# The Data Science Cycle

## Unsupervised Learning - Clustering

DataLab

September 21, 2016

# Outline



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# Supervised Learning vs. Unsupervised Learning

**Supervised learning:**

- Discover patterns in the data that relate data attributes with a target (class) attribute.

**Unsupervised learning:**

The data have no target attribute.

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Clustering is often considered synonymous with unsupervised learning.

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# Pattern Recognition

**Definition**

Search for structure in data

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Search for structure in data

## Elements of Numerical Pattern Recognition

1. Process Description
   - Feature Nomination, Test Data, Design Data
2. Feature Analysis
   - Preprocessing, Extraction, Selection, ...
3. **Cluster Analysis**
   - Labeling, Validity, ...
4. Classifier Design
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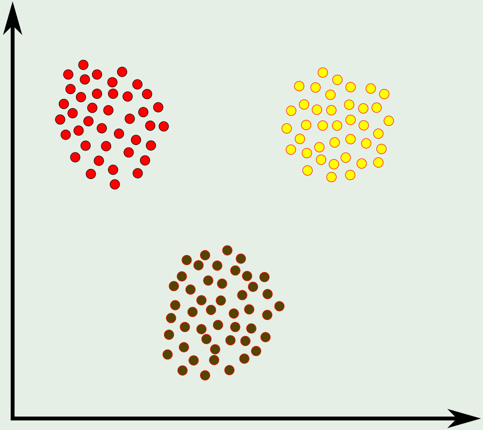
# An illustration

The data set has three natural groups of data points, i.e., 3 natural clusters.



# Examples

**Example 1**

Groups people of similar sizes together to make “small”, “medium” and “large” T-Shirts.

**Example 2**

In marketing, segment customers according to their similarities.

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Clustering!!!

**Basically**

We want to "reveal" the organization of patterns into "sensible" clusters (groups).

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Clustering is one of the most primitive mental activities of humans, used to handle the huge amount of information they receive every day.

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# Aspects of clustering

## A clustering algorithm - They are Many!!!

- Partition clustering.
- Hierarchical clustering.
- etc.

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A distance (similarity, or dissimilarity) function.

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# K-Means - Stuart Lloyd(Circa 1957)

**History**

Invented by Stuart Loyd in Bell Labs to obtain the best quantization in a signal data set.

**Something Notable**

The paper was published until 1982

**Basically given $N$ vectors $x_1, \ldots, x_N \in \mathbb{R}^d$**

It tries to find $k$ points $\mu_1, \ldots, \mu_k \in \mathbb{R}^d$ that minimize the expression (i.e. a partition $S$ of the vector points):

$$\sum_{k=1}^{N} \sum_{i: x_i \in C_k} \|x_i - \mu_k\|^2 = \sum_{k=1}^{N} \sum_{i: x_i \in C_k} (x_i - \mu_k)^T (x_i - \mu_k)$$

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## Definition

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- The $K$-means algorithm partitions the given data into $K$ clusters.
- Each cluster has a cluster center, called centroid.
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# $K$-means algorithm

## The $K$-means algorithm works as follows

Given $k$ as the possible number of cluster:

1. Randomly choose $K$ data points (seeds) to be the initial centroids, cluster centers,
   - $\{\mathbf{v}_1, \cdots, \mathbf{v}_k\}$
2. Assign each data point to the closest centroid
   - $c_i = \arg\min_j \{dist(\mathbf{x}_i - \mathbf{v}_j)\}$
3. Re-compute the centroids using the current cluster memberships.
   - $\mathbf{v}_j = \frac{\sum_{i=1}^{n} I(c_i = j)\mathbf{x}_i}{\sum_{i=1}^{n} I(c_i = j)}$
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# What is the code trying to do?

## It is trying to find a partition $S$

$K$-means tries to find a partition $S$ such that it minimizes the cost function:

$$\min_{S} \sum_{k=1}^{N} \sum_{i:\boldsymbol{x}_i \in C_k} \left(\boldsymbol{x}_i - \boldsymbol{\mu}_k\right)^T \left(\boldsymbol{x}_i - \boldsymbol{\mu}_k\right) \tag{1}$$

## Where $\mu_k$ is the centroid for cluster $C_k$

$$\mu_k = \frac{1}{N_k} \sum_{i:\boldsymbol{x}_i \in C_k} x_i \tag{2}$$

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No (or minimum) re-assignments of data points to different clusters.

## Second

No (or minimum) change of centroids.

