GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

CLUSTER ANALYSIS

LAST TIME:

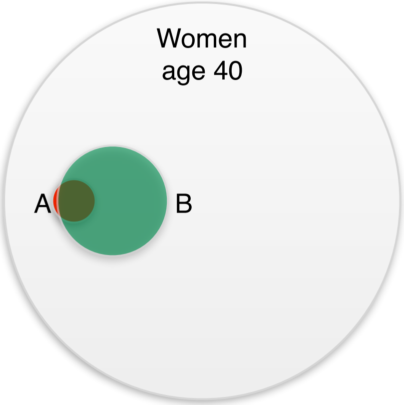
I. INTRO TO PROBABILITY

II. NAÏVE BAYESIAN CLASSIFICATION

EXERCISES:

III. NAÏVE BAYES CLASSIFICATION IN PYTHON

QUESTIONS?



QUESTIONS?

WHAT WAS THE MOST INTERESTING THING YOU LEARNT?

WHAT WAS THE HARDEST TO GRASP?

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

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The goal is to extract and enhance the natural structure of the data

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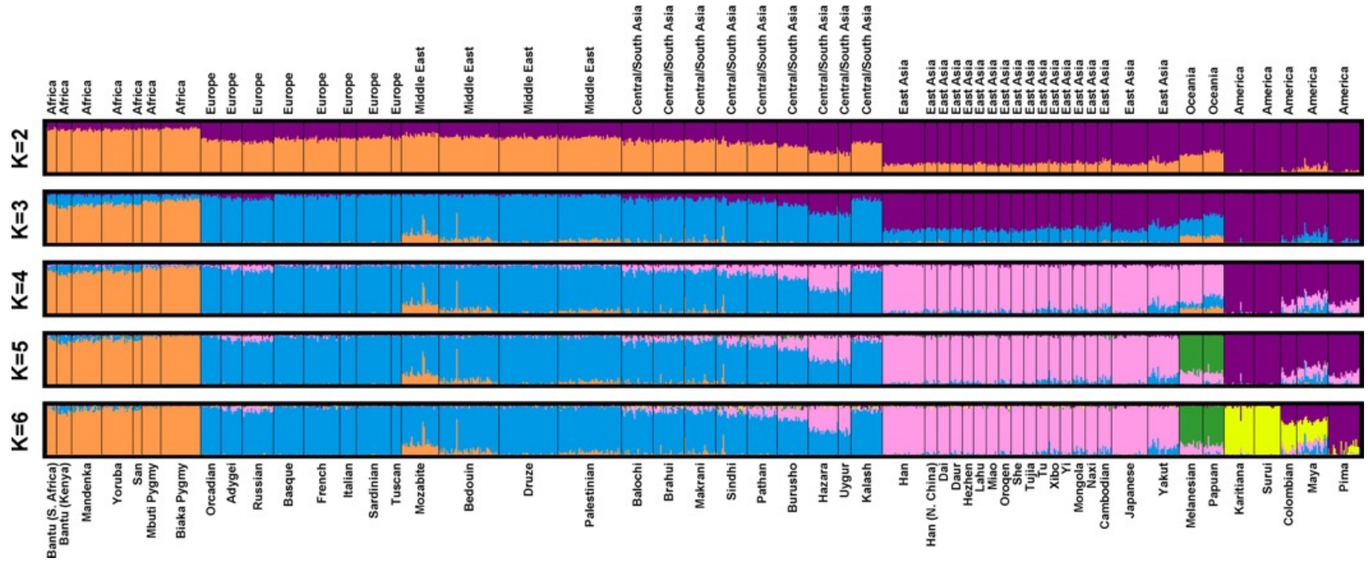

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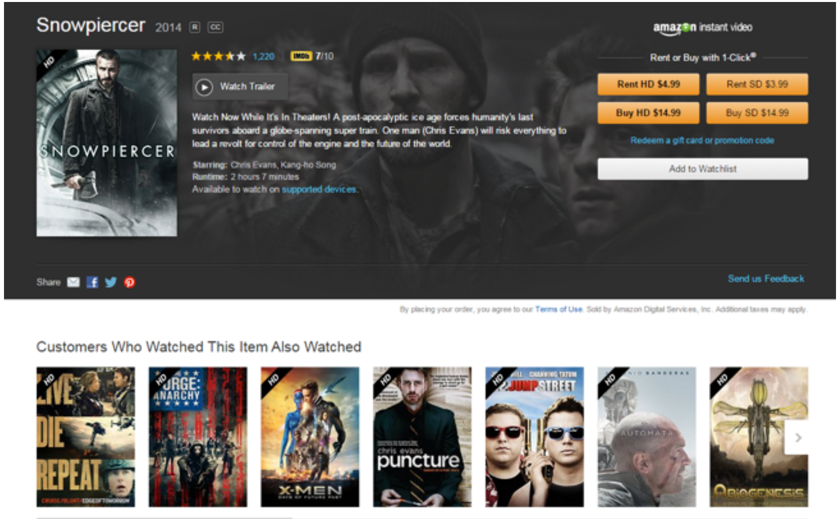

