GENERAL ASSEMBLY

DATA SCIENCE
CLUSTERING

I. UNSUPERVISED LEARNING

Supervised learning has clear objectives:

- Accurately predict unseen test cases
- Understand which features affect the response, and how

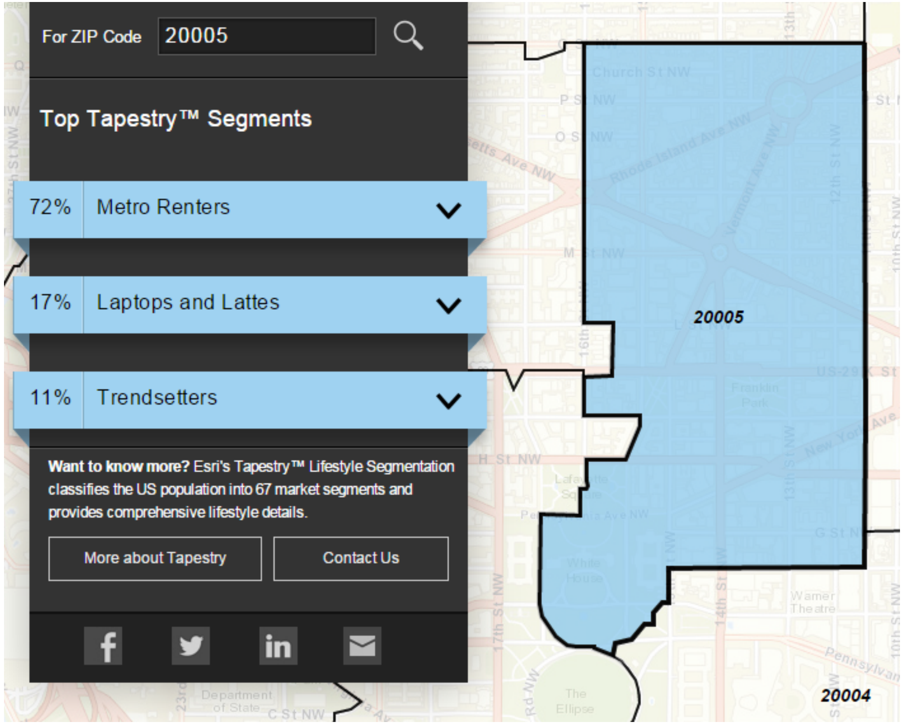
You can evaluate how well you are doing!

Unsupervised learning has fuzzy objectives:

- Find groups of observations that behave similarly
- Find features that behave similarly

It’s difficult to evaluate how well you are doing!

Classify US residential neighborhoods into 67 unique segments based on demographic and socioeconomic characteristics



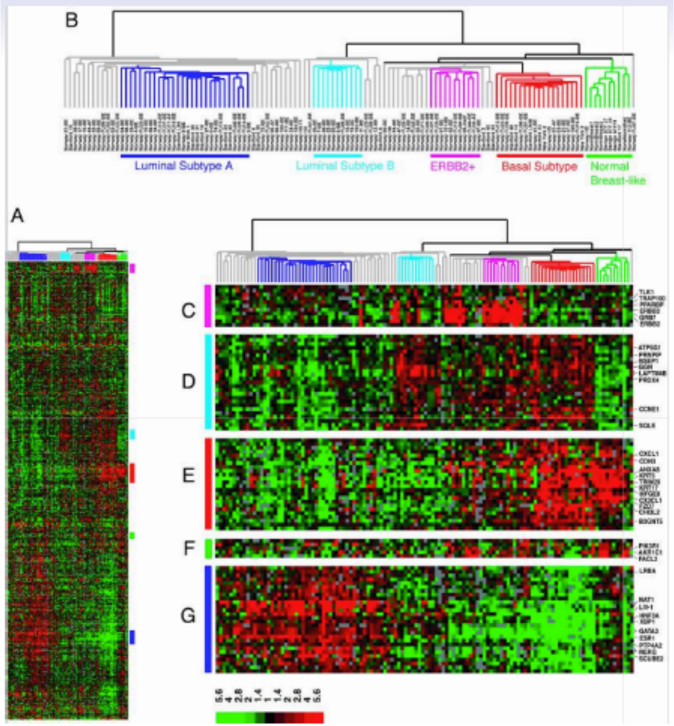
Metro Renters:

Young, mobile, educated, or still in school, we live alone or with a roommate in rented apartments or condos in the center of the city. Long hours and hard work don't deter us; we're willing to take risks to get to the top of our professions… We buy groceries at Whole Foods and Trader Joe's and shop for clothes at Banana Republic, Nordstrom, and Gap. We practice yoga, go skiing, and attend Pilates sessions.