- $C_j$ is cluster $j$.
- $m_j$ is the centroid of cluster $C_j$.

$$SSE = \sum_{j=1}^{k} \sum_{x \in C_j} dist(x, m_j)^2$$

# What Stopping/convergence criterion should we use?

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1. Supervised Learning vs. Unsupervised Learning
   - Supervised vs Unsupervised
   - Clustering
   - Pattern Recognition
   - Aspect of Clustering

2. K-Means Clustering
   - K-Means Clustering
   - Convergence Criterion
   - The Distance Function
   - Example
   - Properties of K-Means

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# The distance function

Actually, we have the following distance functions:

**Euclidean**

$$dixt(\mathbf{x},\mathbf{y}) = ||\mathbf{x}-\mathbf{y}|| = \sqrt{(\mathbf{x}-\mathbf{y})^T(\mathbf{x}-\mathbf{y})}$$

**Manhattan**

$$dixt(\mathbf{x},\mathbf{y}) = ||\mathbf{x}-\mathbf{y}||_1 = \sum_{i=1}^{n} |x_i - y_i|$$

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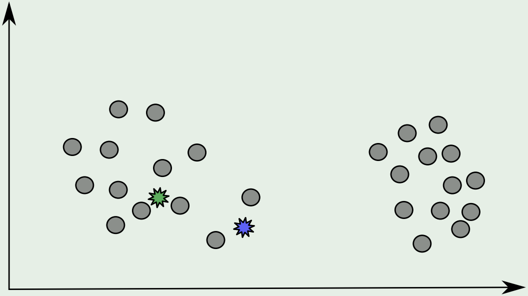
# An example

## Dropping two possible centroids



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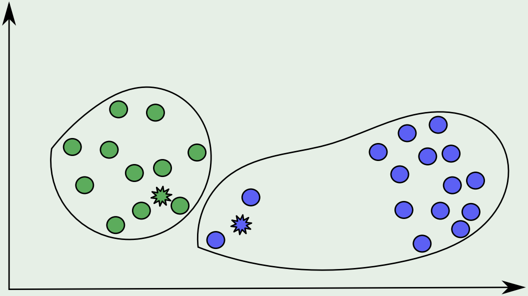
## Calculate the memberships



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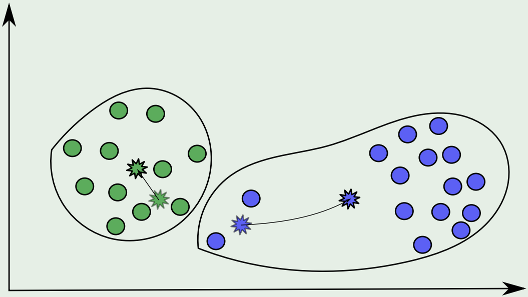

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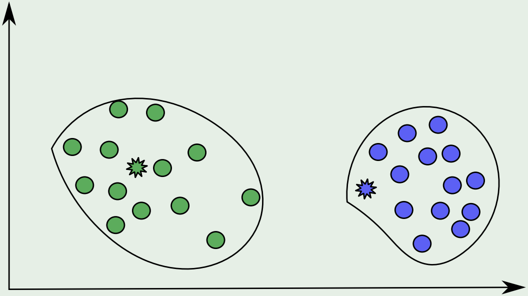

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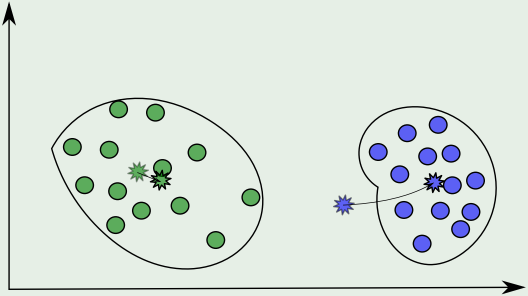
## We re-calculate centroids and keep going



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# Strengths of $K$-means

## Strengths

- Simple: easy to understand and to implement
- Efficient: Time complexity: $O(tKN)$, where $N$ is the number of data points, $K$ is the number of clusters, and $t$ is the number of iterations.
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The algorithm is only applicable if the mean is defined.

