

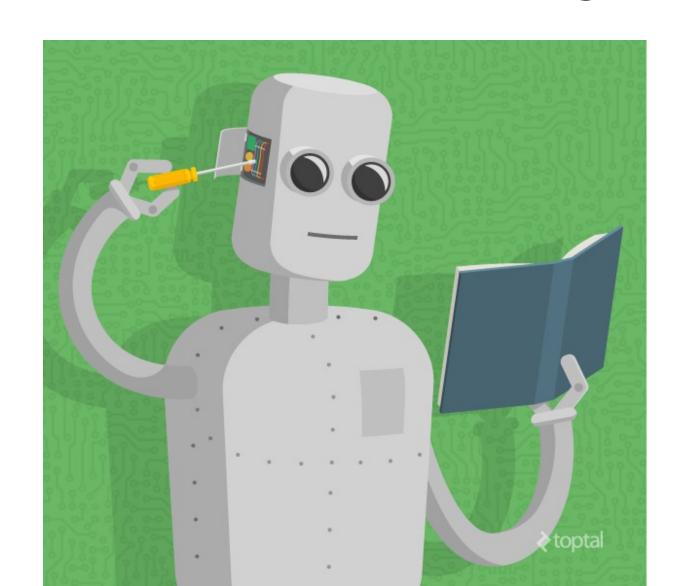
### Target knows your secrets...



"Just wait. We'll be sending you coupons for things you want before you even know you want them." –Andrew Pole, Target statistician

# Clustering

# Unsupervised Machine Learning



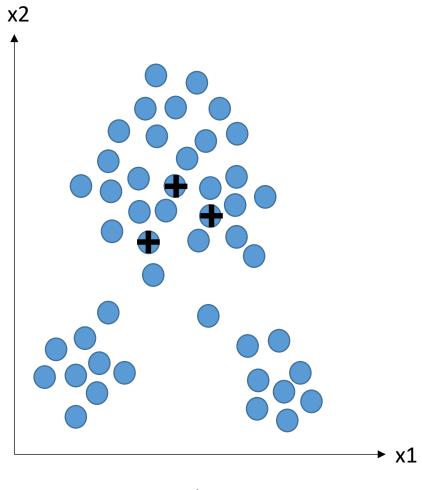
### Clustering

- Cluster analysis divides data into groups (clusters) that are meaningful and/or useful
- Clusters are potential classes and cluster analysis finds them in unlabeled data

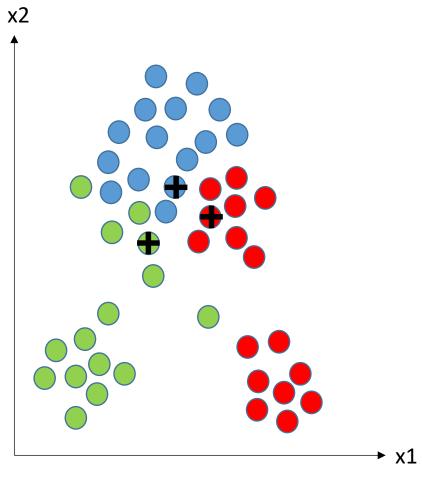
 Items in a cluster should be similar to each other, but different from those outside of their cluster

### K-means algorithm

- Choose K random data points from the training data to be initial centroids
- Each data point is assigned to the closest centroid, to form clusters



