Introduction to Machine Learning

K-Means, K-Meoids, K-Centers and Variations

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January 26, 2023

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

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

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Theorem

- The k-means clustering problem is NP-complete even for $d = 2$.

Reduction

The reduction to an NP-Complete problem

- Exact Cover by 3-Sets problem

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Definition

- Given a finite set U containing exactly $3n$ elements and a collection $\mathcal{C} = \{S_1, S_2, ..., S_l\}$ of subsets of U each of which contains exactly 3 elements, Are there n sets in $\mathcal{C}$ such that their union is U?

However

There are efficient heuristic and approximation algorithms

- Which can solve this problem

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History

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Basically given N vectors $\boldsymbol{x}_1, ..., \boldsymbol{x}_N \in \mathbb{R}^d$

It tries to find k points $\boldsymbol{\mu}_1, ..., \boldsymbol{\mu}_k \in \mathbb{R}^d$ that minimize the expression (i.e. a partition S of the vector points):

$$\sum_{k=1}^{N} \sum_{i:\boldsymbol{x}_i \in C_k} \|\boldsymbol{x}_i - \boldsymbol{\mu}_k\|^2 = \sum_{k=1}^{N} \sum_{i:\boldsymbol{x}_i \in C_k} (\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T (\boldsymbol{x}_i - \boldsymbol{\mu}_k)$$

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- Each cluster has a cluster center, called centroid.

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- Each cluster has a cluster center, called centroid.
- K is specified by the user.

K-means algorithm

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   - $\{\mathbf{v}_1, \cdots, \mathbf{v}_k\}$

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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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4. If a convergence criterion is not met, go to 2.

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:

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

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Where μ_k is the centroid for cluster C_k

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

Where N_k is the number of samples in the cluster C_k.

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Minimum decrease in the sum of squared error (SSE),

- C_k is cluster k.
- $\mathbf{v}_k$ is the centroid of cluster C_k.

$$SSE = \sum_{k=1}^{K} \sum_{x \in c_k} dist\left(\mathbf{x}, \mathbf{v}_k\right)^2$$

Outline

The distance function

Actually, we have the following distance functions:

Euclidean

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

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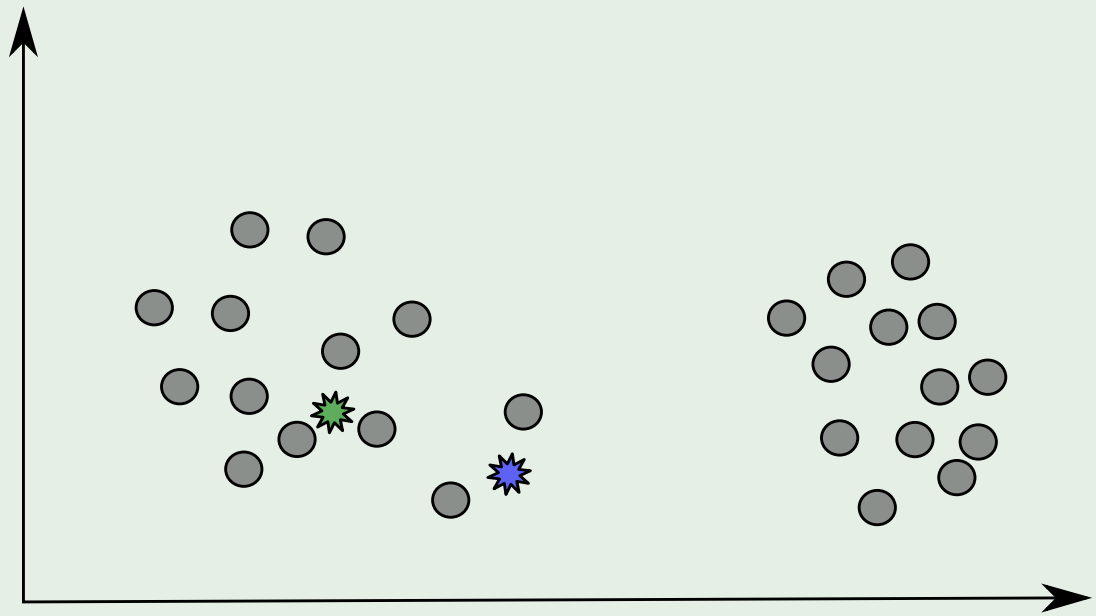
Outline