Source: http://www.esri.com/landing-pages/tapestry/

CLUSTERING EXAMPLE

Classify a tissue sample into one of several cancer classes, based on gene expression data



- Each column is a woman with breast cancer (n=88)
- Each row is a gene (p=8000)
- Color represents level of gene expression

Goal: Locate subcategories of breast cancer showing different gene expressions

Technique: Hierarchical clustering applied to the columns, resulting in six sub-groups of patients

Source: https://class.stanford.edu/c4x/HumanitiesScience/StatLearning/asset/introduction.pdf

II. CLUSTER ANALYSIS

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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

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.

III. 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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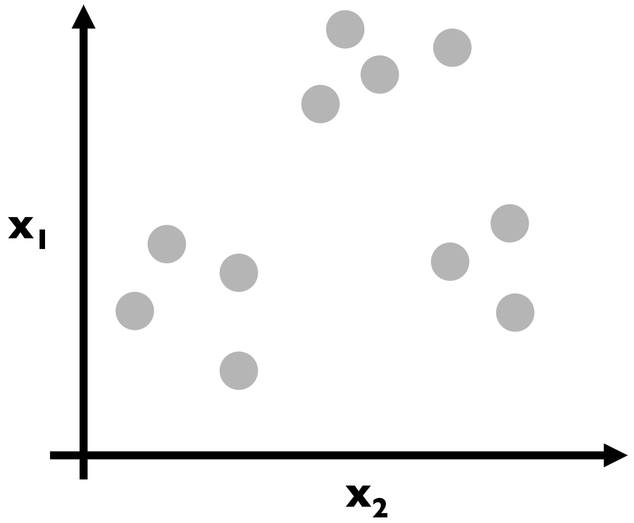

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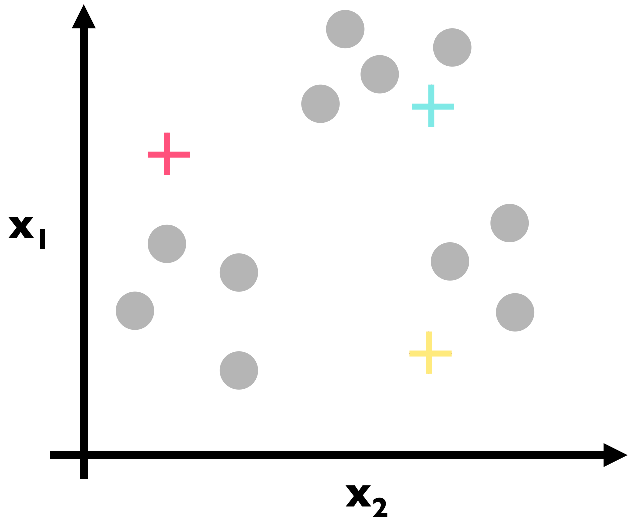

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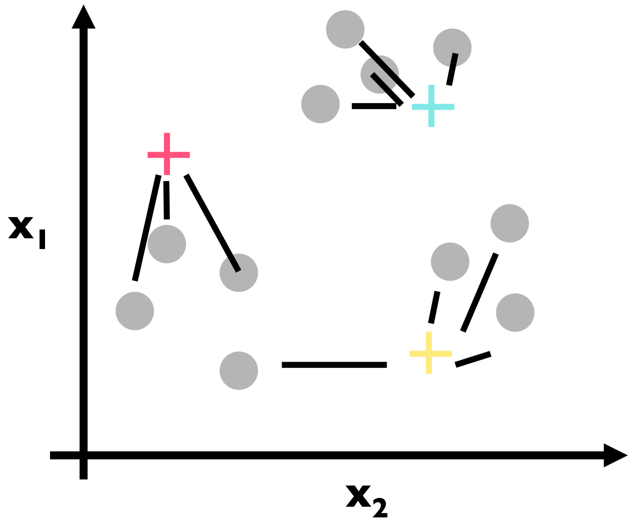

