Introduction to Machine Learning

K-Means and K-Centers

Andres Mendez-Vazquez

February 25, 2019

Outline

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The Hardness of K-means clustering

Definition

- Given a multiset $S \subseteq \mathbb{R}^d$, an integer k and $L \in \mathbb{R}$, is there a subset $T \subset \mathbb{R}^d$ with $|T| = k$ such that

$$\sum_{\boldsymbol{x} \in S} \min_{\boldsymbol{t} \in T} \|\boldsymbol{x} - \boldsymbol{t}\|^2 \leq L?$$

Theorem

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The reduction to an NP-Complete problem

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However

There are efficient heuristic and approximation algorithms

- Which can solve this problem

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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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- 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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It is trying to find a partition S

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

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Where μ_k is the centroid for cluster C_k

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

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- C_k is cluster k.
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$$dist(\mathbf{x}, \mathbf{y}) = ||\mathbf{x} - \mathbf{y}|| = \sqrt{(\mathbf{x} - \mathbf{y})^T (\mathbf{x} - \mathbf{y})}$$

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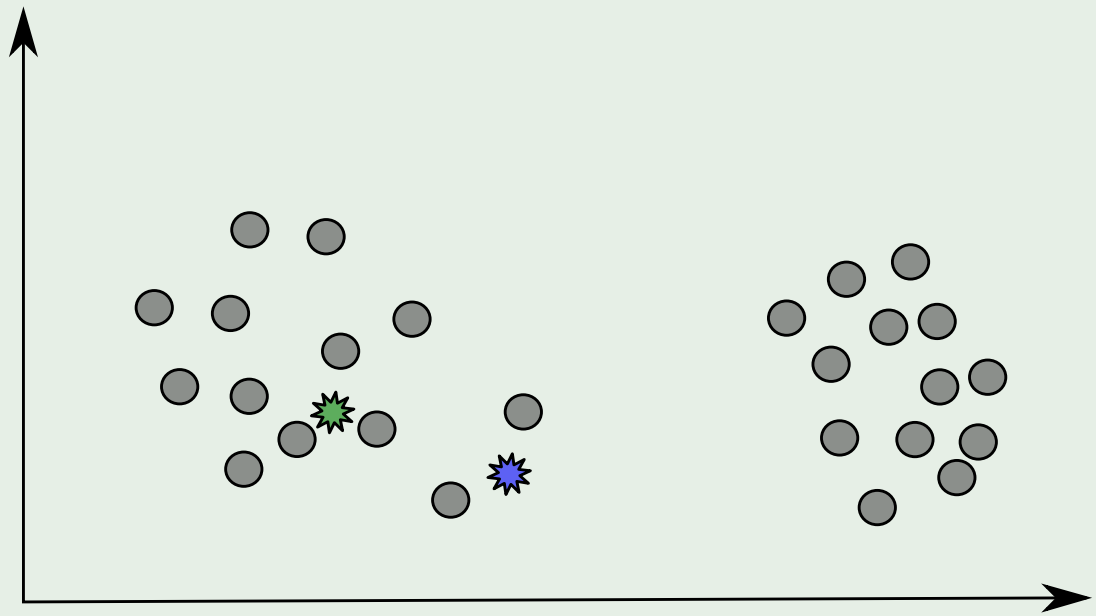
An example

Dropping two possible centroids



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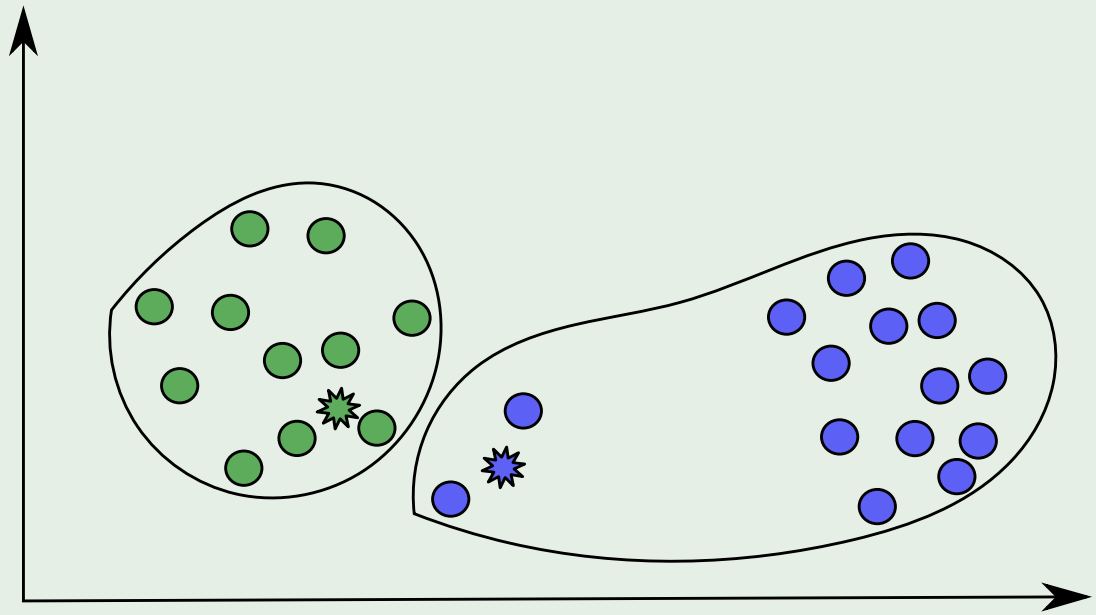
Calculate the memberships



