GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 11: K-MEANS CLUSTERING

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

EXERCISES:
II. K-MEANS CLUSTERING IN R

	continuous	*categorical*
supervised	regression	classification
unsupervised	dimension reduction	clustering

KNN

	KNN
linear	N

	KNN
linear	N
scalability	+/-

	KNN
linear	N
scalability	+/-
interpretation	-

	KNN
linear	N
scalability	+/-
interpretation	-
configuration	+

	KNN
linear	N
scalability	+/-
interpretation	-
configuration	+
specification	-

	KNN
linear	N
scalability	+/-
interpretation	-
configuration	+
specification	-
overfitting	> K

	KNN	Logistic
linear	N	Y
scalability	+/-	+
interpretation	-	+
configuration	+	+
specification	-	+
overfitting	> K	L1 / L2

	KNN	Logistic	NB
linear	N	Y	Y
scalability	+/-	+	+
interpretation	-	+	+
configuration	+	+	+
specification	-	+	+
overfitting	> K	L1 / L2	Prior

	KNN	Logistic	NB	RF
linear	N	Y	Y	N
scalability	+/-	+	+	-
interpretation	-	+	+	-
configuration	+	+	+	+
specification	-	+	+	+
overfitting	> K	L1 / L2	Prior	n tree

	KNN	Logistic	NB	RF	SVM
linear	N	Y	Y	N	Y/N
scalability	+/-	+	+	-	-
interpretation	-	+	+	-	-
configuration	+	+	+	+	-
specification	-	+	+	+	-
overfitting	> K	L1 / L2	Prior	n tree	C-cost

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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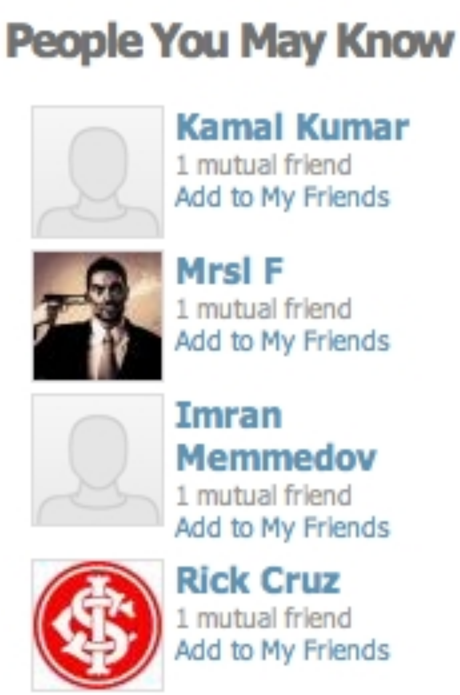
Clustering provides a *layer of abstraction* from individual data points.

The goal is to extract and enhance the natural structure of the data (not to impose arbitrary structure!)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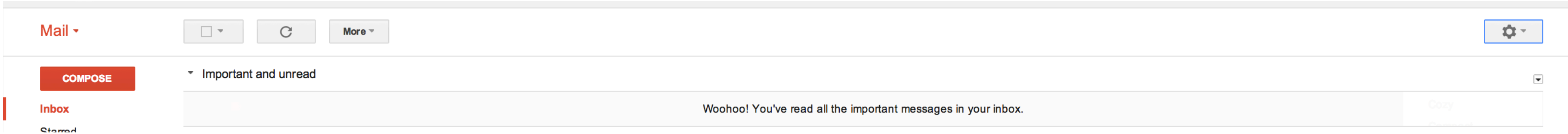
1 mutual friend
Add to My Friends
Mrsl F
1 mutual friend
Add to My Friends
Imran Memmedov
1 mutual friend
Add to My Friends
Rick Cruz
1 mutual friend
Add to My Friends



Priority Inbox: Unsupervised Learning

Group mails into groups and decide which group represents important mails

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Chris Pine (Actor), Zachary Quinto (Actor), J.J. Abrams (Director) | Rated: PG-13 | Format: Blu-ray

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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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partition – each point belongs to exactly one cluster

Q: How are these partitions determined?

