INTRO TO DATA SCIENCE

CLUSTER ANALYSIS

I. CLUSTER ANALYSIS
II. THE K-MEANS ALGORITHM
III. CHOOSING K
IV. EXAMPLE

I. CLUSTER ANALYSIS

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

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

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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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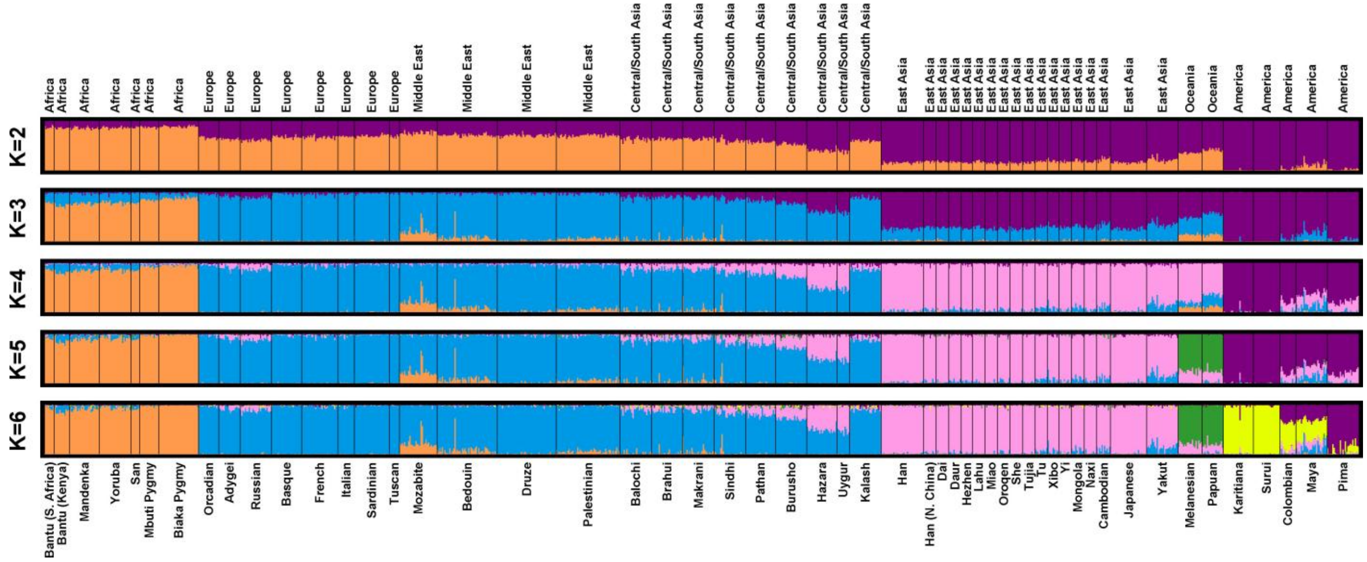

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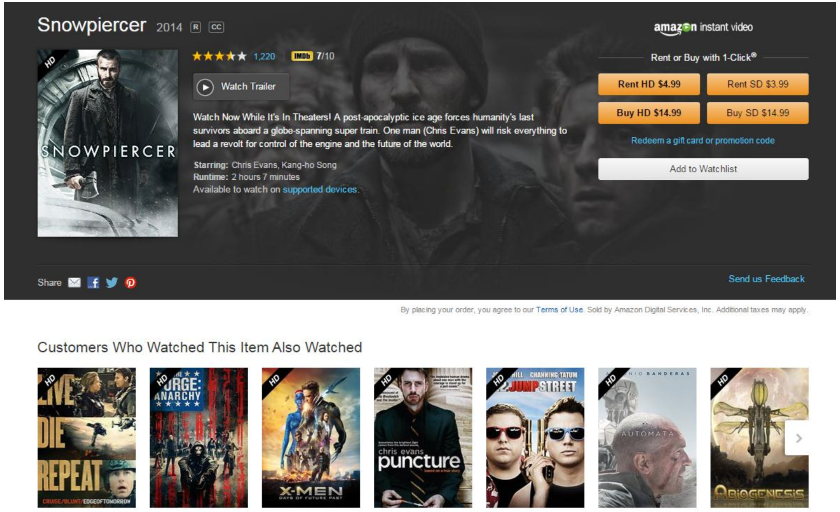