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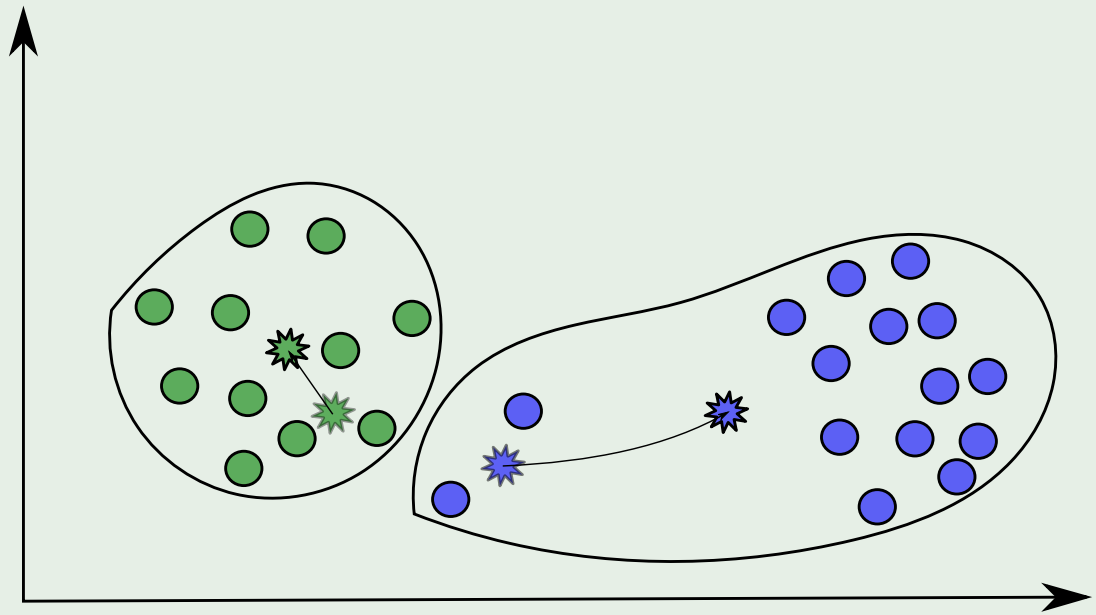
We re-calculate centroids



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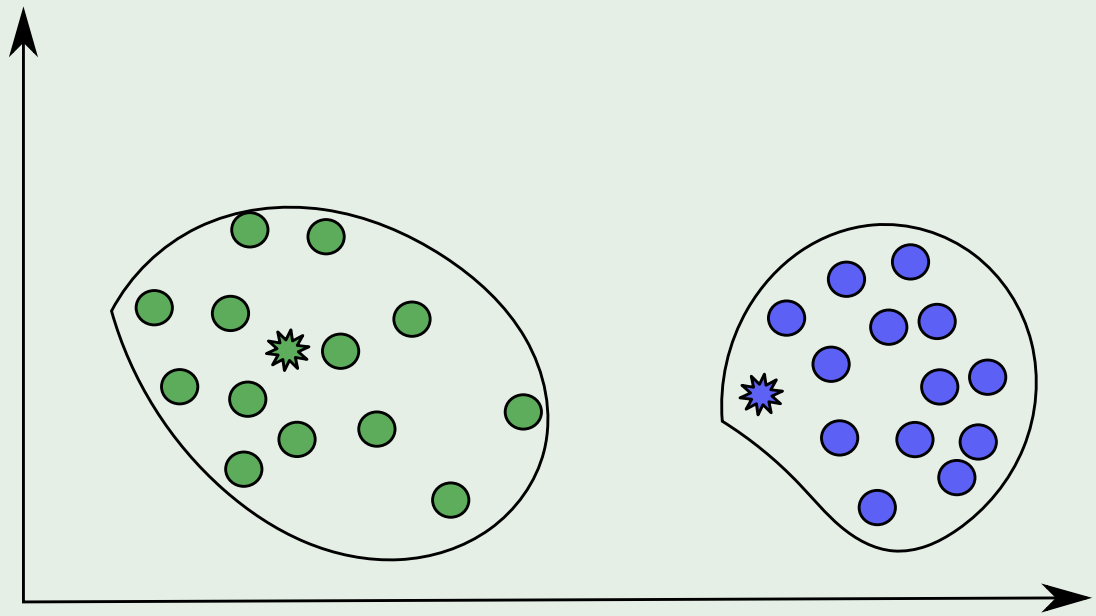
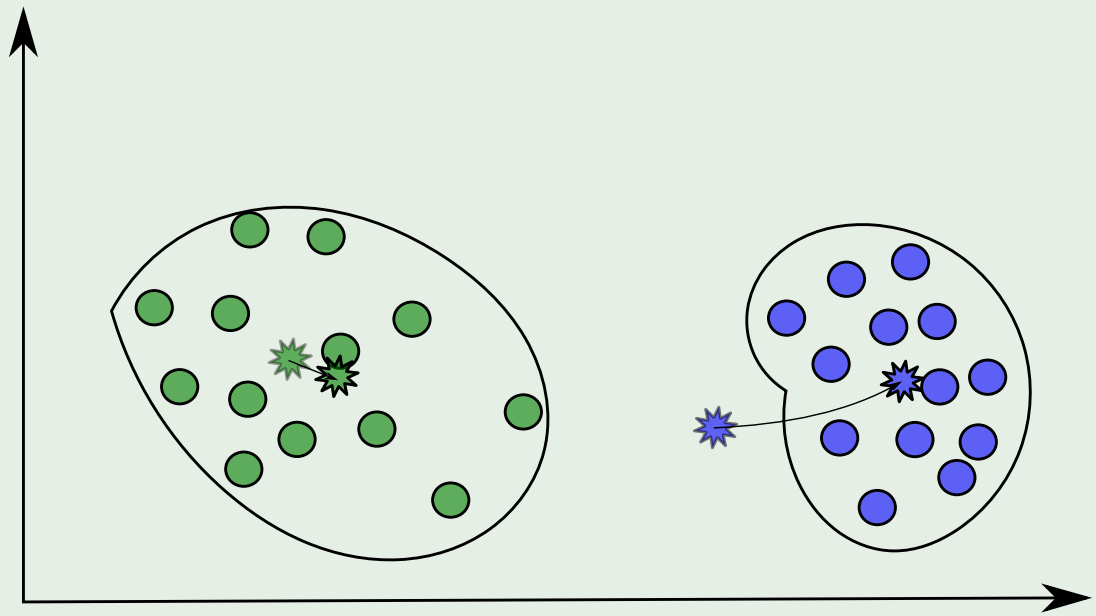