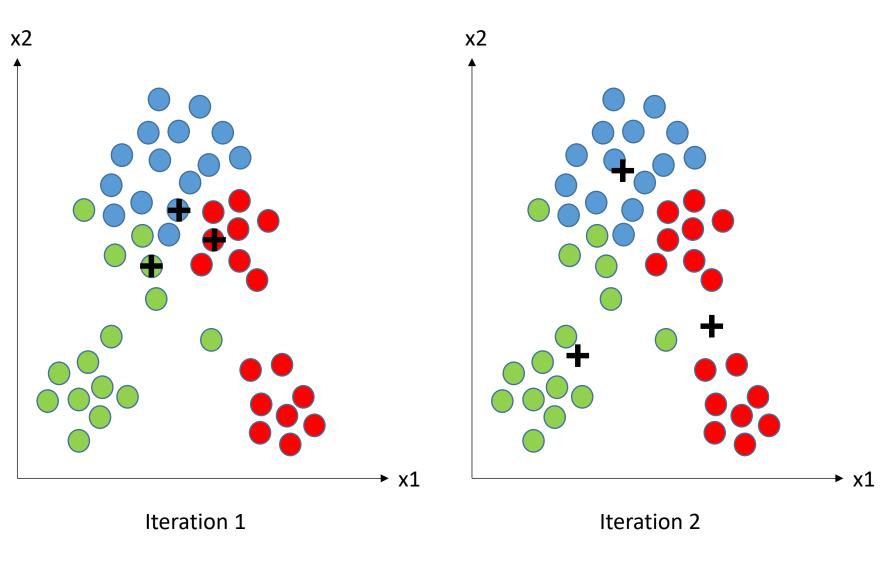
Iteration 1

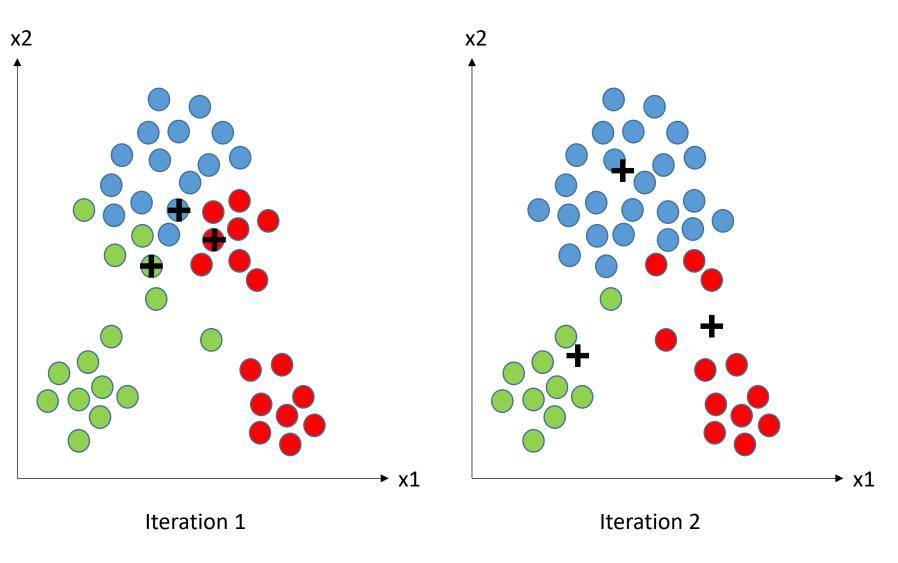


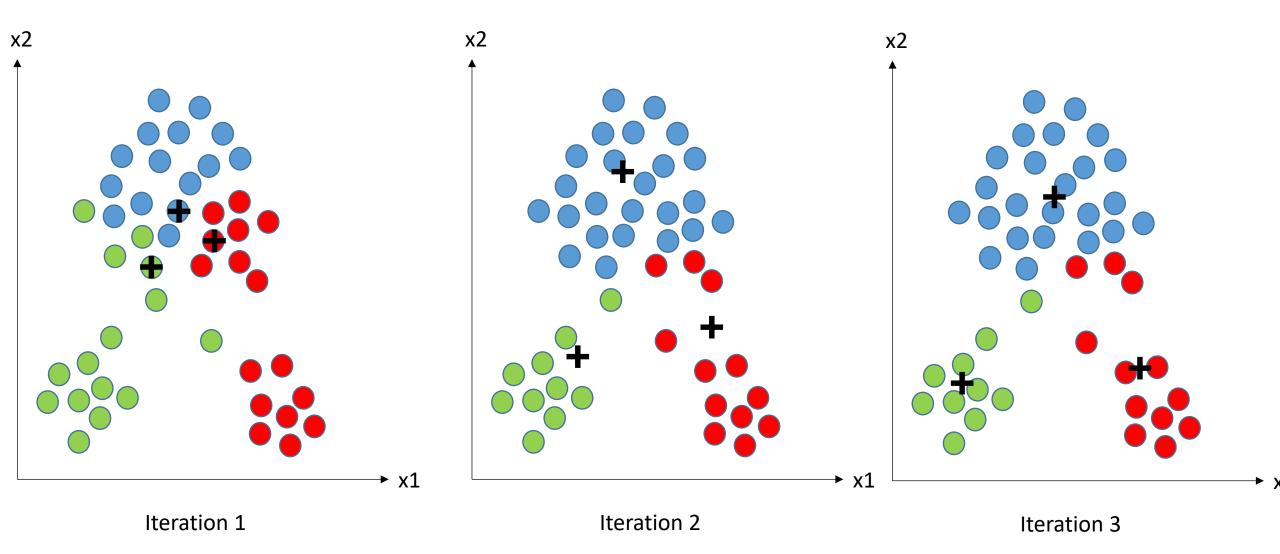
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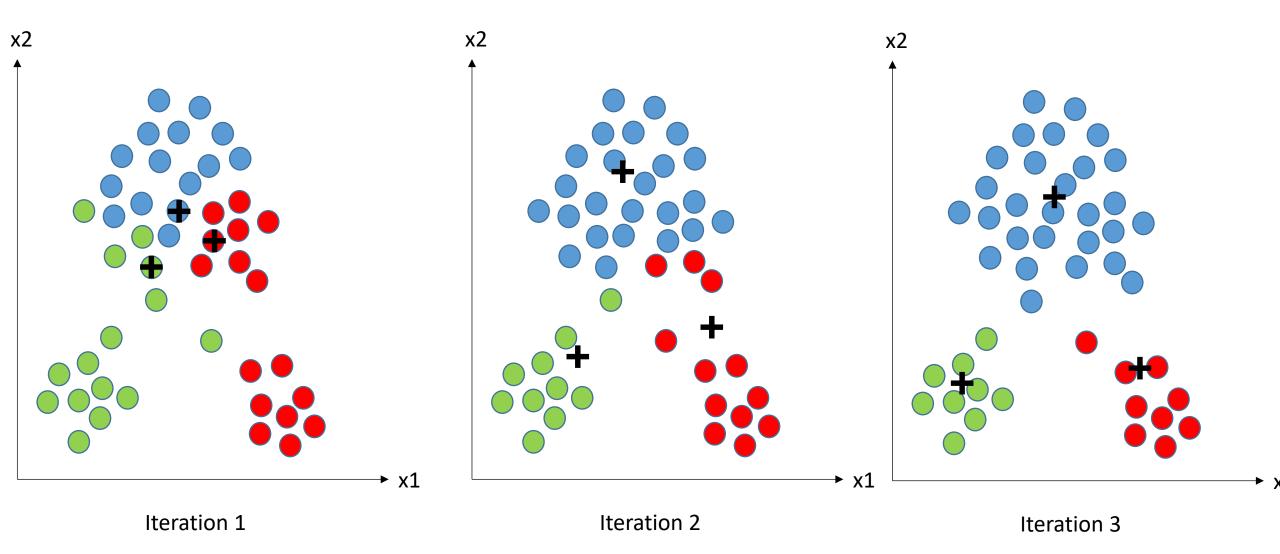
### K-means algorithm

- Choose K random data points from the training data to be initial centroids
- Each data point is assigned to the closest centroid, to form clusters
- Update the centroid of each cluster based on the mean of the points assigned to that cluster
- Re-assign points to their closest centroid