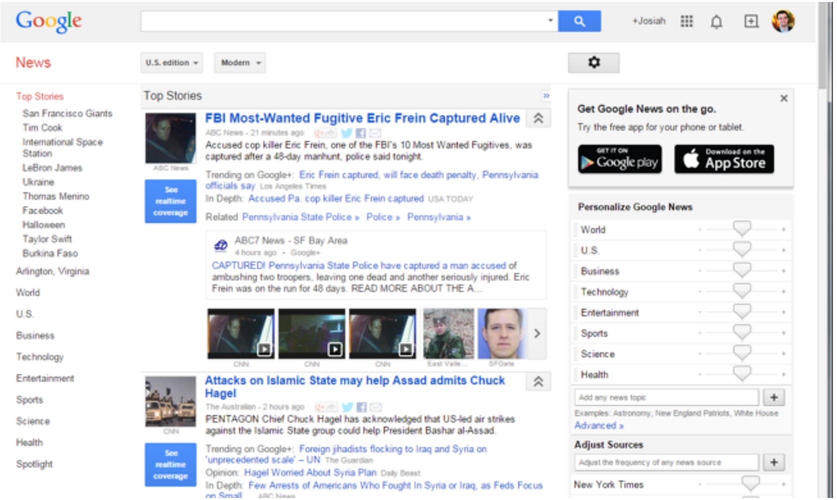

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http://i.huffpost.com/gen/1563531/thumbs/o-GROCERY-STORE-facebook.jpg

There are many kinds of classification procedures. For our class, we will be focusing on K-means clustering, which is one of the most popular clustering algorithms.

K-means is an iterative method that partitions a data set into k clusters.

II. K-MEANS CLUSTERING

Q: How does the algorithm work?

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*

Q: How do you choose the initial centroid positions?

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

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In the case of k-means clustering, the similarity metric is the ***Euclidian distance****:*

$$d(x_1, x_2) = \sqrt{\sum_{i=1}^{N} (x_{1i} - x_{2i})^2}$$

Q: How do we re-compute the positions of the centers at each iteration of the algorithm?

A: By calculating the centroid (i.e., the geometric center)

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) or on the points (eg, if no more than x% change clusters between iterations).

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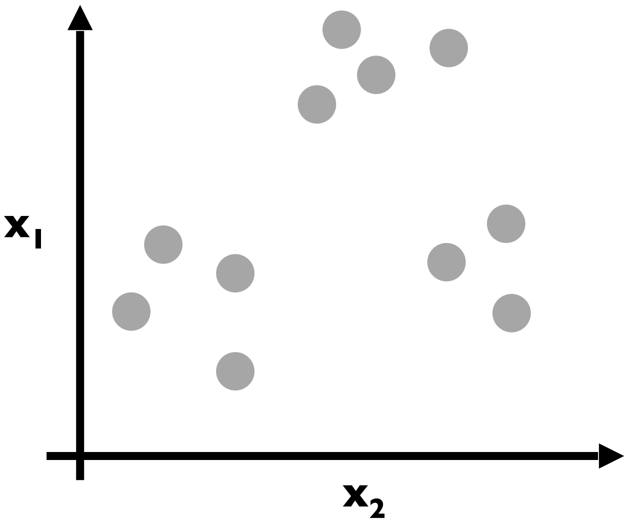

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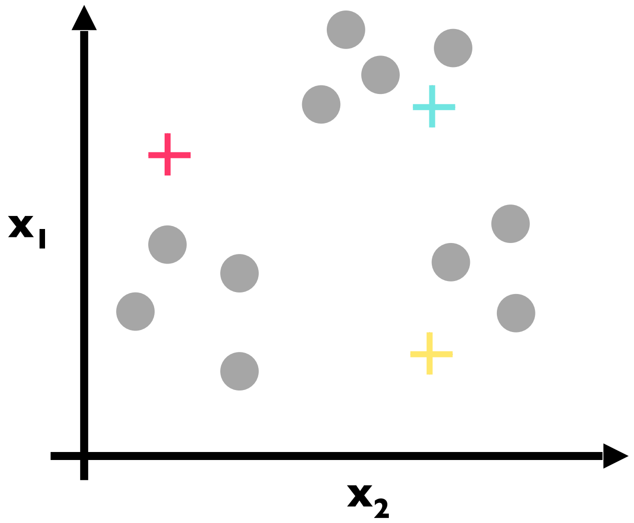