An example

We re-calculate centroids and keep going



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Strengths of K-means

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- 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.
- Since both K and t are small. K-means is considered a linear algorithm.

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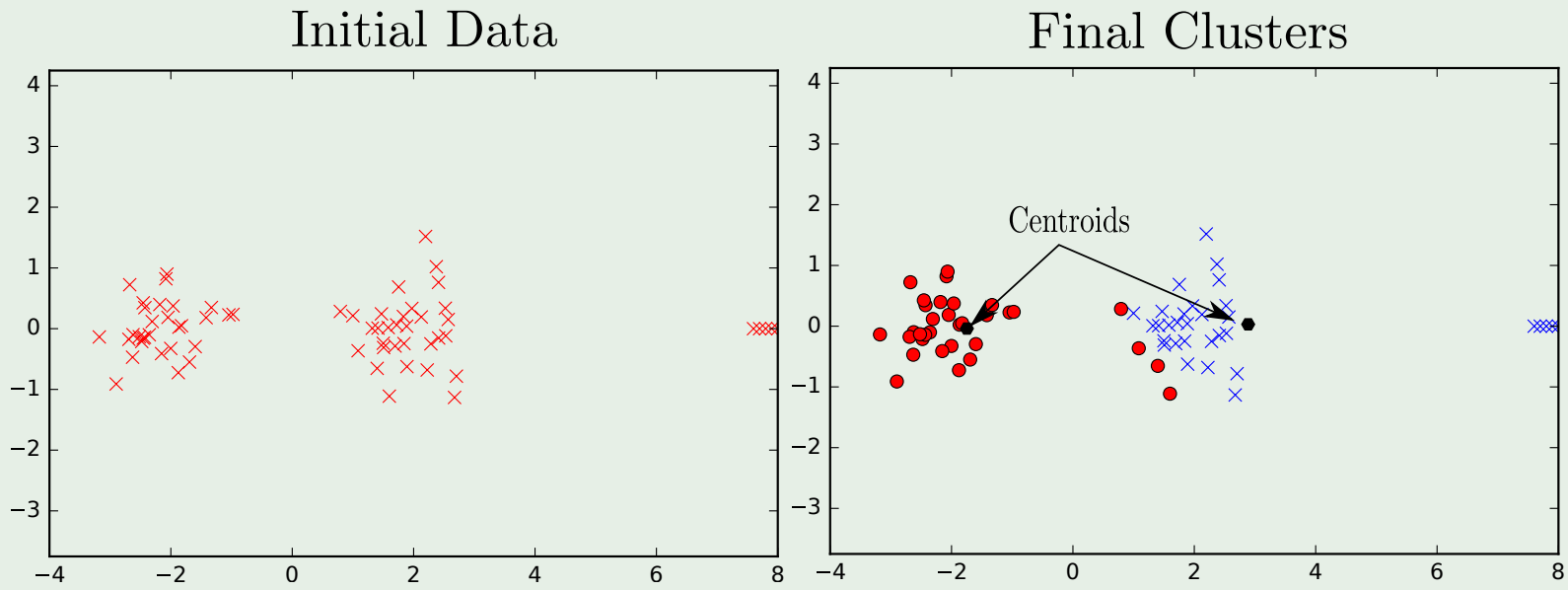
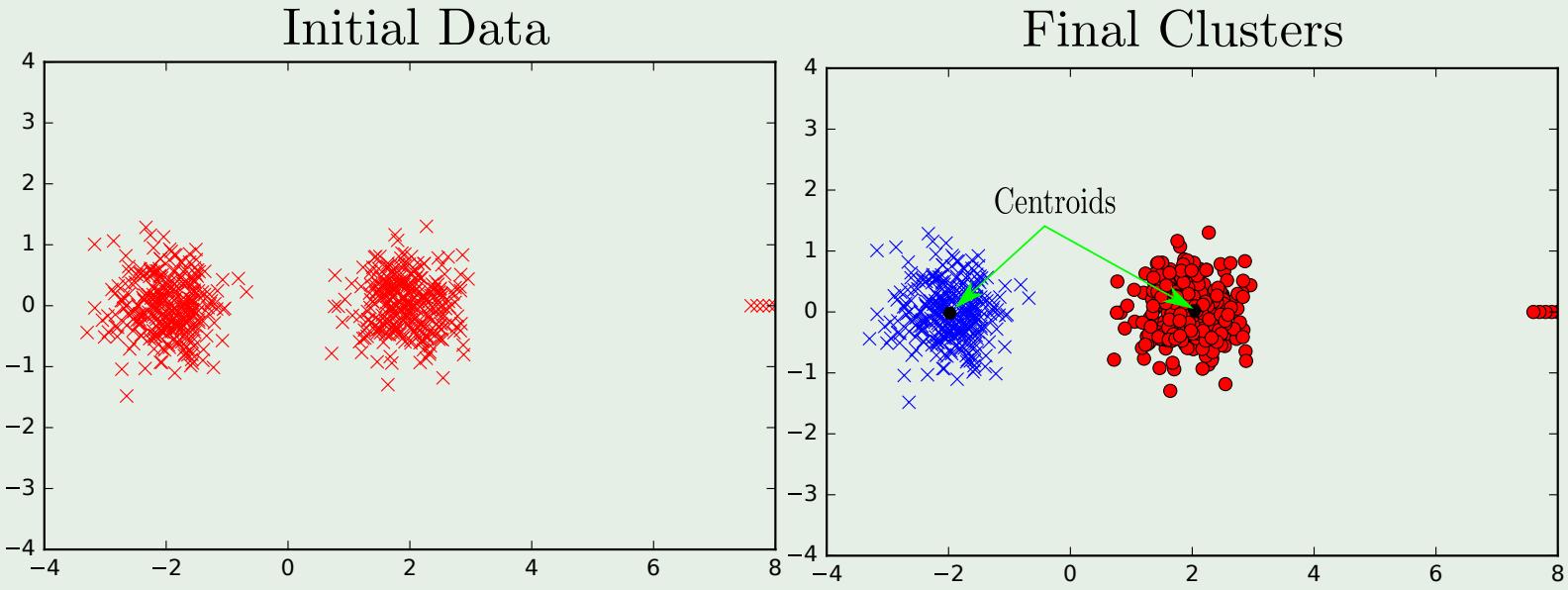
Weaknesses of K-means: Problems with outliers