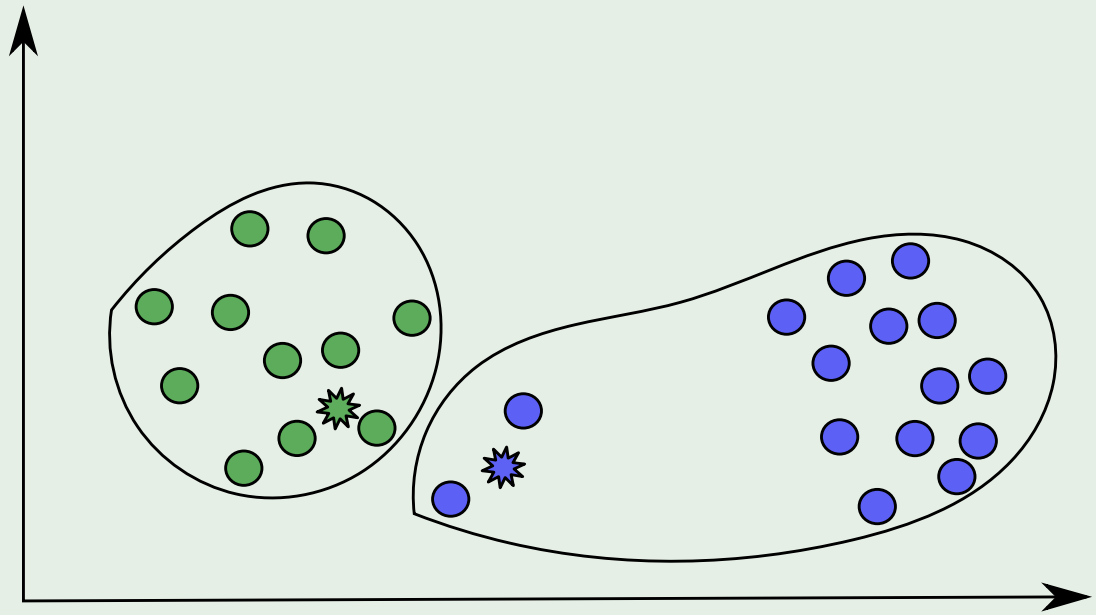
An example

Dropping two possible centroids



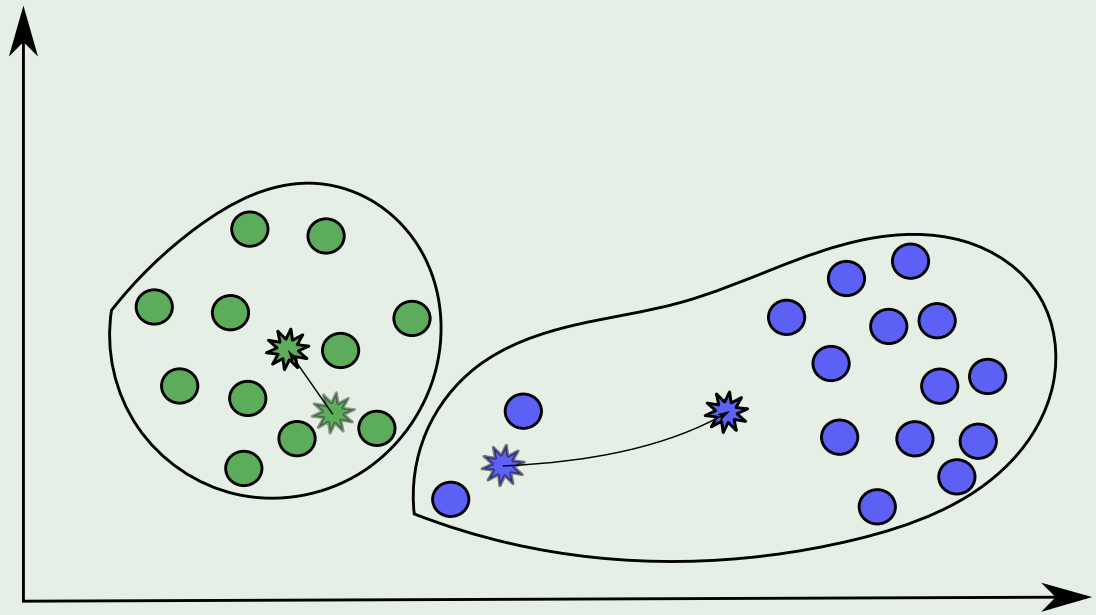
An example

Calculate the memberships



An example

We re-calculate centroids



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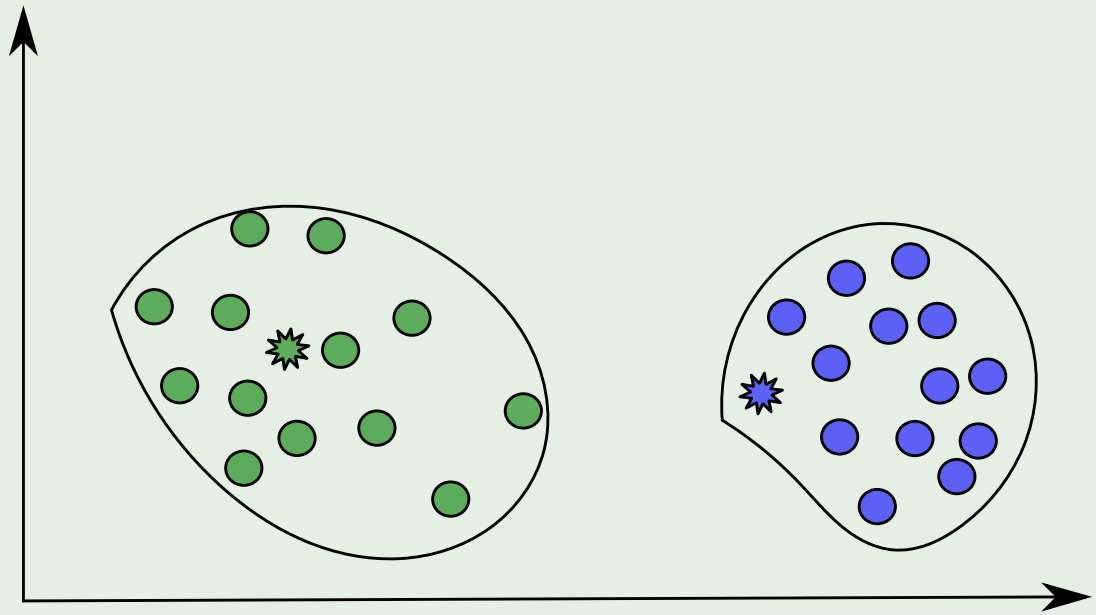
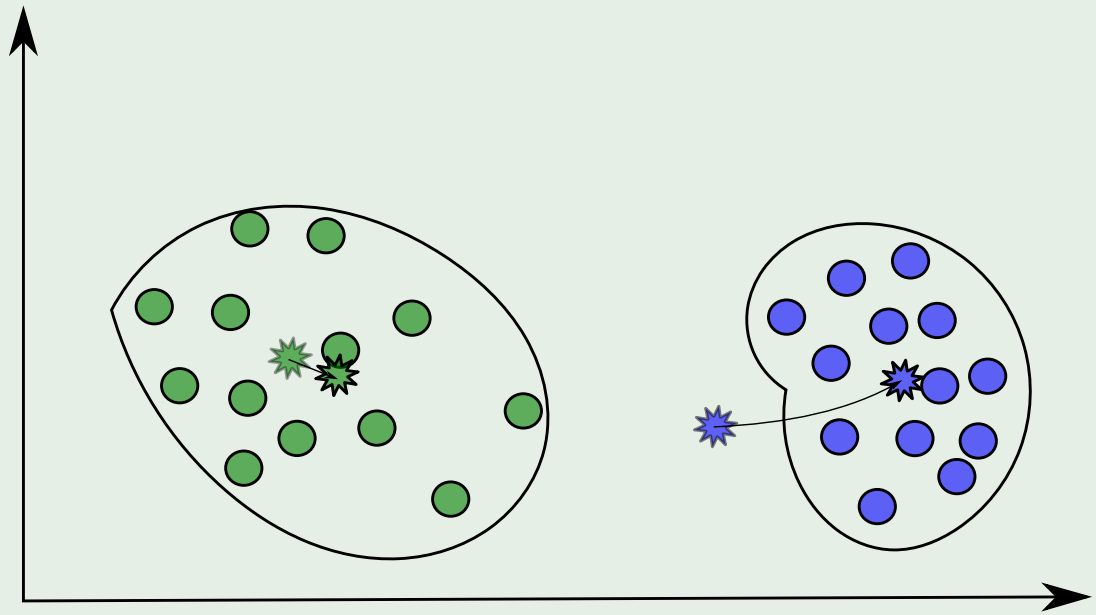


An example

We re-calculate centroids and keep going



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K-means is the most popular clustering algorithm.

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Popularity

K-means is the most popular clustering algorithm.

Note that

It terminates at a local optimum if SSE is used. The global optimum is hard to find due to complexity.

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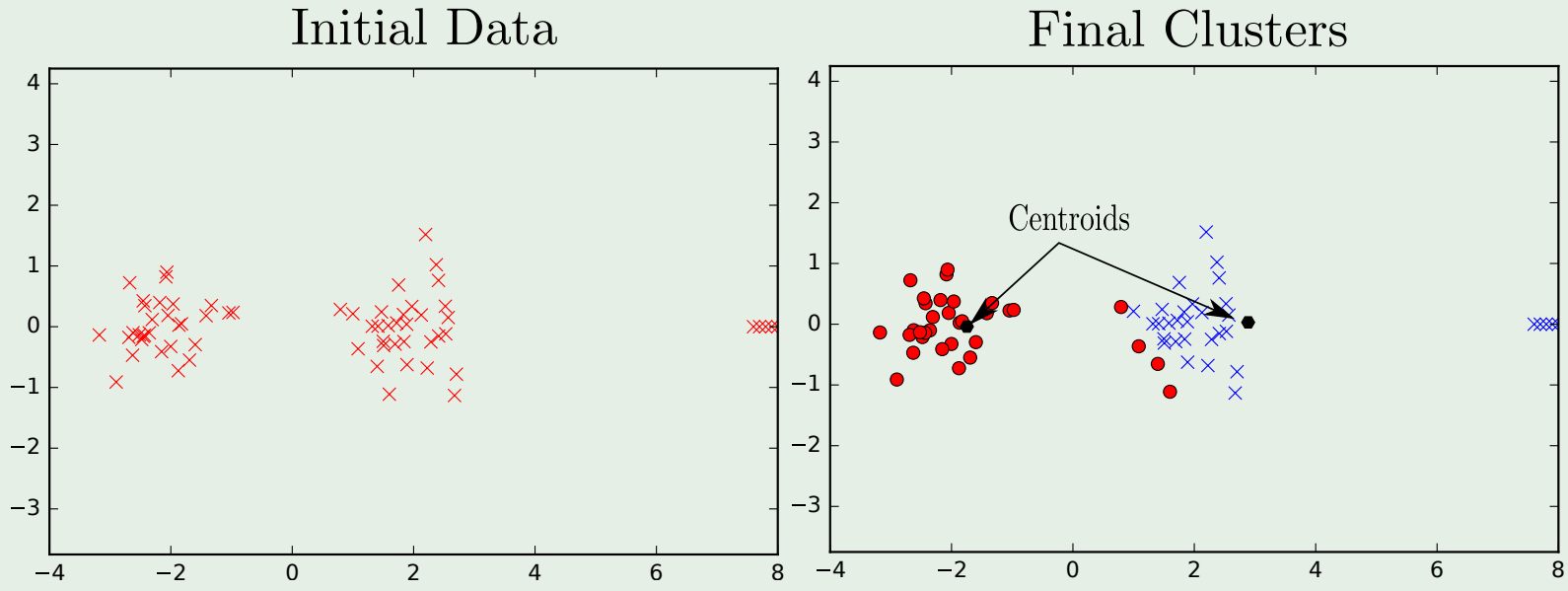
- Outliers are data points that are very far away from other data points.
- Outliers could be errors in the data recording or some special data points with very different values.