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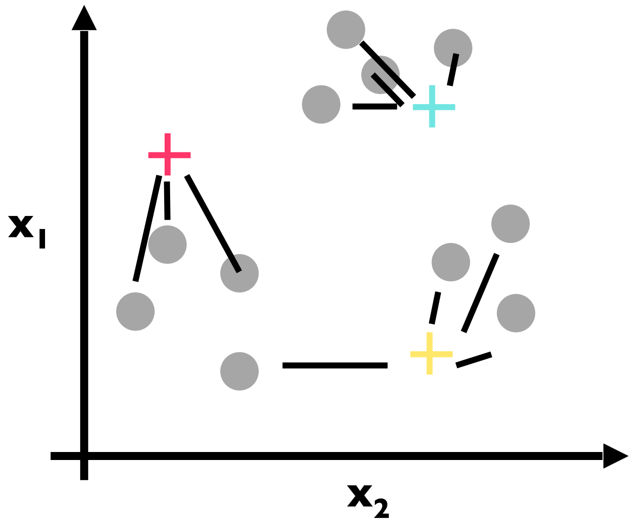

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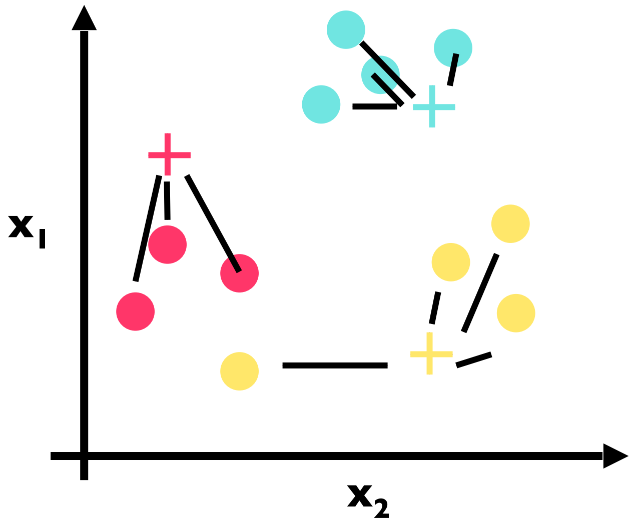

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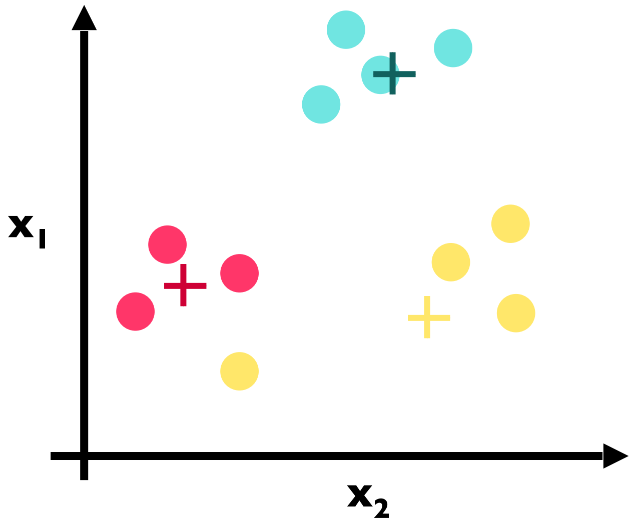

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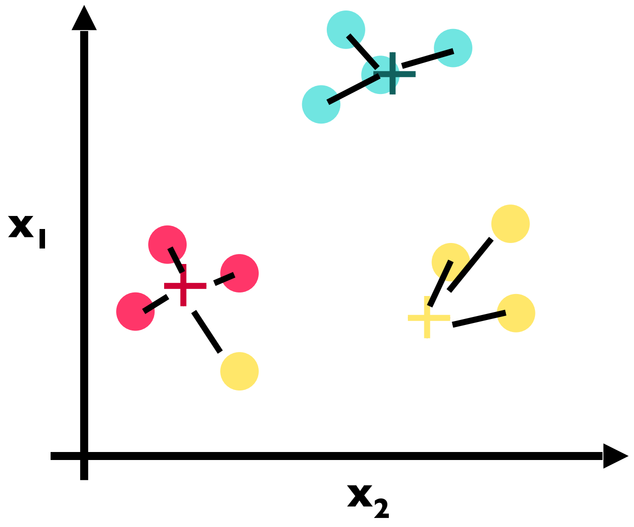