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.

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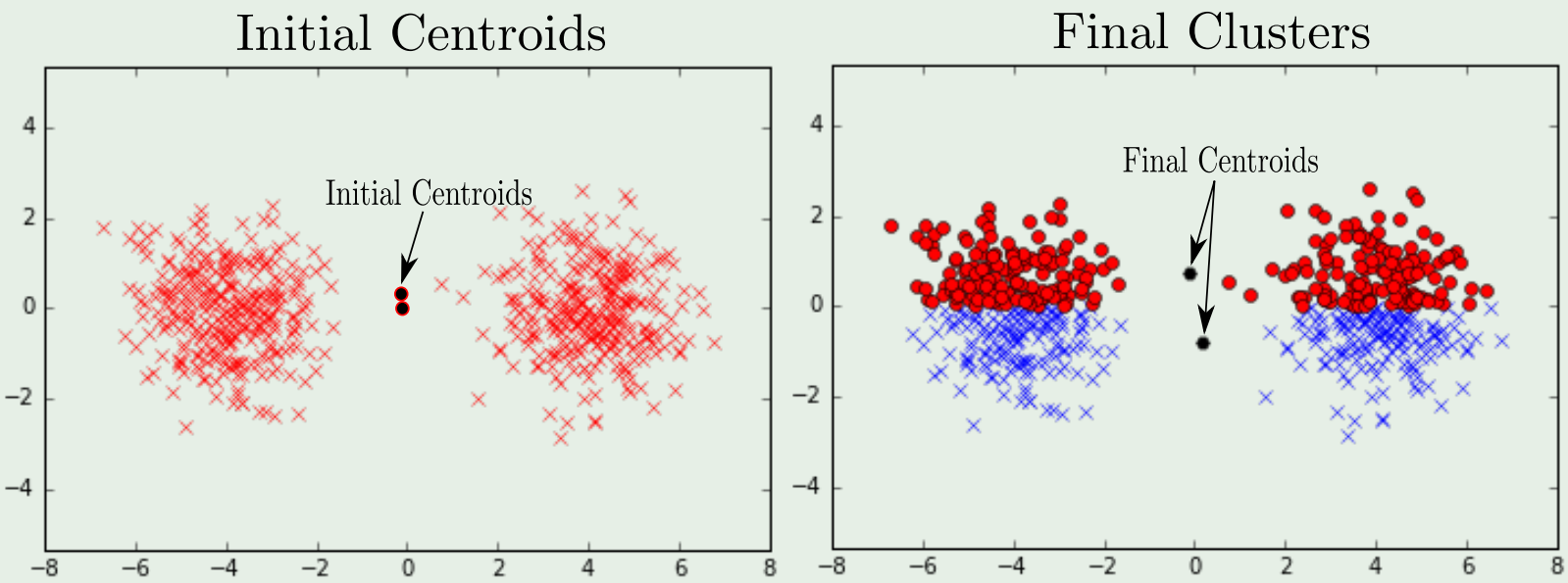
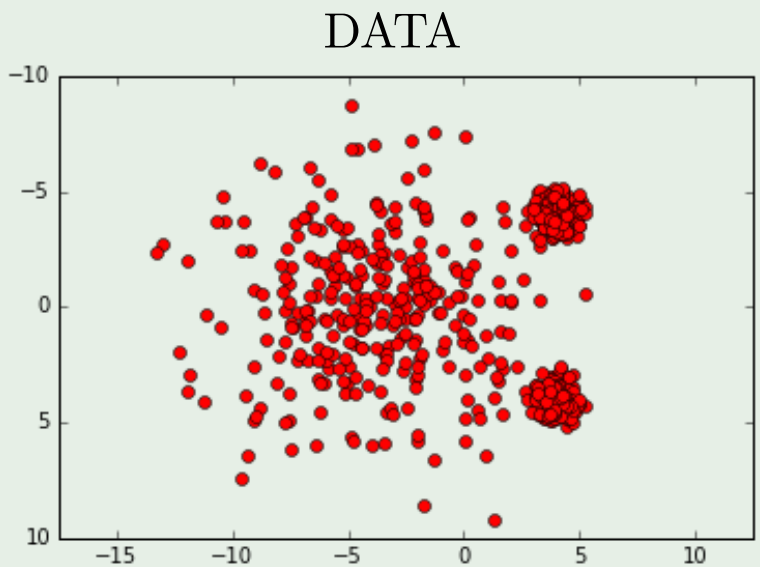
Weaknesses of K-means (cont...)