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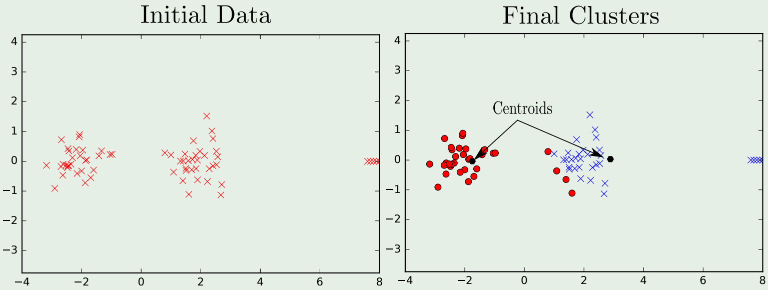
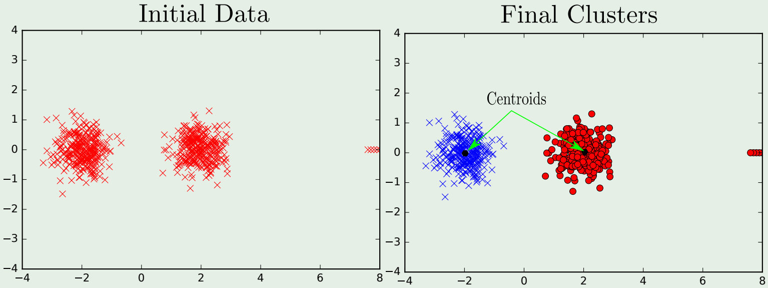
# Weaknesses of $K$-means: Problems with outliers

## A series of outliers



# Weaknesses of $K$-means: Problems with outliers

## Nevertheless, if you have more dense clusters



# Weaknesses of $K$-means: How to deal with outliers

**One method**

To remove some data points in the clustering process that are much further away from the centroids than other data points.

- To be safe, we may want to monitor these possible outliers over a few iterations and then decide to remove them.

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**Another method**

To perform random sampling.

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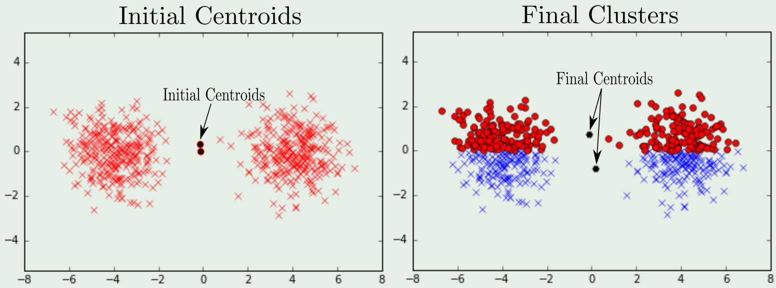
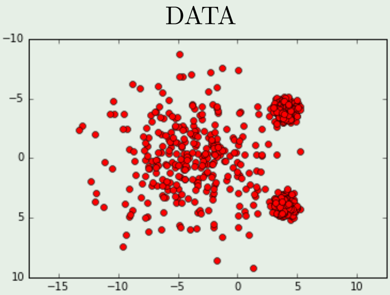
# Weaknesses of $K$-means (cont...)

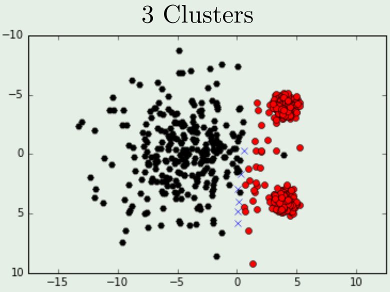
## The algorithm is sensitive to initial seeds



# Weaknesses of $K$-means : Different Densities

## We have three cluster nevertheless

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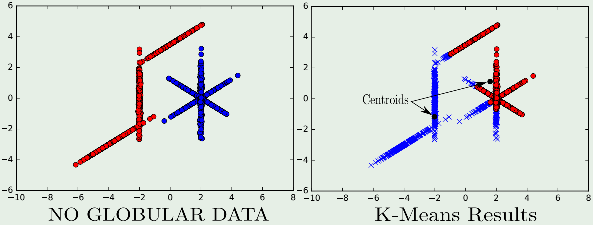
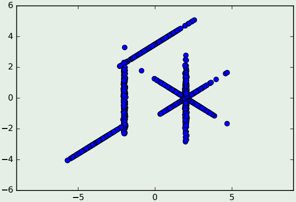
# Weaknesses of $K$-means: Non-globular Shapes

**Here, we notice that $K$-means may only detect globular shapes**

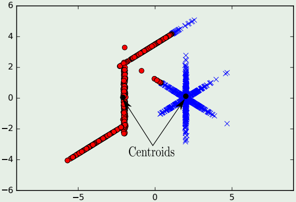


# Weaknesses of $K$-means: Non-globular Shapes

## However, it sometimes work better than expected




NO GLOBULAR DATA




K-Means Results