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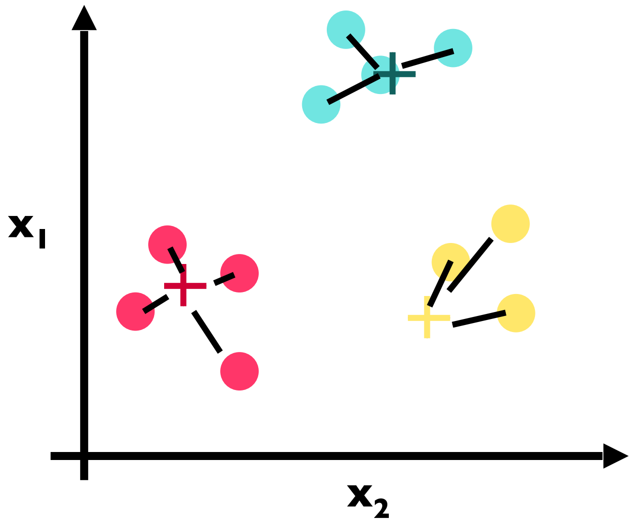

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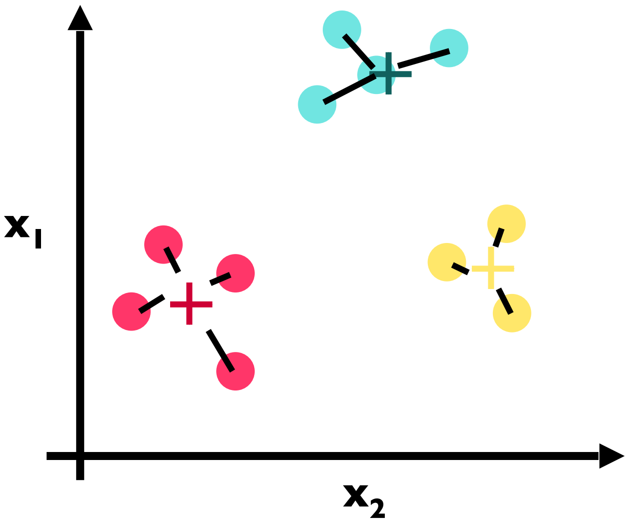

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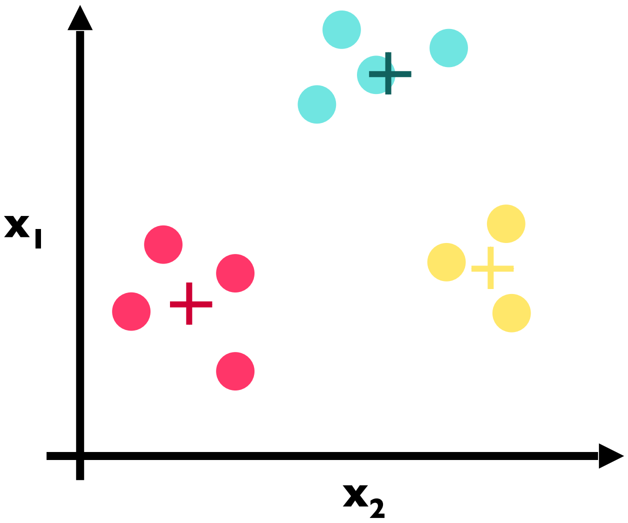