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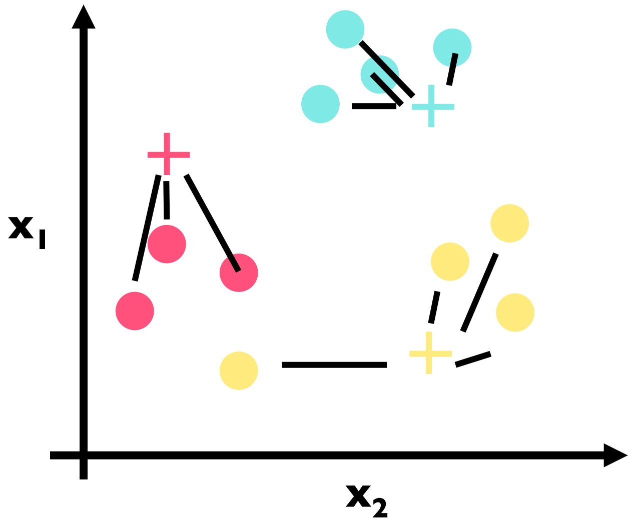

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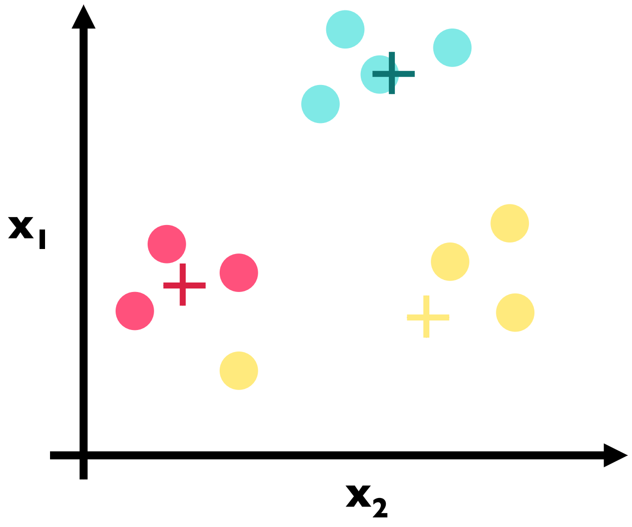

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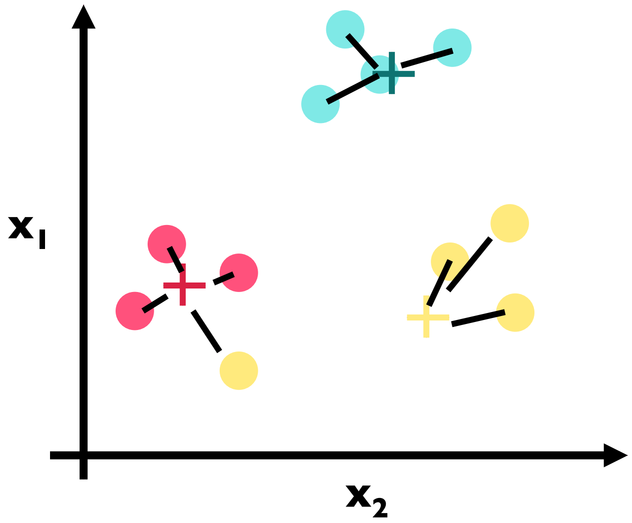

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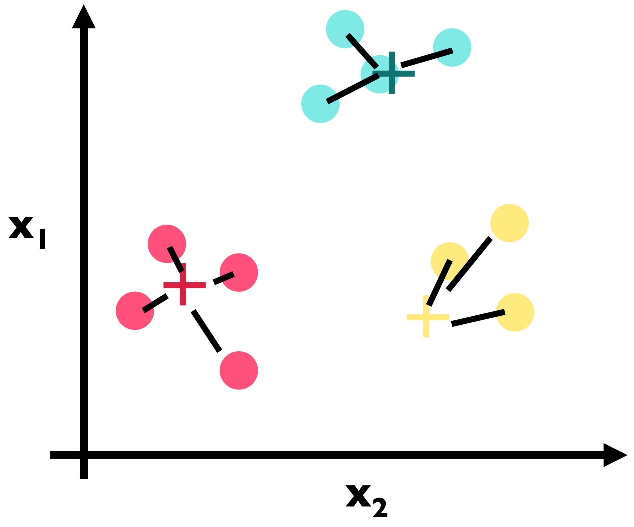