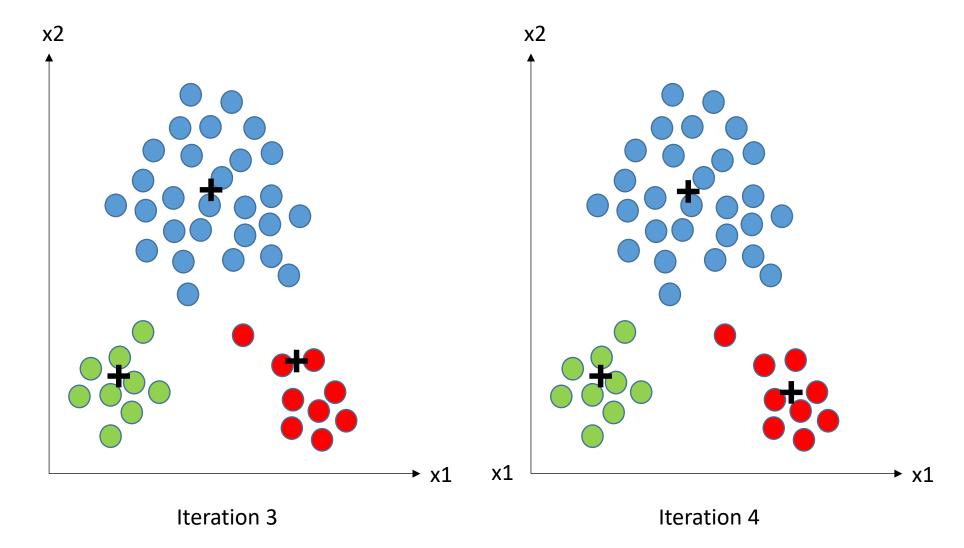






### K-means algorithm

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- Update the centroid of each cluster based on the points assigned to that cluster
- Re-assign points to their closest centroid
- Repeat until no point changes cluster (or equivalently, no centroid changes)



### Objective Function

- The goal of clustering is usually specified by an objective function and a proximity measure
- With a proximity measure of Euclidian Distance, the objective is to minimize the sum of the squared error (SSE), or scatter

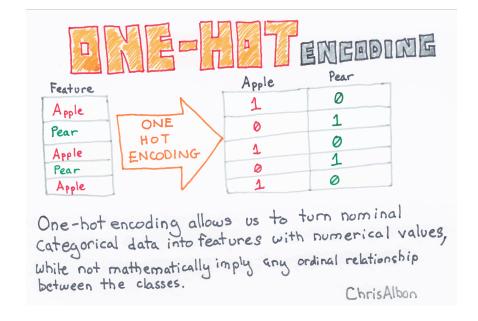
$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist(c_i, x)^2$$
 Where K is the number of clusters  $C_i$  is the i<sup>th</sup> cluster  $C_i$  is the centroid of cluster  $C_i$ 

x is a data point

 Proximity measure, centroid definition, and objective function differ depending on the data and the task.