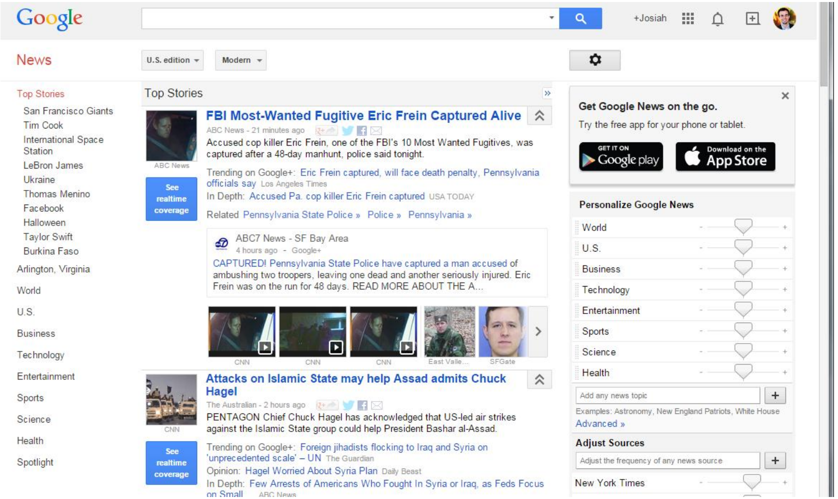

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http://i.huffpost.com/gen/1563531/thumbs/o-GROCERY-STORE-facebook.jpg

There are many kinds of clustering 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*

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- *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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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 recompute 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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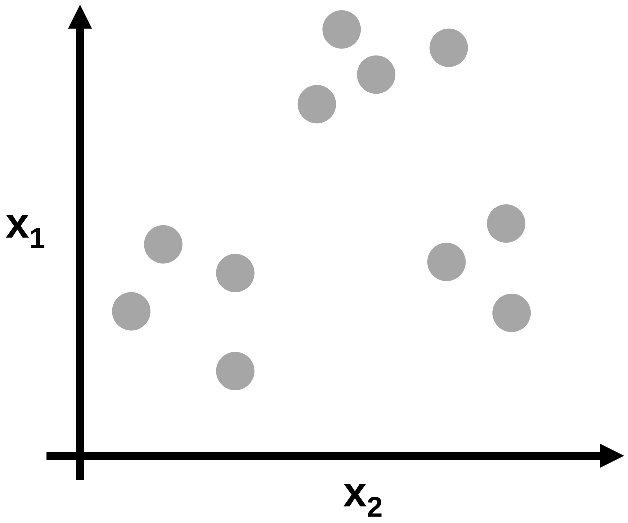

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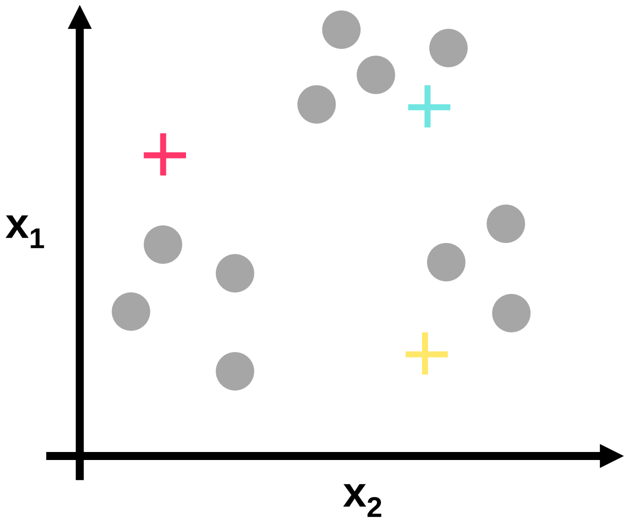

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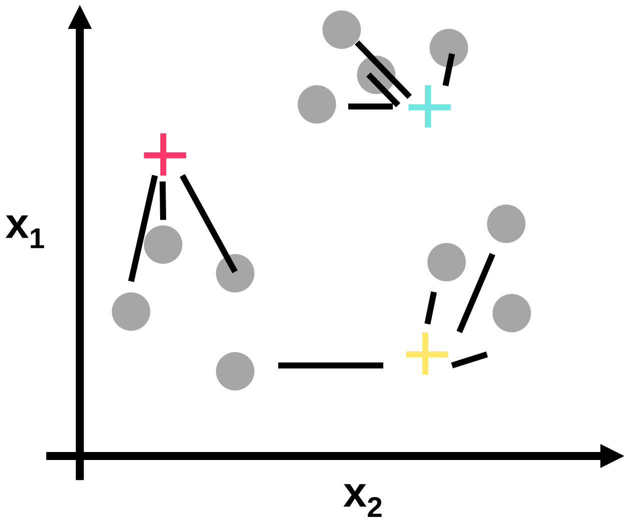