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

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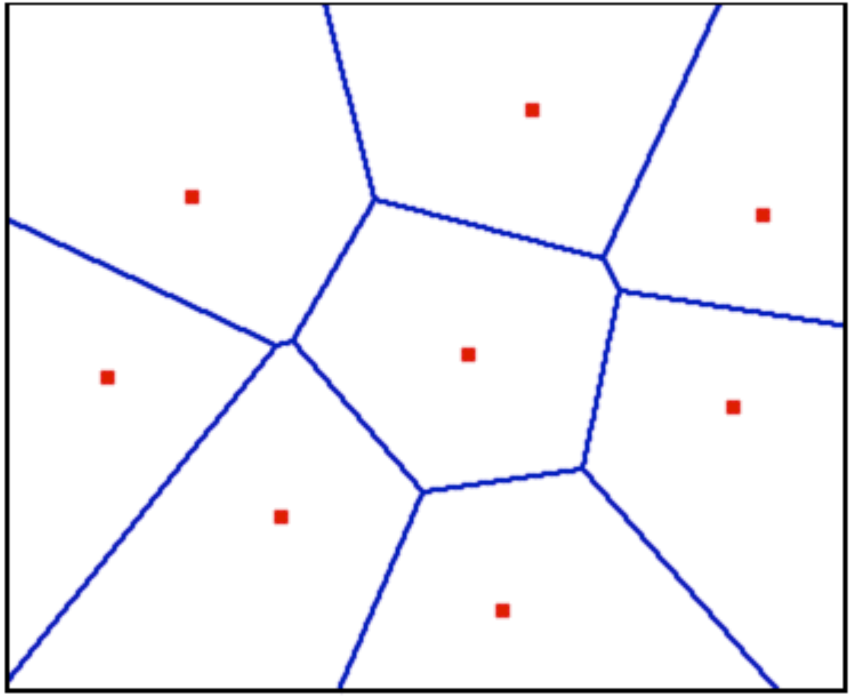
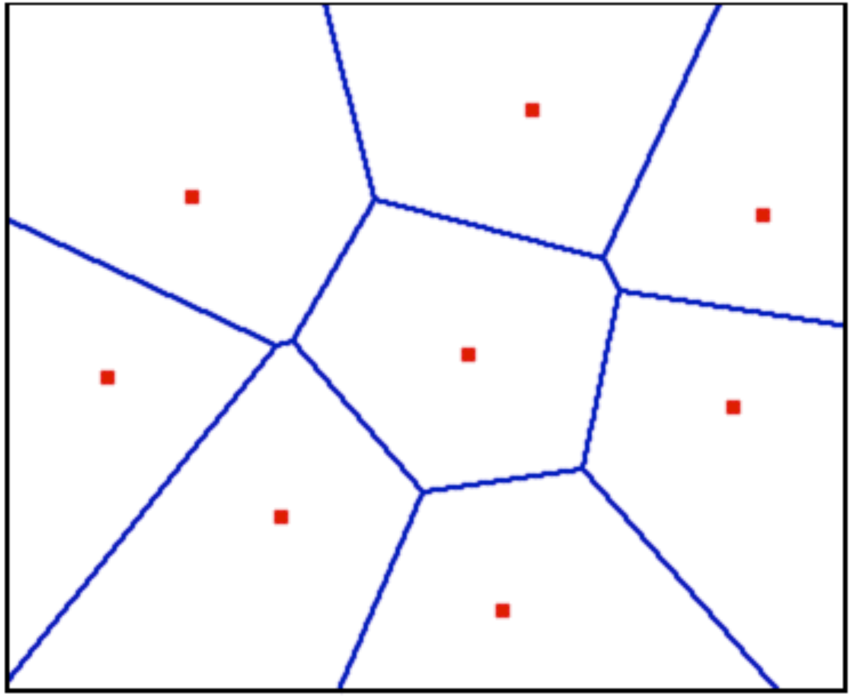
centroid – the mean of the data points in a cluster
→ requires continuous (vector-like) features
→ highlights iterative nature of algorithm

Q: What do these partitions look like?



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*.

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

One important point to keep in mind is that partitions are not scale-invariant!