#### Handling categorical data:

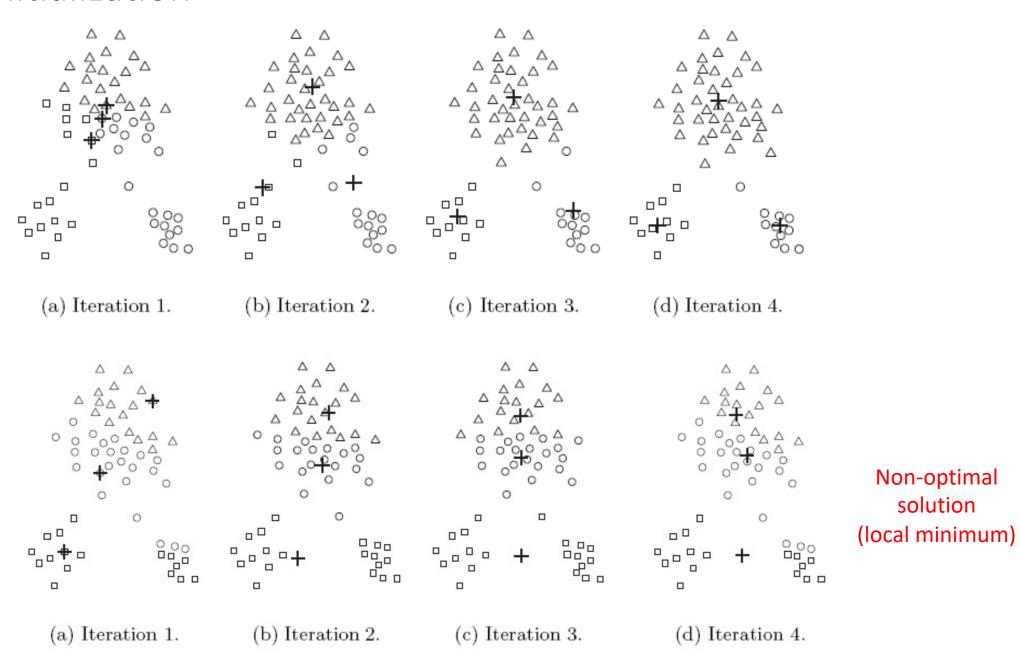
One-hot-encoding



#### Handling empty clusters:

- If no points are assigned to a centroid, choose a new centroid, either:
  - Randomly
  - The point that is farthest away from any current centroid. This
    eliminates the point that currently contributes most to SSE.
  - Choose a replacement from the cluster that has the highest SSE.
     This will split the cluster and typically reduce overall SSE.

#### Centroid Initialization



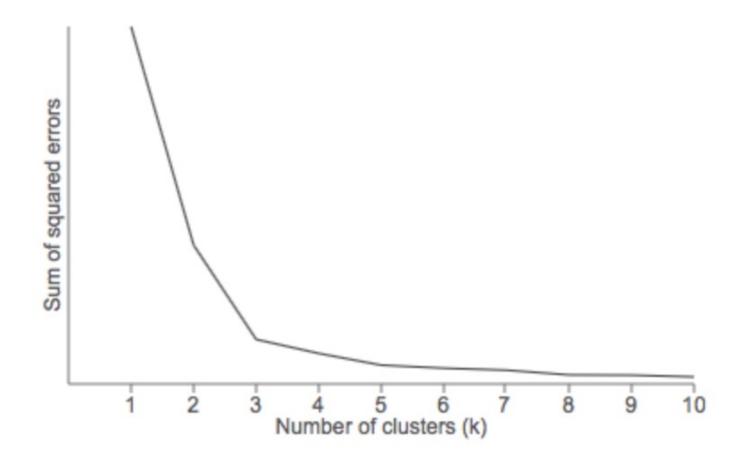
### K-means++

- Choose a random centroid
- Repeat until there are K centroids:
  - Compute distance from every point to its nearest centroid
  - Use squared-distance as a probability distribution for choosing the next centroid (farther are more likely to be selected)

## Choosing the Right K

- Prior knowledge of how many clusters are in the data
- How many clusters are desired for the application
- Let the data tell you how many clusters it naturally has

### Choosing the Right K – Elbow Method



select the value of k at the "elbow" i.e. the point after which the distortion/inertia start decreasing in a linear fashion

### Bisecting K-means

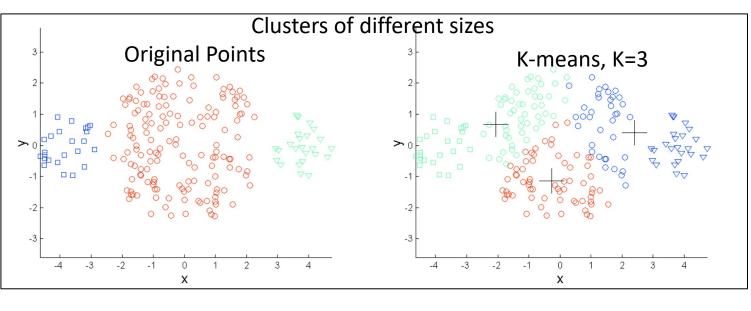
- To obtain K clusters, split the set of all data points into 2 clusters using K-means with K=2
- Choose one of the clusters to split
- Split the chosen cluster using K-means with K=2
- Continue until you have K clusters