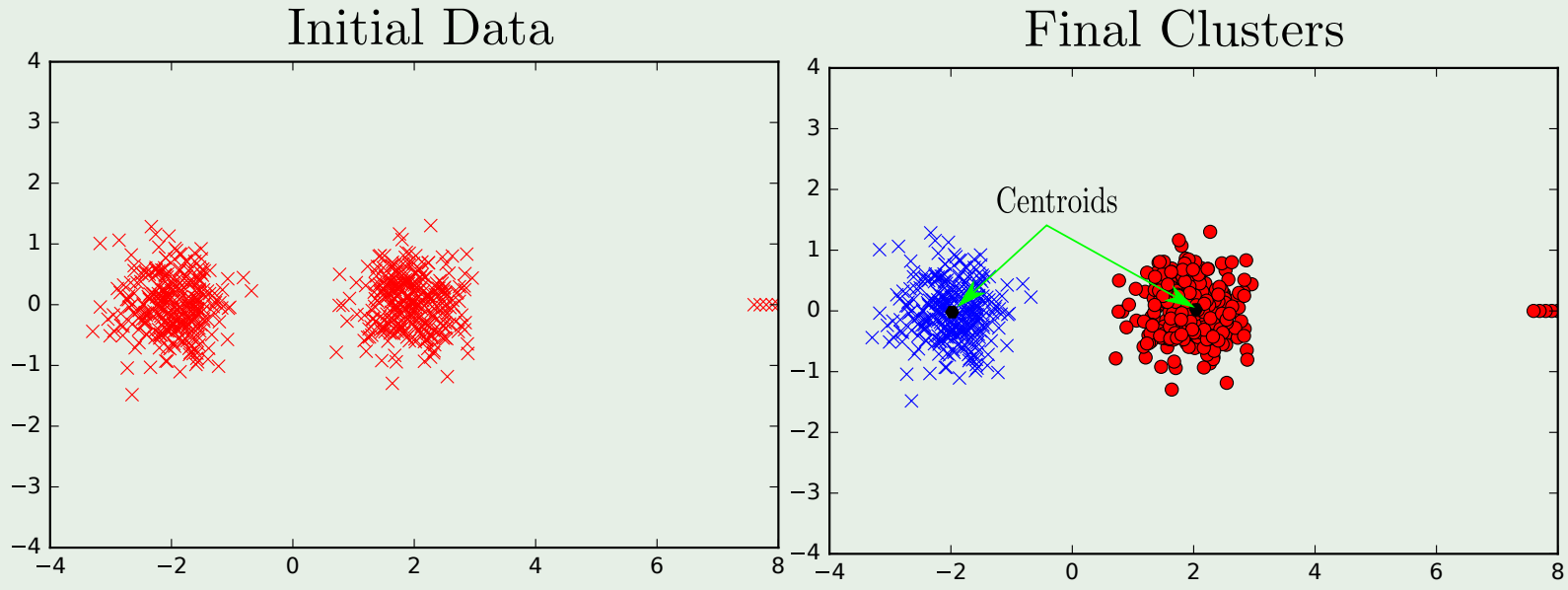
Weaknesses of K-means: Problems with outliers

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

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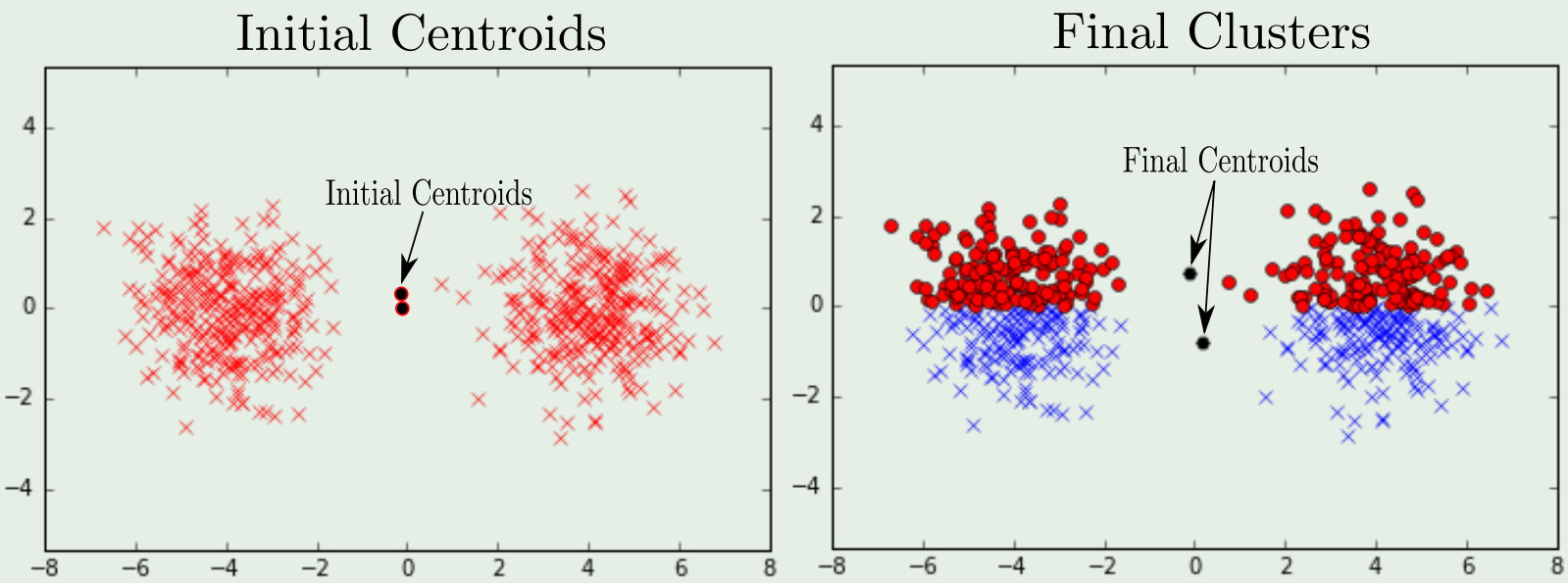
- Since in sampling we only choose a small subset of the data points, the chance of selecting an outlier is very small.
- Assign the rest of the data points to the clusters by distance or similarity comparison, or classification.