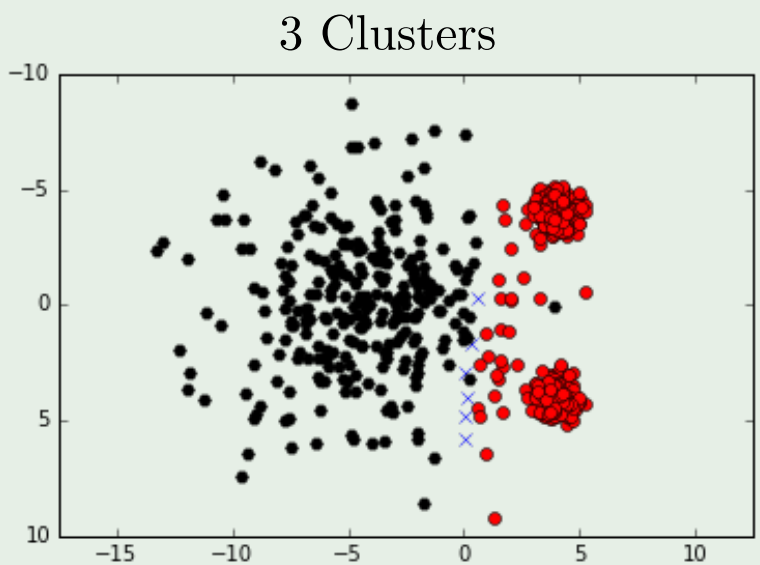
The algorithm is sensitive to initial seeds



Weaknesses of K-means : Different Densities

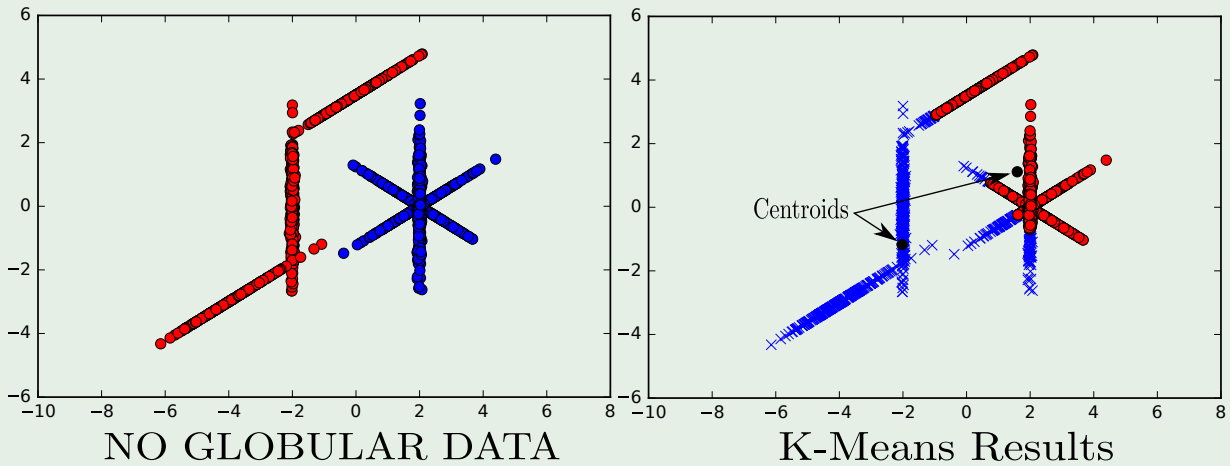
We have three cluster nevertheless





Weaknesses of K-means: Non-globular Shapes

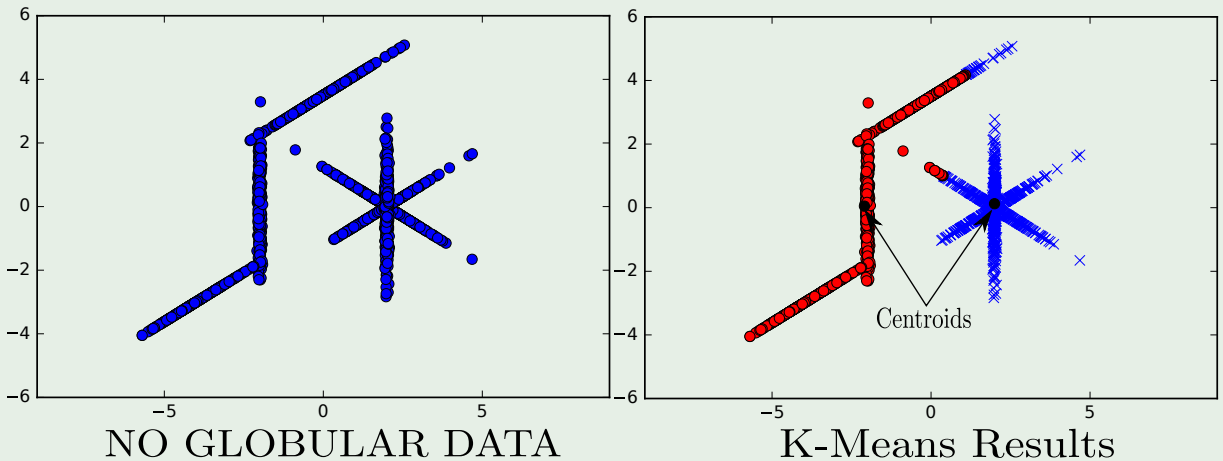
Here, we notice that K-means may only detect globular shapes



NO GLOBULAR DATA K-Means Results

Weaknesses of K-means: Non-globular Shapes

However, it sometimes work better than expected



Outline

The K-center Problem

The input

It is a set of points with distances represented by a weighted graph $G = (V, V \times V)$.