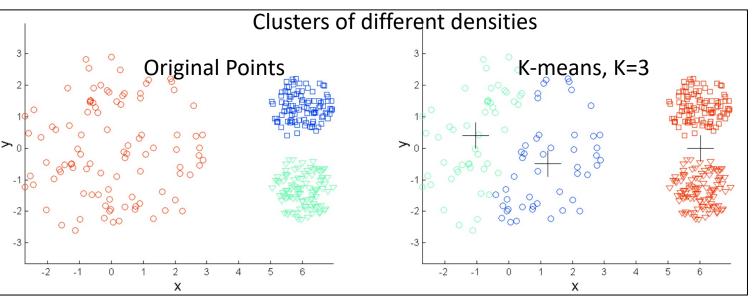
- Less susceptible to initialization problems than K-means
- Shown to converge on better clusters, better overcoming local minimums

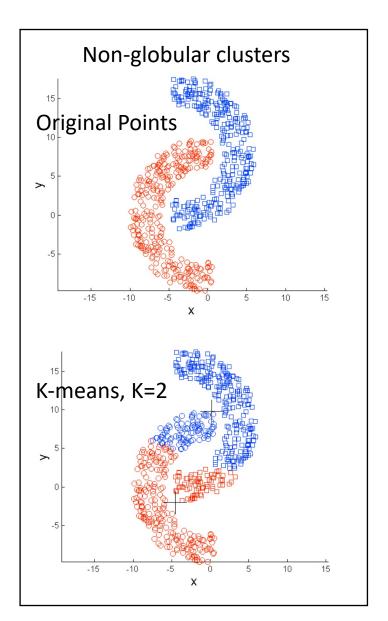
### Characteristics of K-means

- Simple and can be used for a wide variety of data types
- Quite efficient, even when run multiple times
- There are variations (like Bisecting K-means) that are even more efficient and less susceptible to initialization problems
- Outliers can alter results, but outlier detection and removal can be done before clustering
- Curse of Dimensionality: As dimensionality increases, distance and similarity between points lose meaning
- Difficulties with non-globular data, clusters of different sizes, clusters of different densities

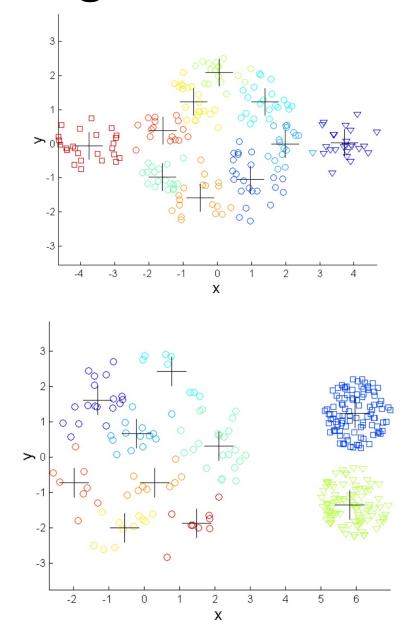
### Weaknesses of K-means

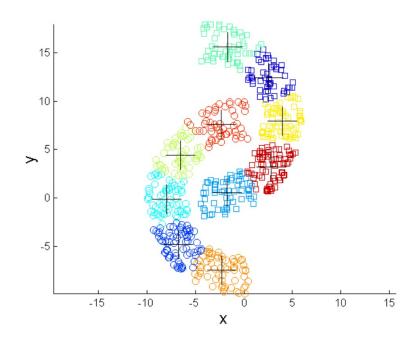






## Increasing K to Overcome Weaknesses





## (Backup) Terminology

- Partitional Clustering: division of dataset into non-overlapping subsets, such that each data object is in exactly one cluster
- Hierarchical Clustering: Clusters can have subclusters. Nested clusters are organized into a tree. Each node in the tree (except leaf nodes) is the union of its children.
- Exclusive Clustering: each object is assigned only to a single cluster
- Overlapping/Non-exclusive clustering: an object can simultaneously belong to more than one cluster
- Fuzzy/Probabilistic Clustering: every object belongs to every cluster with a membership weight from 0 to 1
- Complete Clustering: assigns every object to a cluster
- Partial Clustering: not every object is necessarily assigned to a cluster

### (Backup) K-means Example

Given this dataset with one attribute, cluster it using k-means with k=2. Use data points A and B as the initial centroids.

	A	В	С	D	Е
X1	1	6	8	20	30