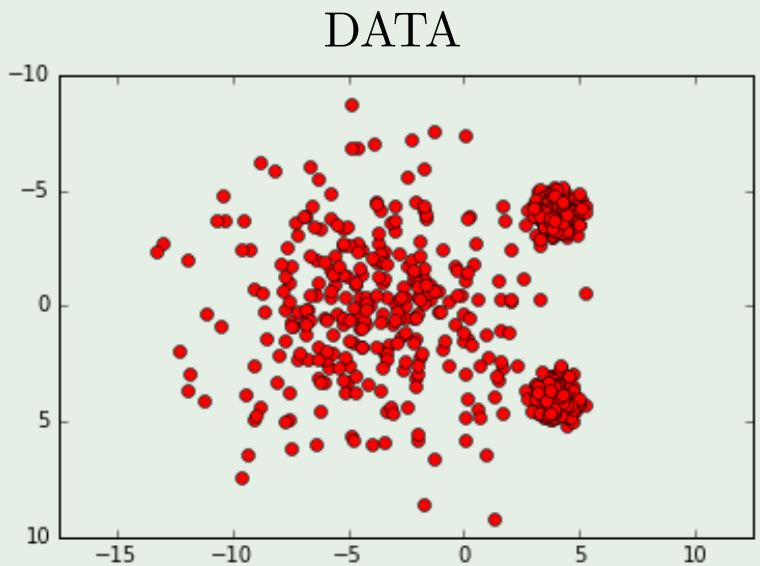
Weaknesses of K-means (cont...)

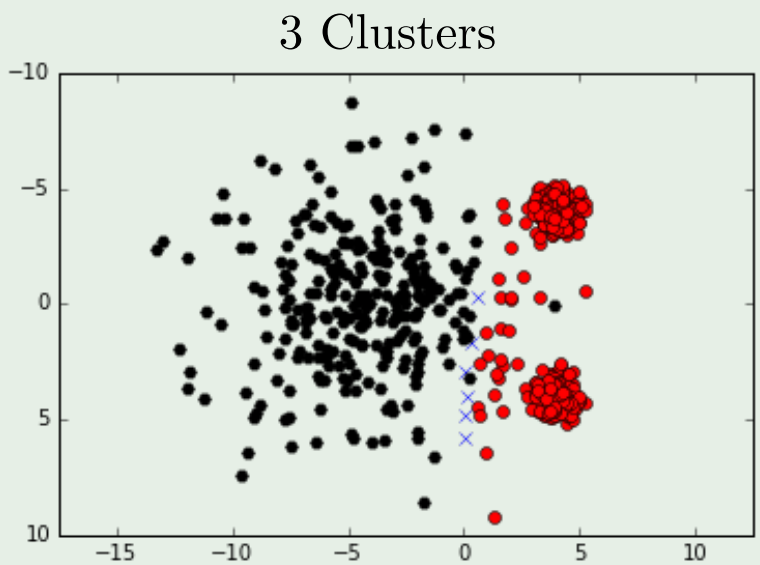
The algorithm is sensitive to initial seeds



Weaknesses of K-means : Different Densities

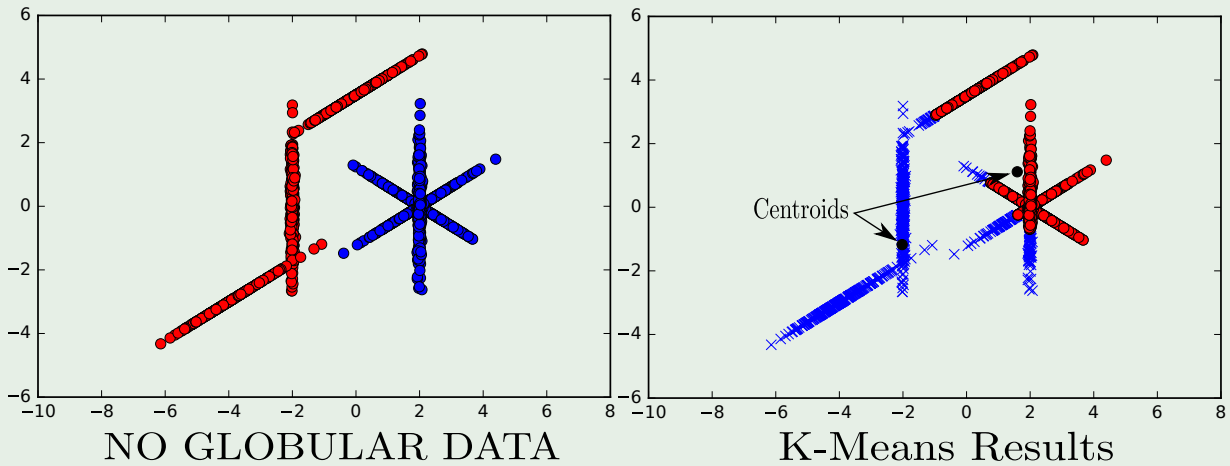
We have three cluster nevertheless





Weaknesses of K-means: Non-globular Shapes

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

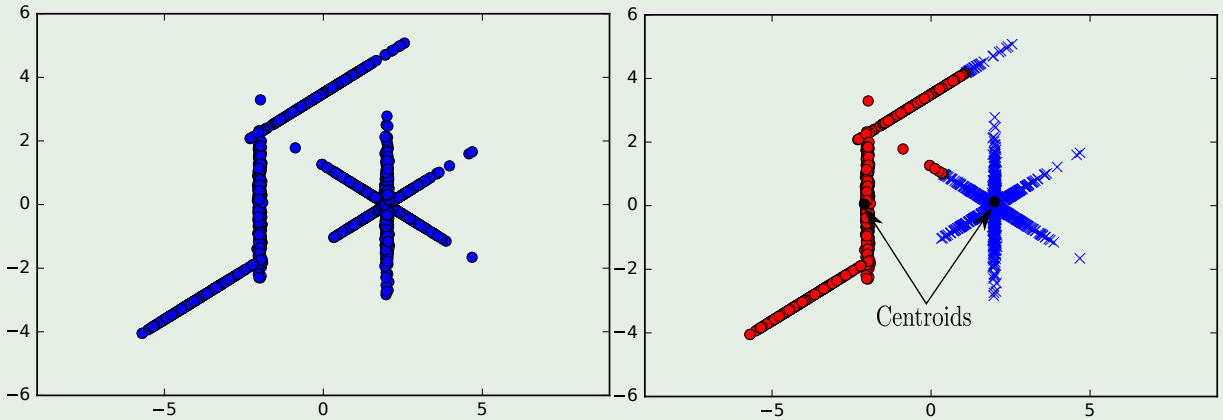


NO GLOBULAR DATA

K-Means Results

Weaknesses of K-means: Non-globular Shapes

However, it sometimes work better than expected



NO GLOBULAR DATA K-Means Results

Outline

Connecting K-Means and PCA

There is a nice connection between both algorithms

- Using
  - Eckhart-Young Theorem
  - SVD
  - Frobenious Norm

What?