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It is a set of points with distances represented by a weighted graph $G = (V, V \times V)$.

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- Select K centroids in G.
- Such that minimize maximum distance of every point to a centroid.

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The Triangle Inequality

Given x, y and z

$$L(x,z) \leq L(x,y) + L(y,z)$$

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Outline

We have a new criterion

Instead of using the K-mean criterion

We use the K-center criterion under the triangle inequality.

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The K-center criterion partitions the points into K clusters so as to minimize the maximum distance of any point to its cluster center.

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Define a cluster size for any cluster C_k as follows.

- The smallest value D for which all points in this cluster C_k are:
  - Within distance D of each other.
  - Or within distance $\frac{D}{2}$ of some point called the cluster center.

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Another Way

We have

Another way to define the cluster size:

- D is the maximum pairwise distance between an arbitrary pair of points in the cluster.
- Or twice the maximum distance between a data point and a chosen centroid.

Thus

Denoting the cluster size of C_k by D_k, we have that the cluster size of partition (the way the points are grouped) S by:

$$D = \max_{k=1,\ldots,K} D_k \tag{3}$$

In another words

The cluster size of a partition composed of multiple clusters is the maximum size of these clusters.

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Comparison with K-means

We use the following distance for comparison

In order to compare these methods, we use Euclidean distance.

In K-means we assume the distance between vectors is the squared Euclidean distance

K-means tries to find a partition S that minimizes:

$$\min_{S} \sum_{k=1}^{N} \sum_{i:x_i \in C_k} (\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T (\boldsymbol{x}_i - \boldsymbol{\mu}_k) \tag{4}$$

Where μ_k is the centroid for cluster C_k

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i:x_i \in C_k} \boldsymbol{x}_i \tag{5}$$

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K-center, on the other hand, minimizes the worst case distance to these centroids

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Where

$\boldsymbol{\mu}_k$ is called the "centroid", but may not be the mean vector.

- Moreover, among the clusters, only the worst cluster matters, whose farthest data point yields the maximum distance to the centroid comparing with the farthest data points of the other clusters.

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In other words

First

This minimax type of problem is much harder to solve than solving the objective function of k-means.

Another formulation of K-center minimizes the worst case pairwise distance instead of using centroids

$$\min_{S} \max_{k=1,\ldots,K} \max_{i,j:x_i,x_j \in C_k} L\left(x_i, x_j\right) \tag{7}$$

With

$L\left(x_i, x_j\right)$ denotes any distance between a pair of objects in the same cluster.

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Greedy Algorithm for K-Center

Main Idea

The idea behind the Greedy Algorithm is to choose a subset H from the original dataset S consisting of K points that are farthest apart from each other.

Intuition

Since the points in set H are far apart then the worst-case scenario has been taken care of and hopefully the cluster size for the partition is small.

Thus

Each point $h_k \in H$ represents one cluster or subset of points C_k.

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Then

Something Notable

We can think of it as a centroid.

However

Technically it is not a centroid because it tends to be at the boundary of a cluster, but conceptually we can think of it as a centroid.

Important

The way that we partition these points given the centroids is the same as in K-means, that is, the nearest-neighbor rule.

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Specifically

We do the following

For every point x_i, in order to see which cluster C_k it is partitioned into, we compute its distance to each cluster centroid as follows, and find out which centroid is the closest:

$$L\left(\boldsymbol{x}_i, \boldsymbol{h}_k\right) = \min_{k'=1,\ldots,K} L\left(\boldsymbol{x}_i, \boldsymbol{h}_{k'}\right) \tag{8}$$

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Important

For K-center clustering

We only need pairwise distance $L(\boldsymbol{x}_i, \boldsymbol{x}_j)$ for any $\boldsymbol{x}_i, \boldsymbol{x}_j \in S$.

Where

$\boldsymbol{x}_i$ can be a non-vector representation of the objects.

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Properties

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The greedy algorithm achieves an approximation factor of 2 as the distance measure L satisfies the triangle inequality.

Thus, we have that

$$D^* = \min_{S} \max_{k=1,\ldots,K} \max_{i,j:x_i,x_j \in C_k} L(x_i, x_j) \tag{9}$$

Then, we have the following guarantee for the greedy algorithm

$$D \leq 2D^* \tag{10}$$

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Setup

First

Set H denotes the set of cluster centroids or cluster of representative objects $\{\boldsymbol{h}_1, ..., \boldsymbol{h}_k\} \subset S$.

Second

Let $cluster\,(\boldsymbol{x}_i)$ be the identity of the cluster $\boldsymbol{x}_i \in S$ belongs to.

Third

The distance $dist\,(\boldsymbol{x}_i)$ is the distance between $\boldsymbol{x}_i$ and its closest cluster representative object (centroid):

$$dist\,(\boldsymbol{x}_i) = \min_{h_j \in H} L\,(\boldsymbol{x}_i, \boldsymbol{h}_j) \tag{11}$$

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- We generate one cluster centroid first and then add others one by one until we get K clusters.
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1. $dist\left(\boldsymbol{x}_i\right) = L\left(\boldsymbol{x}_i, \boldsymbol{h}_1\right)$.
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- The $dist\left(\boldsymbol{x}_i\right)$ is the computed distance between $\boldsymbol{x}_j$ and $\boldsymbol{h}_1$.
- Because so far we only have one cluster, we will assign a cluster label 1 to every $\boldsymbol{x}_j$.