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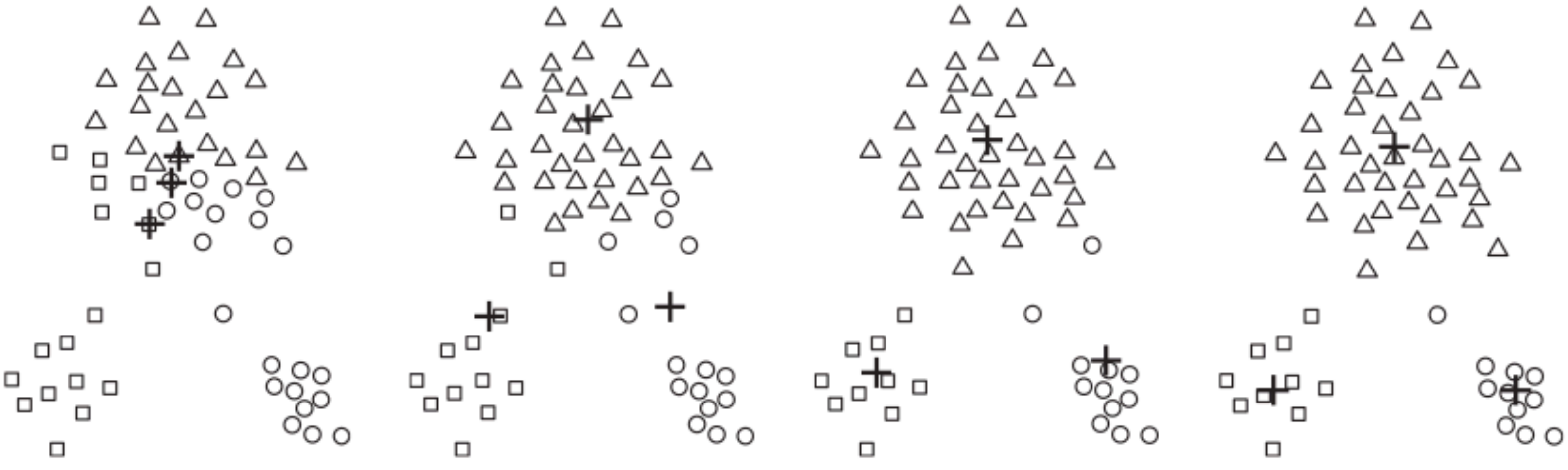
Therefore it’s important to think about your data representation before applying a clustering algorithm.

These graphs show two different representations of the same data:

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



(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

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

Q: How do you choose the initial centroid positions?

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- randomly (but may yield divergent behavior)

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- randomly (but may yield divergent behavior)
- perform alternative clustering task, use resulting centroids as initial k-means centroids

Q: How do you determine which centroid is the nearest?

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

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.