Theorem

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Frobenious Matrix Norm

$$\|A\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2} = \sqrt{\text{trace}\,(A^T A)}$$

The Eckhart-Young Theorem

Theorem

- Let A be a real $m \times n$ matrix. Then for any $k \in \mathbb{N}$ and any $m \times m$ orthogonal projection matrix P of rank k, we have

$$\|A - P_k A\|_F \leq \|A - PA\|_F$$

  - with $P_k = \sum_{i=1}^{k} \boldsymbol{u}_i \boldsymbol{u}_i^T$

Thus

We have the Covariance matrix

$$S = \frac{1}{N-1} \sum_{i=1}^{N} (\boldsymbol{x}_i - \overline{\boldsymbol{x}}) (\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T$$

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Therefore, we have the following decomposition

$$S = U \Sigma U^T$$

- Where $UU^T = I$ and U is a $d \times d$ matrix

Orthogonal Projection

Therefore, we have that U is a orthogonal projection

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Now, we can re-write k-means

$$f_{k-\text{mean}} = \min_{\mu_1,\ldots\mu_k} \sum_{i\in[n]} \min_{j\in[k]} \|\boldsymbol{x}_i - \mu_j\|^2$$

Then

PCA can also re-write the cost function

$$f_{PCA} = \min_{P_k} \sum_{i \in [n]} \|\boldsymbol{x}_i - P_k \boldsymbol{x}_i\|^2 = \min_{P_k} \sum_{i \in [n]} \min_{\boldsymbol{y}_i \in P_k} \|\boldsymbol{x}_i - \boldsymbol{y}_i\|^2$$

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Where

- Given that P_k is a projection into dimension k and $\boldsymbol{y} \in P_k$ means that $P_k \boldsymbol{y} = \boldsymbol{y}$

Basically

This is what we do when reducing the

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Something Notable

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Furthermore

$$\arg\min_{y \in P} \|\boldsymbol{x} - \boldsymbol{y}\| = P\boldsymbol{x}$$

Thus, using the Eckhart-Young Theorem

Assume P_k^* which contains the k optimal centers

- Given that $\mu_j \in P_k^*$

$$
\begin{aligned}
&\geq \sum_{i \in [n]} \min_{\boldsymbol{y}_i \in P_k^*} \|\boldsymbol{x}_i - \boldsymbol{y}_i\|^2 \\
&\geq \min_{P_k} \sum_{i \in [n]} \min_{\boldsymbol{y}_i \in P_k} \|\boldsymbol{x}_i - \boldsymbol{y}_i\|^2 \\
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Therefore, given $P\boldsymbol{x}_i = \boldsymbol{y}_i$ and $\widehat{\mu}_j = P\mu_j$

- Where the $\widehat{S}$ and $\widehat{\mu}$ are the assignments and centers of the projected points $\boldsymbol{y}_i$:

$$= \sum_{j\in[k]} \sum_{i\in S_j} \|\boldsymbol{y}_i - \widehat{\mu}_j\|^2$$

$$\geq \sum_{j\in[k]} \sum_{i\in \widehat{S}_j} \|\boldsymbol{y}_i - \widehat{\mu}_j\|^2 = f^*_{k-\text{means}}$$

Therefore

Now, consider solving k-means on the points $\boldsymbol{y}_i$ instead

- They are embedded into dimension exactly k by projection P_k

Therefore, given $P\boldsymbol{x}_i = \boldsymbol{y}_i$ and $\widehat{\mu}_j = P\mu_j$

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$$\begin{aligned}\sum_{j\in[k]}\sum_{i\in S_j}\|\boldsymbol{x}_i-\mu_j\|^2 &\geq \sum_{j\in[k]}\sum_{i\in S_j}\|P\boldsymbol{x}_i-P\mu_j\|^2\\ &= \sum_{j\in[k]}\sum_{i\in S_j}\|\boldsymbol{y}_i-\widehat{\mu}_j\|^2\\ &\geq \sum_{j\in[k]}\sum_{i\in \widehat{S}_j}\|\boldsymbol{y}_i-\widehat{\mu}_j\|^2 = f^*_{k-\text{means}}\end{aligned}$$

Therefore, your best beat

Steps

1. Compute the PCA of the points x_i into dimension k.

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2. Solve k-means on the points y_i in dimension k.
3. Output the resulting clusters and centers.

Given that

We have that

$$f_{new} = \sum_{j \in [k]} \sum_{i \in S_j^*} \left\| \boldsymbol{x}_i - \mu_j^* \right\|^2 = *$$

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Finally

$$** = \sum_{i \in [n]} \left\| \boldsymbol{x}_i - \boldsymbol{y}_i \right\|^2 + \sum_{j \in [k]} \sum_{i \in S_j^*} \left\| \boldsymbol{y}_i - \mu_j^* \right\|^2$$

Therefore, we have

Something Notable

$$f_{PCA} + f^*_{k-means} \leq 2 f_{k-means}$$

Outline

Until now, we have assumed a Euclidean metric space

Important step

- The cluster representatives $m_1, ..., m_k$ in are taken to be the means of the currently assigned clusters.

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- The cluster representatives $m_1, ..., m_k$ in are taken to be the means of the currently assigned clusters.

We can generalize this by using a dissimilarity $D(\boldsymbol{x}_i, \boldsymbol{x}_{i'})$

- By using an explicit optimization with respect to $m_1, ..., m_k$

Outline

Algorithm K-meoids

Step 1

- For a given cluster assignment C find the observation in the cluster minimizing total distance to other points in that cluster:

$$i_k^* = \arg \min_{\{i|C(i)=k\}} \sum_{C(i')=k} D\left(\boldsymbol{x}_i, \boldsymbol{x}_{i'}\right)$$

  - Then $m_k = \boldsymbol{x}_{i_k^*}$ $k = 1, ..., K$ are the current estimates of the cluster centers.

Now

Step 2

- Given a current set of cluster centers $m_1, ..., m_k$, minimize the total error by assigning each observation to the closest (current) cluster center:

$$C(i) = \arg \min_{1 \leq k \leq K} D(\boldsymbol{x}_i, m_k)$$

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Iterate over steps 1 and 2

- Until the assignments do not change.

Outline

Complexity

Problem, solving the first step has a complexity for $k = 1, ..., K$

$$O\left(N_k^2\right)$$

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Given a set of cluster "centers," $\{i_1, i_2, ..., i_K\}$

- Given the new assignments

$$C(i) = \arg \min_{1 \leq k \leq K} D(\boldsymbol{x}_i, m_k)$$

  - It requires a complexity of $O(KN)$ as before.

Therefore

We have that

- K-medoids is more computationally intensive than K-means.

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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Theorem (In the general case for any distance)

It is NP-hard to approximate the general K-center problem within any factor α.

Therefore

We change the distance to be constrained by

The Triangle Inequality

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The Triangle Inequality

Given x, y and z

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

Outline

We have a new criterion

Instead of using the K-mean criterion

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New Criterion

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

Explanation

Setup

Suppose we have a data set A that contains N objects.

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Now

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.

Another Way

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Another way to define the cluster size:

- D is the maximum pairwise distance between an arbitrary pair of points in the cluster.
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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:

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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

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

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Where μ_k is the centroid for cluster C_k

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

Now, what about the K-centers

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

$$\min_{S} \max_{k=1,\ldots,K} \max_{i:x_i \in C_k} (\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T (\boldsymbol{x}_i - \boldsymbol{\mu}_k) \tag{6}$$

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Properties

- The above objective function shows that for each cluster, only the worst scenario matters, that is, the farthest data point to the centroid.

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Properties

- The above objective function shows that for each cluster, only the worst scenario matters, that is, the farthest data point to the centroid.
- 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.

In other words

First

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

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

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

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With

$L\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)$ denotes any distance between a pair of objects in the same cluster.

Outline

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.

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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.

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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 $\boldsymbol{h}_k \in H$ represents one cluster or subset of points C_k.

Then

Something Notable

We can think of it as a centroid.

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Important

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

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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We do the following

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Thus

Whichever centroid with the minimum distance is selected as the cluster for x_i.