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Step 3

For $i = 2$ to K

1. $D = \max_{\boldsymbol{x}_j : \boldsymbol{x}_j \in S - H} dist\left(\boldsymbol{x}_j\right)$
2. Choose $\boldsymbol{h}_i \in S - H$ such that $dist\left(\boldsymbol{h}_i\right) == D$
3. $H = H \cup \{\boldsymbol{h}_i\}$
4. for $j = 1$ to N
5. if $L\left(\boldsymbol{x}_j, \boldsymbol{h}_i\right) \leq dist\left(\boldsymbol{x}_j\right)$
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2. Choose $\boldsymbol{h}_i \in S - H$ such that $dist\left(\boldsymbol{h}_i\right) == D$
3. $H = H \cup \{\boldsymbol{h}_i\}$
4. for $j = 1$ to N
5. if $L\left(\boldsymbol{x}_j, \boldsymbol{h}_i\right) \leq dist\left(\boldsymbol{x}_j\right)$
6. $dist\left(\boldsymbol{x}_j\right) = L\left(\boldsymbol{x}_j, \boldsymbol{h}_i\right)$
7. $cluster\left(\boldsymbol{x}_j\right) = i$

Thus

As the algorithm progresses

- We gradually add more and more cluster centroids, beginning with 2 until we get to K.
- At each iteration, we find among all of the points which are not yet included in the set, a worst point:
  - Worst in the sense that this point has maximum distance to its corresponding centroid.

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Implementation

We can use the following for implementation

- The disjoint-set data structure with the following operations:
  - MakeSet
  - Find
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  - Remove Iteratively through the disjoint trees.

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Although

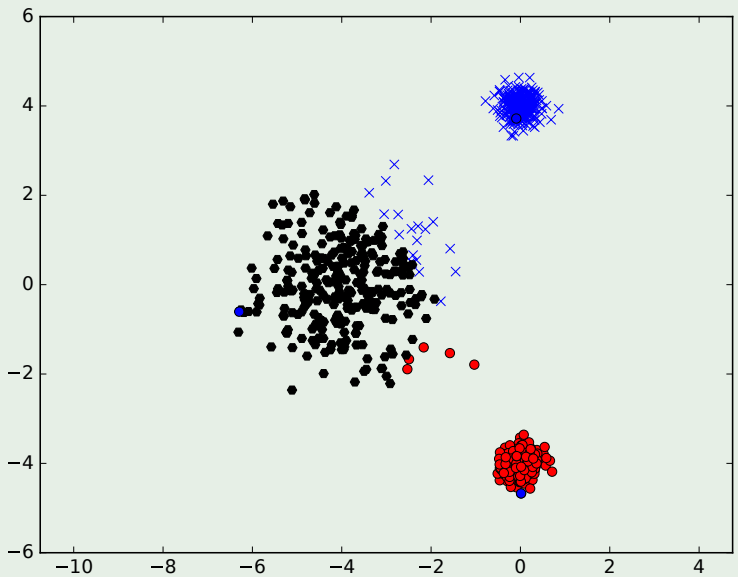
Other things need to be taken in consideration

I will allow to you to think about them

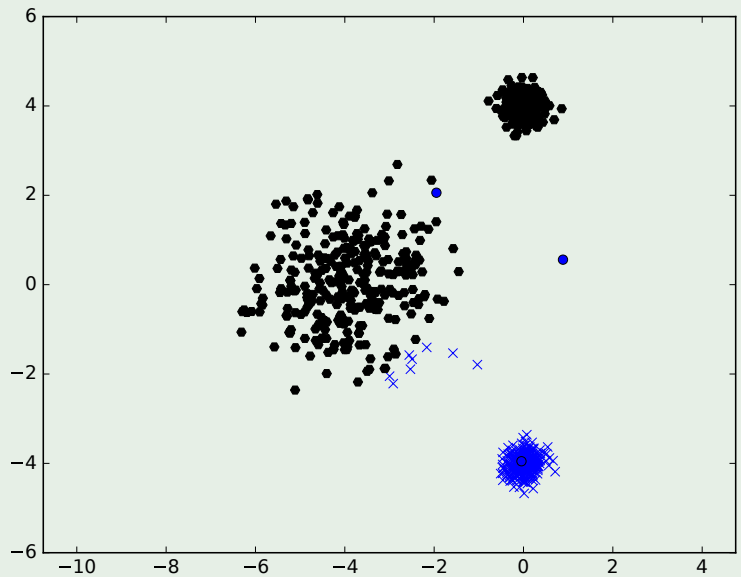
Outline

Example

Running the k-center and k-means algorithms allows to see that for different densities k-center is more robust