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III. CLUSTER VALIDATION

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.*

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

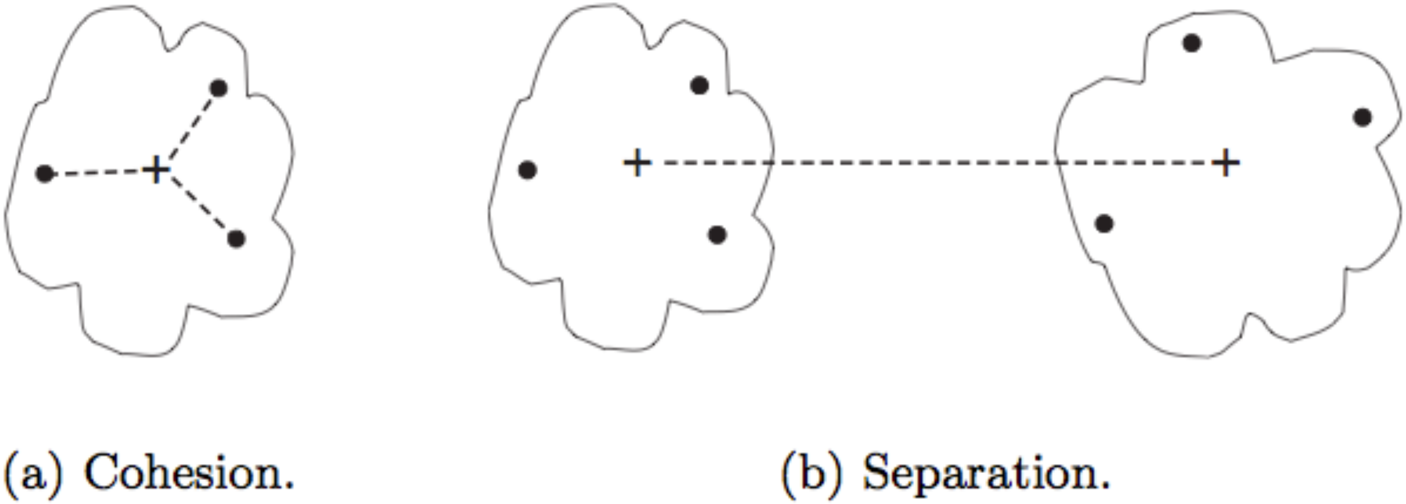

Figure 8.28. Prototype-based view of cluster cohesion and separation.

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

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.

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 SSE or SC for different values of k.

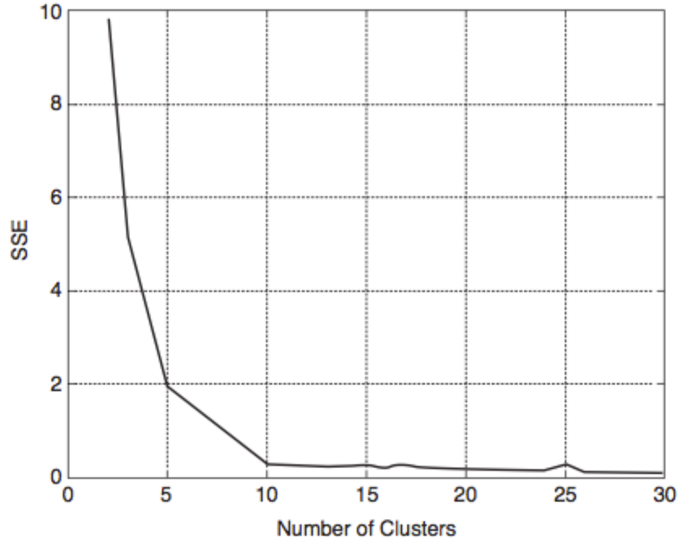

Figure 8.32. SSE versus number of clusters for the data of Figure 8.29.

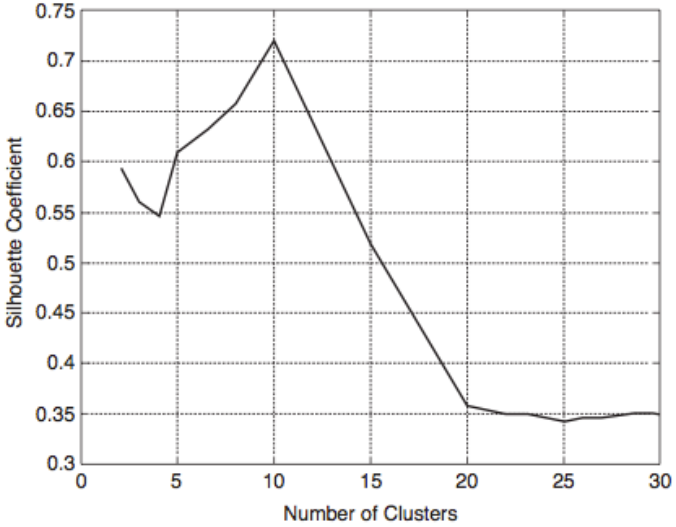

Figure 8.33. Average silhouette coefficient versus number of clusters for the data of Figure 8.29.

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

Strengths:

K-means is a popular algorithm because of its computational efficiency and simple and intuitive nature.

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Weaknesses:

However, K-means is highly scale dependent, and is not suitable for data with widely varying shapes and densities.

EX: K-MEANS CLUSTERING