Important

For K-center clustering

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

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As long we can calculate

$L(\boldsymbol{x}_i, \boldsymbol{x}_j)$ which makes the K-center more general than the K-means.

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Something Notable

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

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Thus, we have that

$$D^* = \min_S \max_{k=1,\ldots,K} \max_{i,j:x_i,x_j \in C_k} L(\boldsymbol{x}_i, \boldsymbol{x}_j) \tag{9}$$

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Thus, we have that

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Then, we have the following guarantee for the greedy algorithm

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

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K-center does not provide a locally optimal solution.

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K-center does not provide a locally optimal solution.

We can get only a solution

Guaranteeing to be within a certain performance range of the theoretical optimal solution.

Outline

Setup

First

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

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

Setup

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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 $dist\,(x_i)$ is the distance between x_i and its closest cluster representative object (centroid):

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

The Main Idea

Something Notable

We always assign $\boldsymbol{x}_i$ to the closest centroid. Therefore $dist\left(\boldsymbol{x}_i\right)$ is the minimum distance between $\boldsymbol{x}_i$ and any centroid.

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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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The Algorithm is Iterative

- We generate one cluster centroid first and then add others one by one until we get K clusters.
- The set of centroids H starts with only a single centroid, $\boldsymbol{h}_1$.

Outline

Algorithm

Step 1

- Randomly select an object $\boldsymbol{x}_j$ from S, let $\boldsymbol{h}_1 = \boldsymbol{x}_j,\ H = \{\boldsymbol{h}_1\}$.

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For $j = 1$ to n:

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In other words

- The $dist\left(x_i\right)$ is the computed distance between $\boldsymbol{x}_j$ and $\boldsymbol{h}_1$.

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- The $dist\left(x_i\right)$ 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 $\boldsymbol{x}_j$.

Algorithm

Step 3

For $i = 2$ to K

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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

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- To stress gain, points already included in H are not among the consideration.

Outline

Implementation

We can use the following for implementation

- The disjoint-set data structure with the following operations:

Implementation

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- The disjoint-set data structure with the following operations:
  - MakeSet
  - Find

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Of course it is necessary to have extra fields for the necessary distances

Thus, each node-element for the sets must have a field $dist(\boldsymbol{x}_j)$ such that

$$dist(\boldsymbol{x}_j) = L(\boldsymbol{x}_j, Find(\boldsymbol{x}_j)) \tag{12}$$

Although

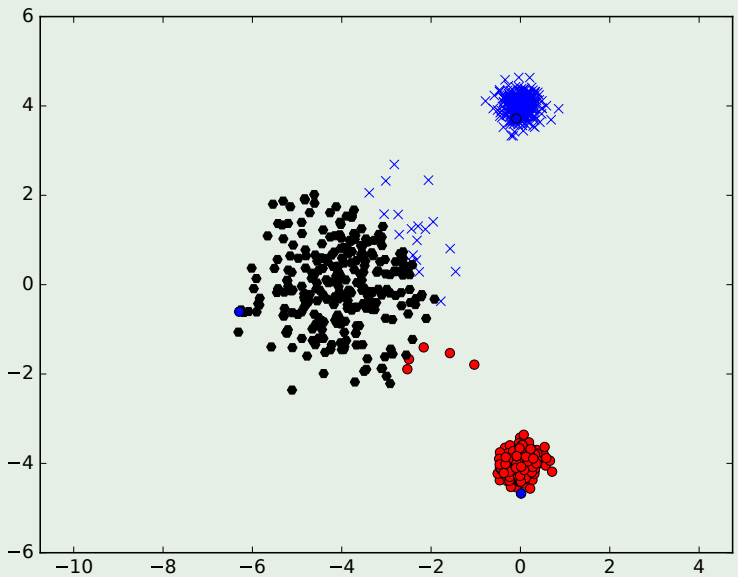
Other things need to be taken in consideration