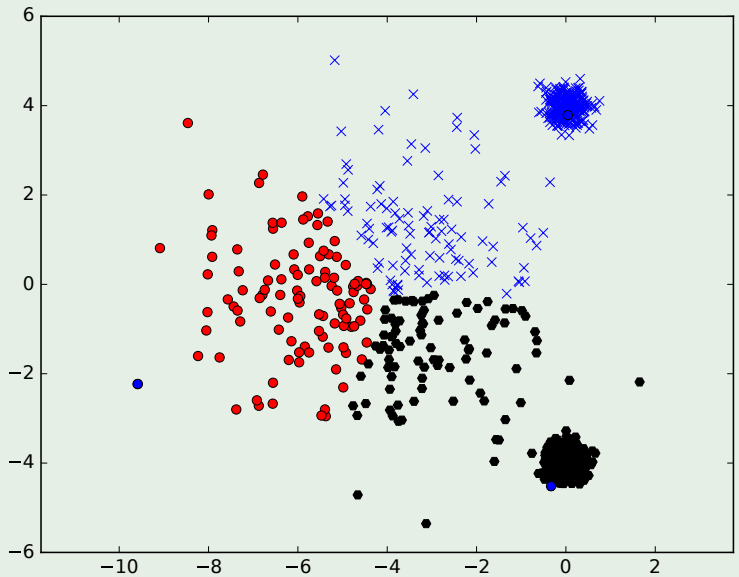
K-Center



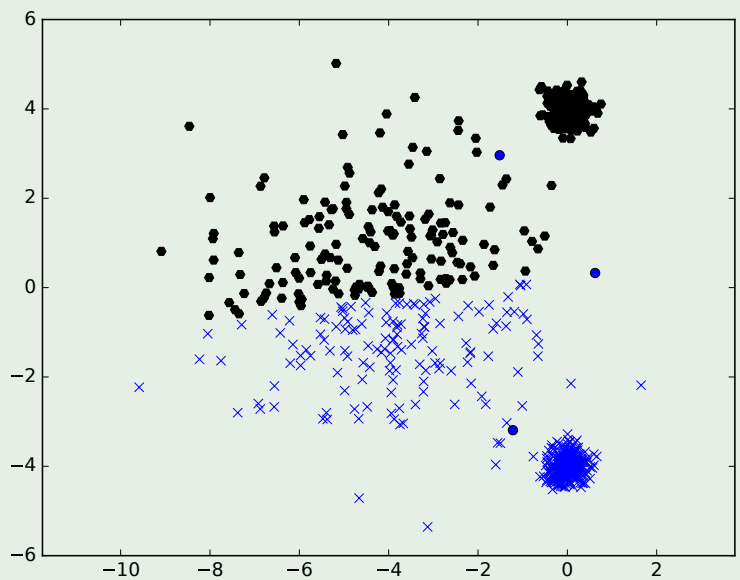
K-Means

Example

Decreasing the density of one of the clusters, we see a degradation on the clusters



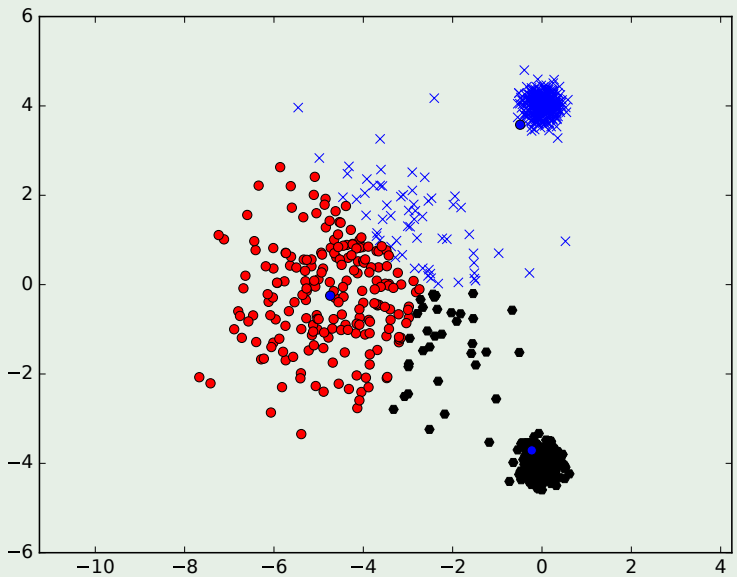
K-Center



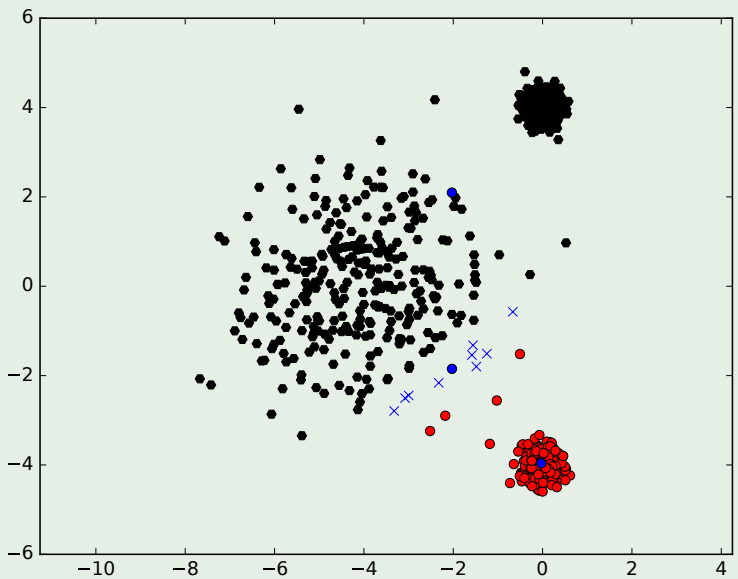
K-Means

Using Centroids of the K-center to initialize K-mean

Thus, we can use the centroids of K-center to try to improve upon K-means to a certain degree



K-Means using the K-Center Centroids



K-Means using random centroids

Outline

The Running Time

We have that

The running time of the algorithm is $O(KN)$, where K is the number of clusters generated and N is the size of the data set.

Why?

Because K-center only requires pairwise distance between any point and the centroids.

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