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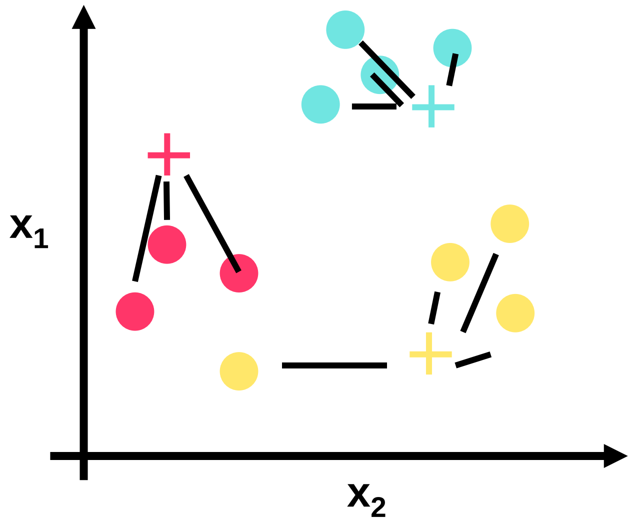

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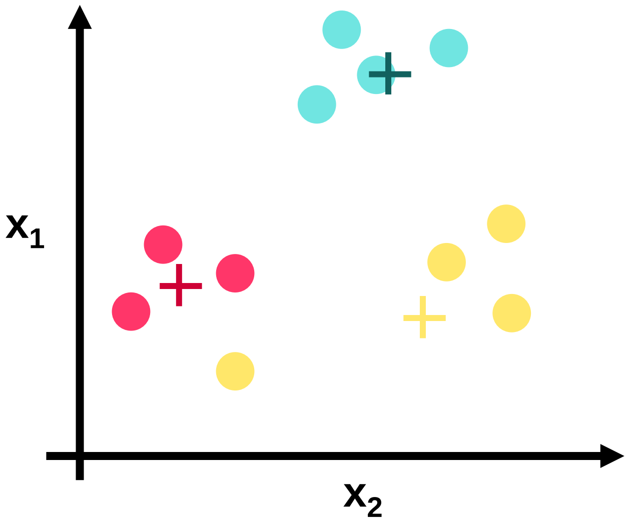

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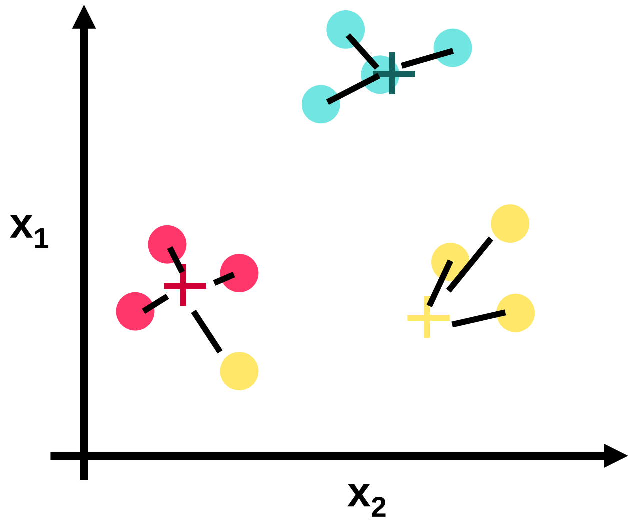

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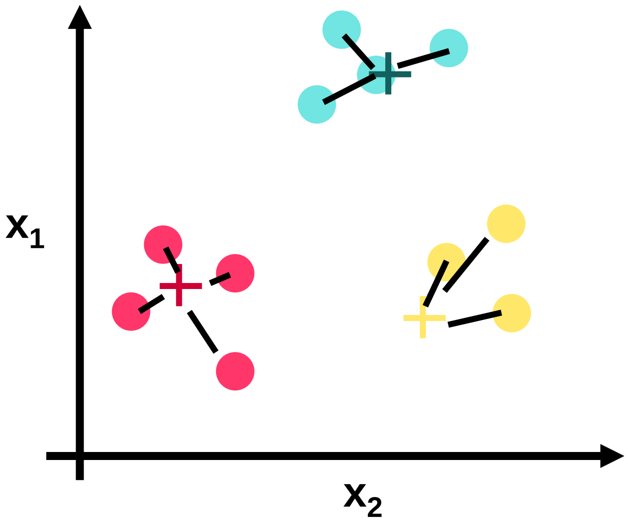