I will allow to you to think about them

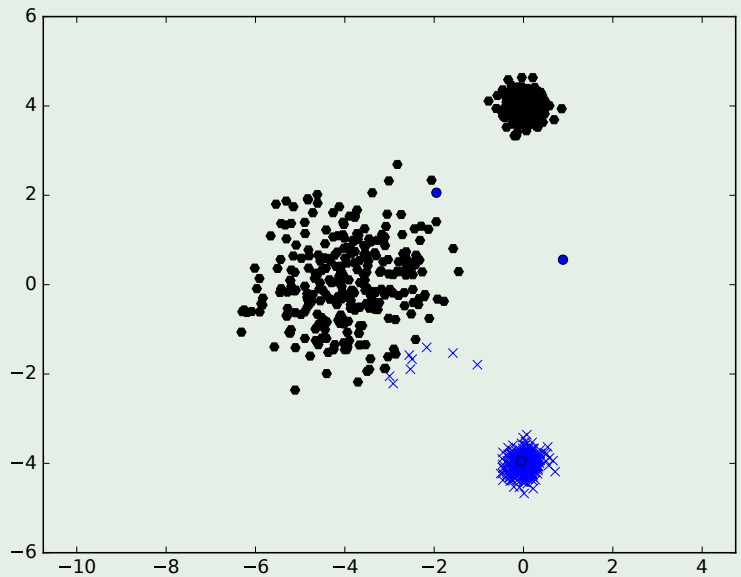
Outline

Example

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



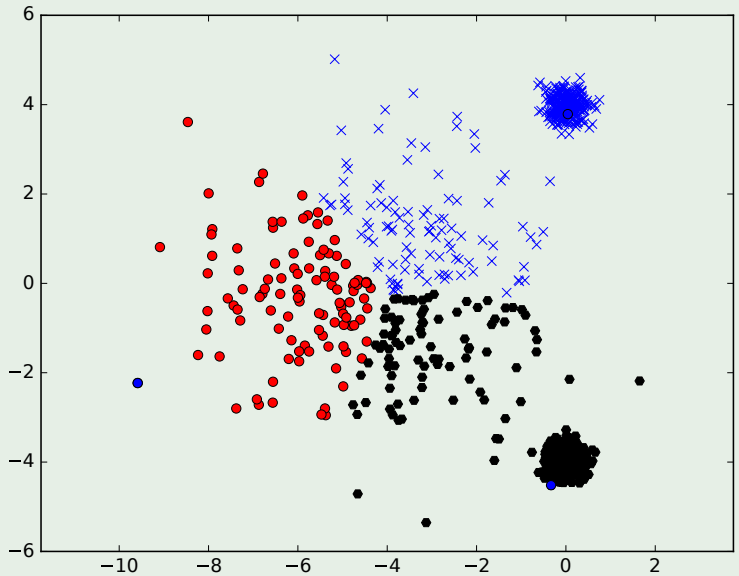
K-Center



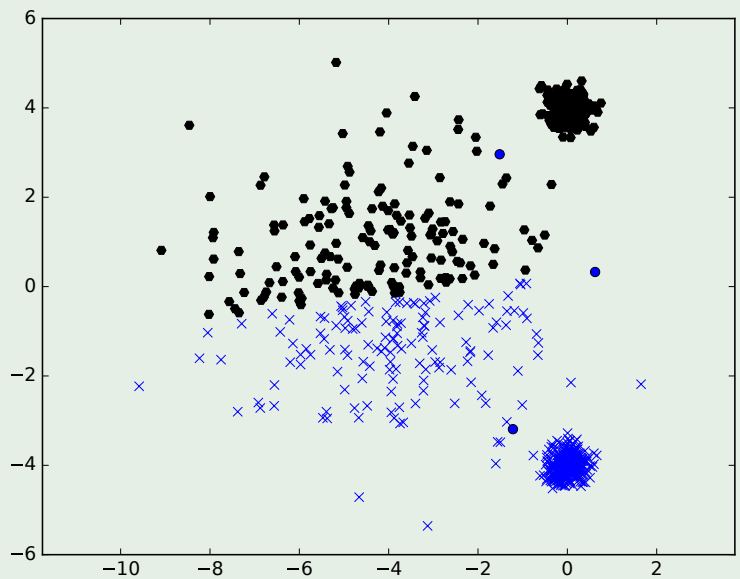
K-Means

Example

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



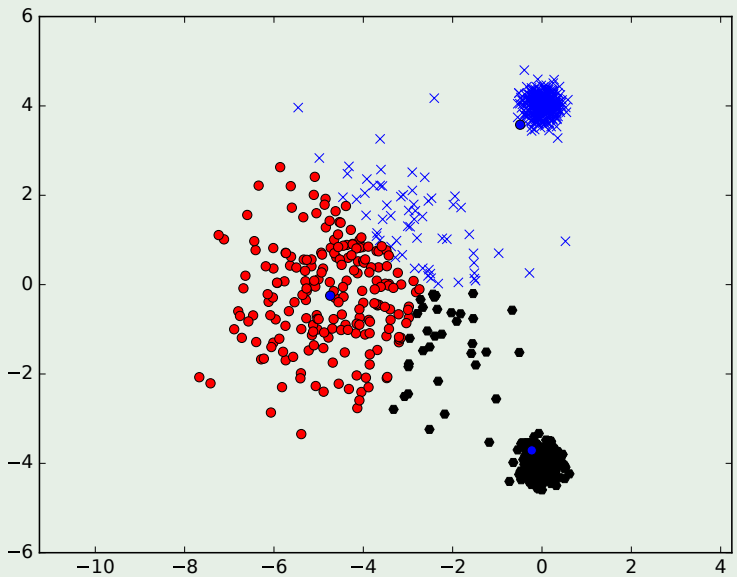
K-Center



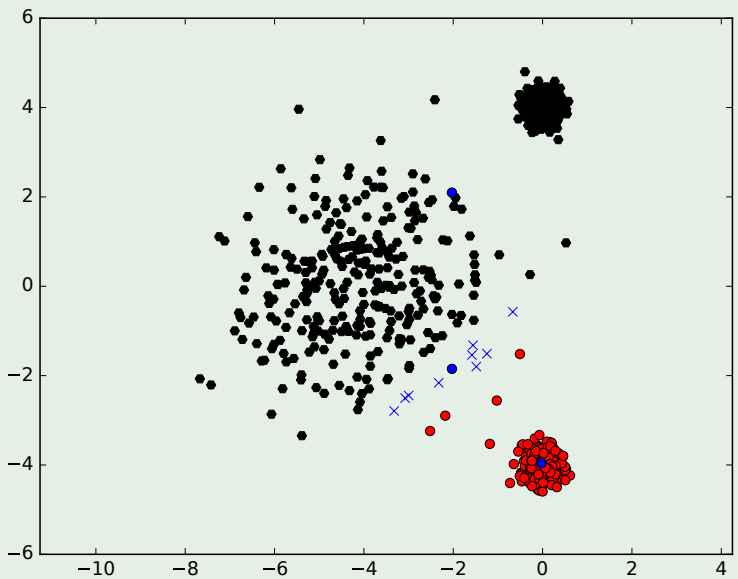
K-Means

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

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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.

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Why?

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

Main Bound of the K-center algorithm

Lemma

Given the distance measure L satisfying the **triangle inequality**.

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Main Bound of the K-center algorithm

Lemma

Given the distance measure L satisfying the **triangle inequality**.

- If the partition obtained by the greedy algorithm is $\widetilde{S}$ and the optimal partition be S^*, such that the cluster size of $\widetilde{S}$ be $\widetilde{D}$ and the one for S^* is D^*, then

$$\widetilde{D} \leq 2D^* \tag{13}$$

Outline

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If we look only at the first j centroid

It generates a partition j with size D_j and also:

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Why?

- Because $D = \max_{\boldsymbol{x}_j : \boldsymbol{x}_j \in S - H} dist\left(\boldsymbol{x}_j\right)$ and lines 5-7 in the step 3 and using induction!!!

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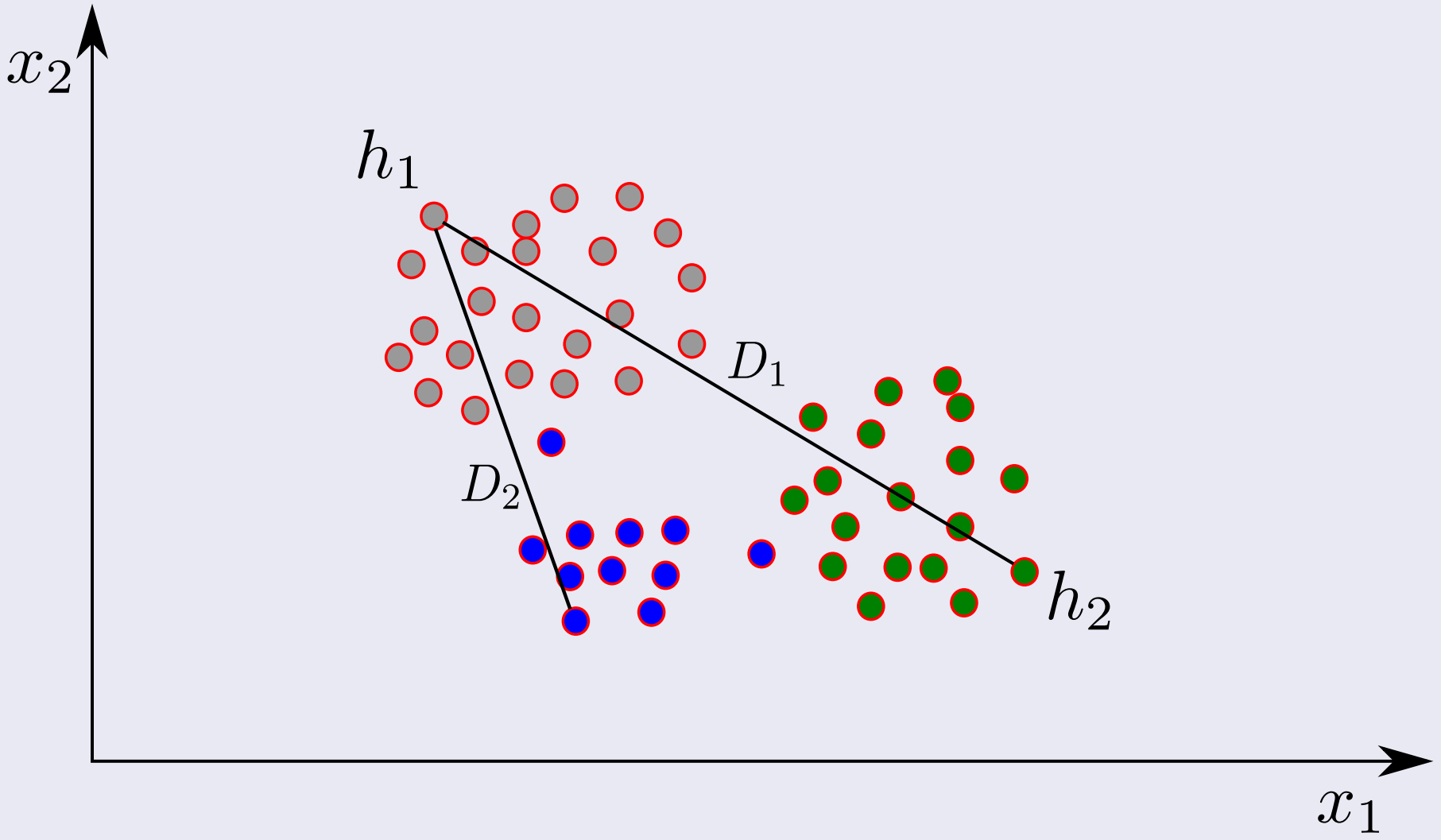
- You can prove that part by yourselves..