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

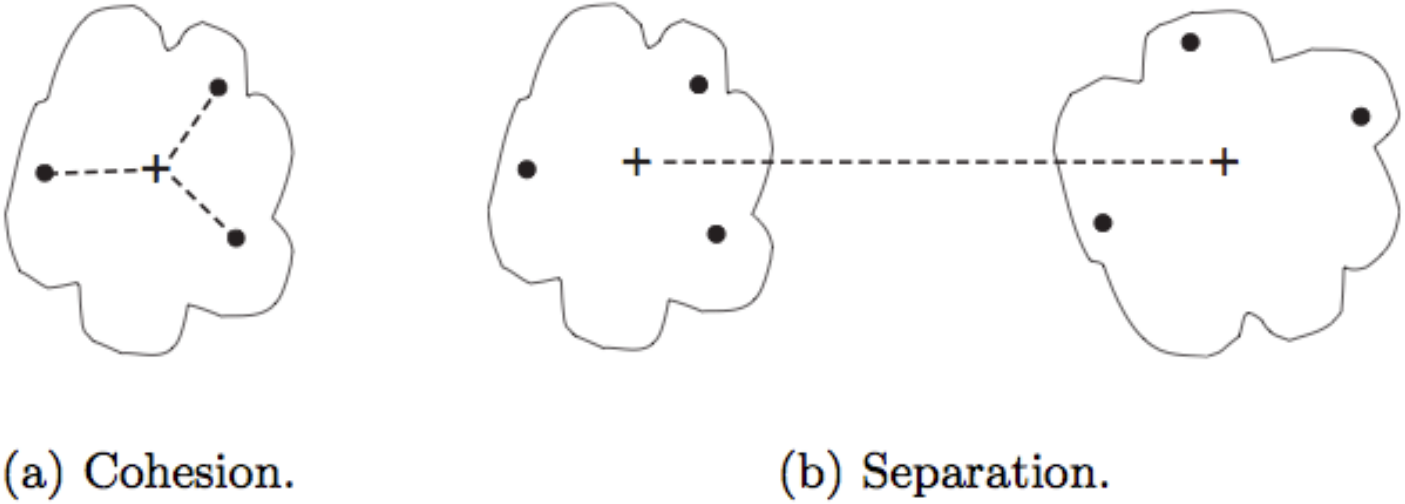

Figure 8.28. Prototype-based view of cluster cohesion and separation.

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 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.

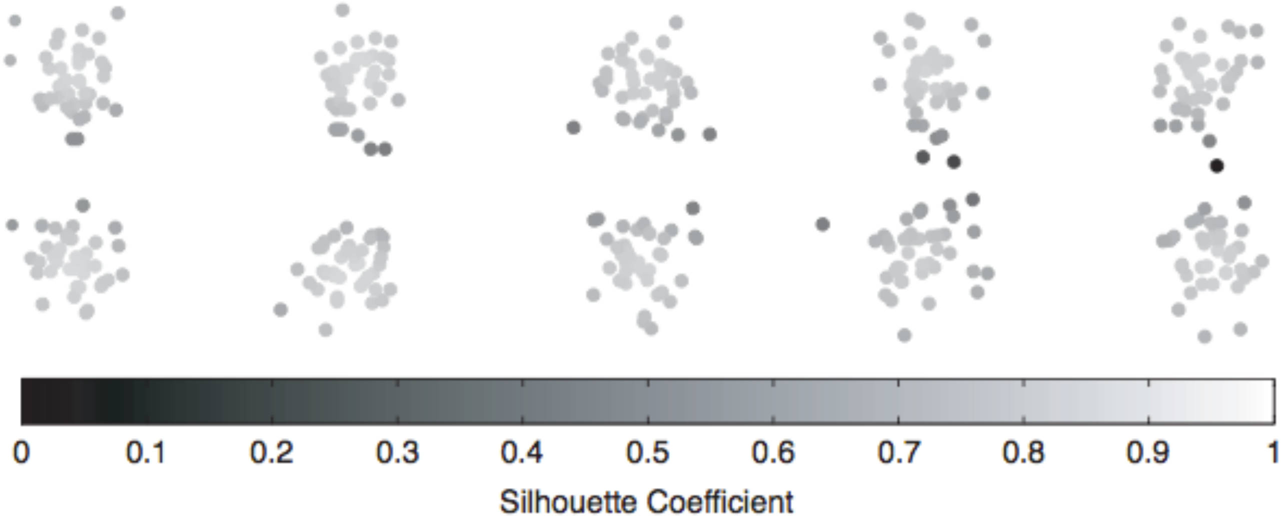

Figure 8.29. Silhouette coefficients for points in ten clusters.

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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$$SC_{total} = \frac{1}{k} \sum_{1}^{k} SC(C_i)$$