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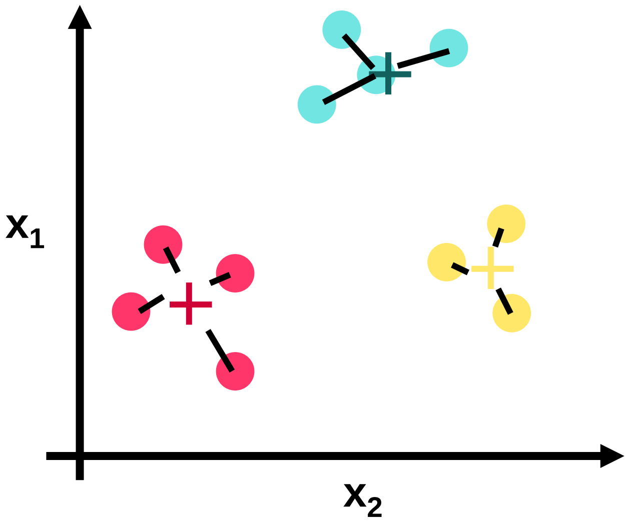

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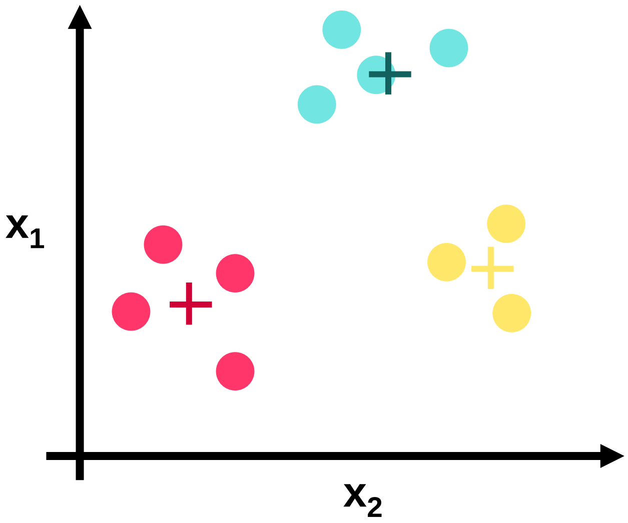

III. CLUSTER VALIDATION

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.*

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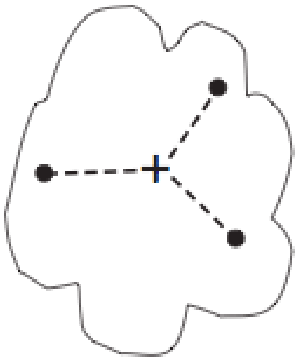
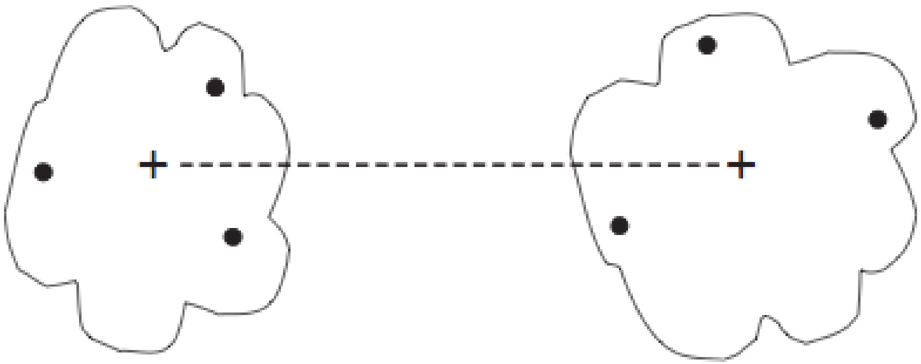
Separation *measures clustering effectiveness between clusters.*

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



(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

One useful measure than combines the ideas of cohesion and separation is the **silhouette coefficient**. *For a single point, this is given by:*

$$SC = \frac{b - a}{\max(a, b)}$$

a = The mean distance between a sample and all other points in the same class.

Source: scikit learn

One useful measure than combines the ideas of cohesion and separation is the **silhouette coefficient**. *For a single point, this is given by:*

$$SC = \frac{b-a}{\max(a,b)}$$

b = The mean distance between a sample and all other points in the next nearest cluster.

Source: scikit learn

Generally, this formula simplifies to the following:

$$SC = 1 - \frac{a}{b}$$

This is because generally b > a:

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:

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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 SC for different values of k.

A: Another commonly used metric is the within sum of squared errors

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

Strengths:

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Weaknesses:

However, K-means is highly scale dependent, and may produce misleading results for data with widely varying shapes and densities.

EX: K-MEANS CLUSTERING