Graphically

It is easy to see that when the inner loop changes distances



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It is necessary to prove

$$\forall i < j,\ L\left(\boldsymbol{h}_i, \boldsymbol{h}_j\right) \geq D_{j-1} \tag{15}$$

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D_{j-1} is a lower bound for the distance between $\boldsymbol{h}_i$ and $\boldsymbol{h}_j$.

Proof of the Previous Statement

It is possible to see that

$$L\left(\boldsymbol{h}_{j-2}, \boldsymbol{h}_j\right) \geq L\left(\boldsymbol{h}_{j-1}, \boldsymbol{h}_j\right) \tag{16}$$

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How?

Assume it is not true. Then, $L\left(\boldsymbol{h}_{j-2}, \boldsymbol{h}_j\right) < L\left(\boldsymbol{h}_{j-1}, \boldsymbol{h}_j\right)$

Then

We have that given the partition $\widetilde{S}$ generated by the greedy algorithm

- $\boldsymbol{h}_{j-2} \in \widetilde{C}_{j-2}$, $\boldsymbol{h}_{j-2} \in \widetilde{C}_j$ for $\widetilde{C}_{j-2}, \widetilde{C}_j \in \widetilde{S}$
- It is a contradiction because $\boldsymbol{h}_{j-2}$ is generated by the algorithm such that cannot be in any other cluster!!!

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Thus iteratively

$$L\left(\boldsymbol{h}_1, \boldsymbol{h}_j\right) \geq L\left(\boldsymbol{h}_2, \boldsymbol{h}_j\right) \geq L\left(\boldsymbol{h}_3, \boldsymbol{h}_j\right) \geq ... \geq L\left(\boldsymbol{h}_{j-1}, \boldsymbol{h}_j\right) = D_{j-1} \quad (17)$$

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Therefore, D_{j-1} is not only the lower bound for the distance between $\boldsymbol{h}_i$ and $\boldsymbol{h}_j$, it is also the exact boundary for a specific i.

If, we continue with the proof

Now

- Let us consider the optimal partition S^* with K clusters and its size D^*.
  - **Suppose the greedy algorithm generates** the centroids $\widetilde{H} = \{\boldsymbol{h}_1, \boldsymbol{h}_2, ..., \boldsymbol{h}_K\}$.
  - For the proof, we are adding one more, $\boldsymbol{h}_{K+1}$.

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According to the pigeonhole principle, at least two of the centroids among

$\{\boldsymbol{h}_1, \boldsymbol{h}_2, ..., \boldsymbol{h}_K, \boldsymbol{h}_{K+1}\}$will fall into one cluster k of the partition S^*.

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$$L(\boldsymbol{h}_i, \boldsymbol{h}_j) \leq L(\boldsymbol{h}_i, \boldsymbol{h}_k) + L(\boldsymbol{h}_k, \boldsymbol{h}_j) \leq D^* + D^* = 2D^* \tag{19}$$

Then

In addition

Also $L(\boldsymbol{h}_i, \boldsymbol{h}_j) \geq D_{j-1} \geq D_k$ then $D_k \leq 2D^*$

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Given $\widetilde{S}$, the partition generated by the greedy algorithm

We define Δ as

$$\Delta = \max_{\boldsymbol{x}_j : \boldsymbol{x}_j \in \widetilde{S} - \widetilde{H}} \min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in \widetilde{H}} L(\boldsymbol{x}_j, \boldsymbol{h}_k) \tag{20}$$

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Basically

The maximum of all points that are not centroids that minimize the distance to some centroid for the partition generated by the greedy algorithm.

Now, we are ready for the final part

Let $\boldsymbol{h}_{K+1}$ be an element in $\widetilde{S} - \widetilde{H}$

Such that

$$\min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in \widetilde{H}} L\left(\boldsymbol{h}_{K+1}, \boldsymbol{h}_k\right) = \Delta \tag{21}$$

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Thus, we have the following sets

Let $H_k = \{\boldsymbol{h}_1, ..., \boldsymbol{h}_k\}$ with $k = 1, 2, ..., K$.

Now

Consider the distance between $\boldsymbol{h}_i$ and $\boldsymbol{h}_j$ for $i < j \leq K$

- According the greedy algorithm
  $$\min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in H_{j-1}} L\left(\boldsymbol{h}_j, \boldsymbol{h}_k\right) \geq \min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in H_{j-1}} L\left(\boldsymbol{x}_l, \boldsymbol{h}_k\right) \text{ for any } x_l \in \widetilde{S} - H_j$$
- Basically remember that the $\boldsymbol{h}_i$ are obtained by finding the farthest points.

Now, we have

Since $\boldsymbol{h}_{K+1} \in \widetilde{S} - \widetilde{H}$ and $\widetilde{S} - \widetilde{H} \subset \widetilde{S} - H_j$

$$
\begin{aligned}
&\geq \min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in H_{j-1}} L\left(\boldsymbol{h}_{K+1}, \boldsymbol{h}_k\right) \\
&\geq \min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in \widetilde{H}} L\left(\boldsymbol{h}_{K+1}, \boldsymbol{h}_k\right) \\
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We have shown that for any for $i < j \leq K+1$

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We have shown that for any for $i < j \leq K + 1$

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Now

Consider the optimal partition $S^* = \{C_1^*, C_2^*, ..., C_K^*\}$

Thus at least 2 of the $K+1$ elements $h_1, h_2, ..., h_{K+1}$ will be covered by one cluster.

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Assume that

$\boldsymbol{h}_i$ and $\boldsymbol{h}_j$ belong to the same cluster in S^* . Then $L(\boldsymbol{h}_i, \boldsymbol{h}_j) \leq D^*$.

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We have that since $L(\boldsymbol{h}_i, \boldsymbol{h}_j) \geq \Delta$ then $\Delta \leq D^*$

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Consider elements $\boldsymbol{x}_m$ and $\boldsymbol{x}_n$ in any cluster represented by $\boldsymbol{h}_k$

$$L\left(\boldsymbol{x}_m, \boldsymbol{h}_k\right) \leq \Delta \text{ and } L\left(\boldsymbol{x}_n, \boldsymbol{h}_k\right) \leq \Delta \tag{24}$$

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$$L\left(\boldsymbol{x}_m, \boldsymbol{h}_k\right) \leq \Delta \text{ and } L\left(\boldsymbol{x}_n, \boldsymbol{h}_k\right) \leq \Delta \tag{24}$$

By Triangle Inequality

$$L\left(\boldsymbol{x}_m, \boldsymbol{x}_k\right) \leq L\left(\boldsymbol{x}_m, \boldsymbol{h}_k\right) + L\left(\boldsymbol{x}_n, \boldsymbol{h}_k\right) \leq 2\Delta \tag{25}$$

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Finally, there are two elements $\boldsymbol{x}_m$ and $\boldsymbol{x}_n$ in a cluster such that $\widetilde{D} = L\left(\boldsymbol{x}_m, \boldsymbol{x}_n\right)$

$$\widetilde{D} = \max_k \; D_k \leq 2\Delta \leq 2D^* \tag{26}$$