CLUSTERING