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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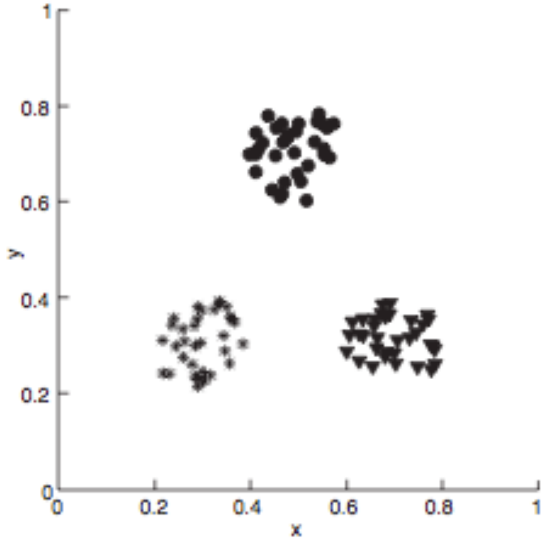
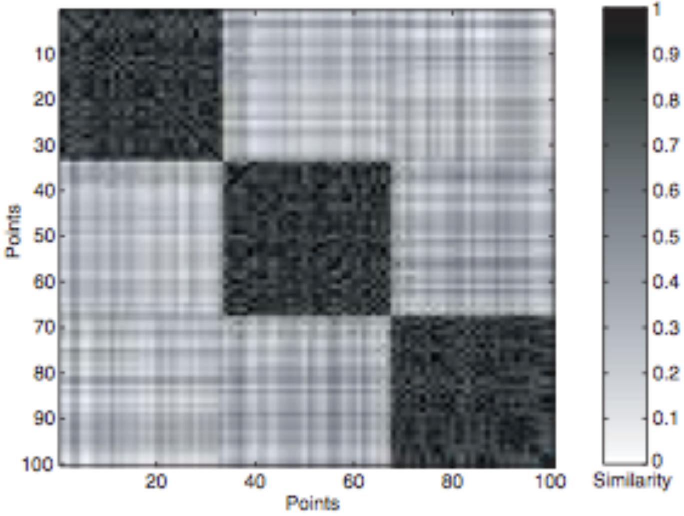
This can be done either graphically or using correlations.



(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?

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.

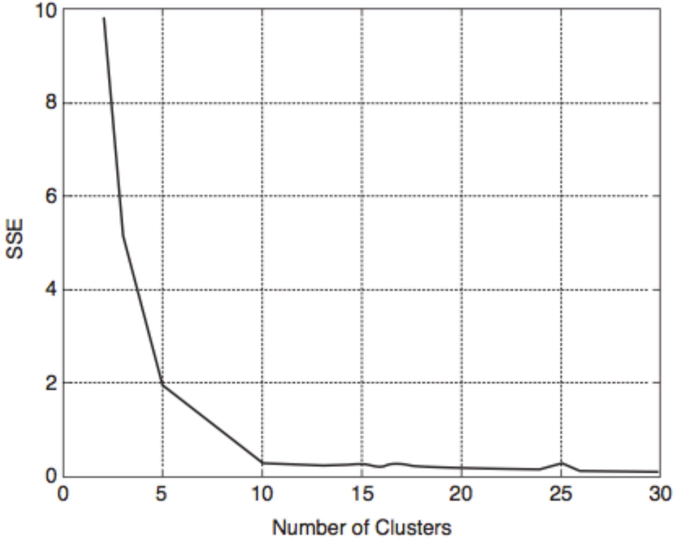

Figure 8.32. SSE versus number of clusters for the data of Figure 8.29.

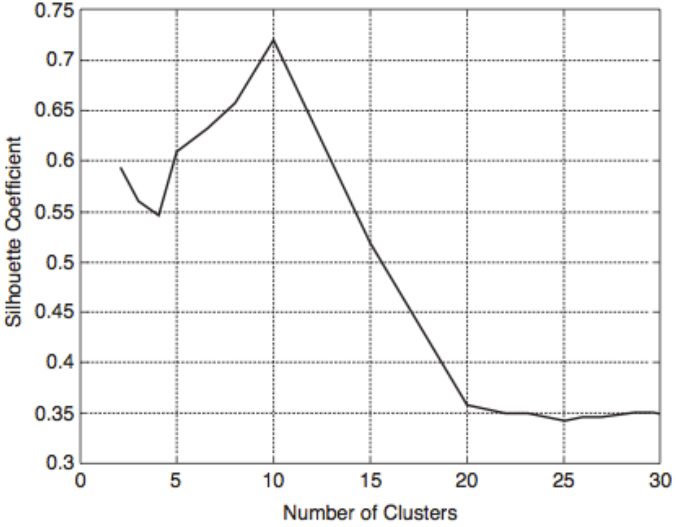

Figure 8.33. Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

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