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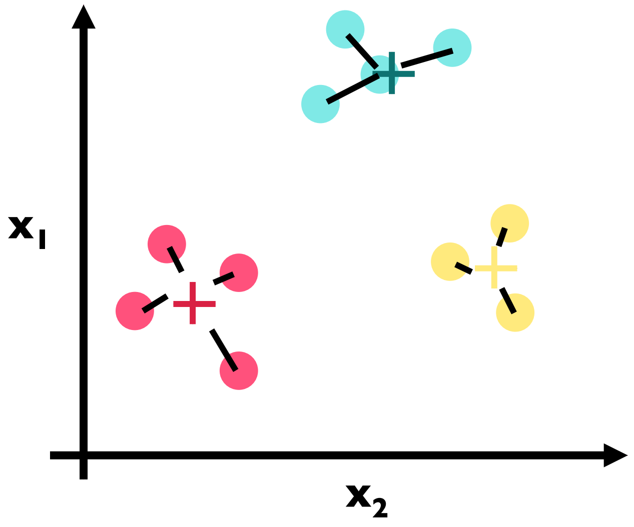

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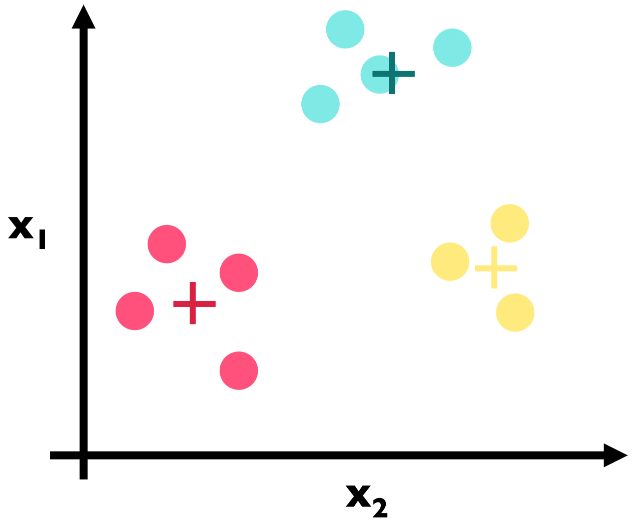

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- randomly (but may yield divergent behavior)
- perform alternative clustering task, use resulting centroids as initial k-means centroids
- start with global centroid, choose point at max distance, repeat (but might select outlier)

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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).

IV. 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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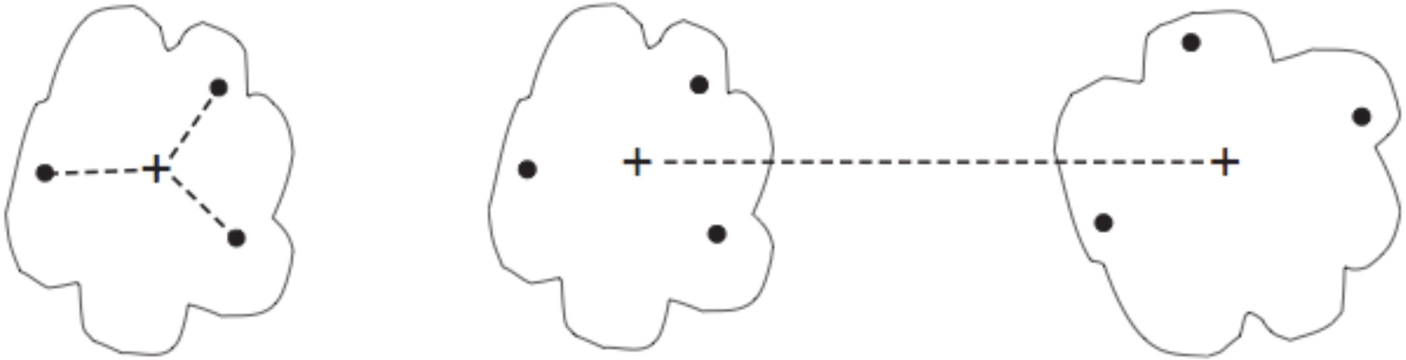
Separation measures clustering effectiveness between clusters.

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



(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 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:

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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?

A: By computing the SC for different values of k.

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 is not suitable for data with widely varying shapes and densities.

V. EXAMPLE