Introduction to Machine Learning

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

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August 4, 2018

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

- Exact Cover by 3-Sets problem

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

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However

There are efficient heuristic and approximation algorithms

- Which can solve this problem

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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 $x_1, ..., x_N \in \mathbb{R}^d$

It tries to find k points $\mu_1, ..., \mu_k \in \mathbb{R}^d$ 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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Let the set of data points (or instances) D be $\{\mathbf{x}_1, \cdots, \mathbf{x}_n\}$ where $\mathbf{x}_i = (x_{i1}, \cdots, x_{ir})^T$:

- 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.
   - $\mathbf{v}_j = \dfrac{\sum_{i=1}^{n} I(c_i = j)\mathbf{x}_i}{\sum_{i=1}^{n} I(c_i = j)}$
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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 μ_k is the centroid for cluster C_k

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

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

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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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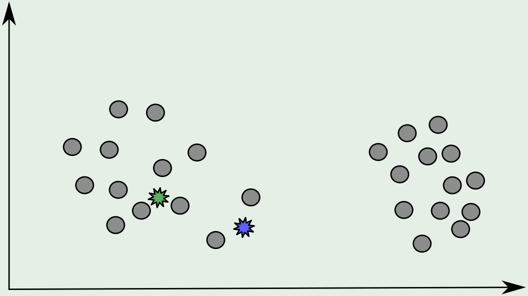
An example

Dropping two possible centroids



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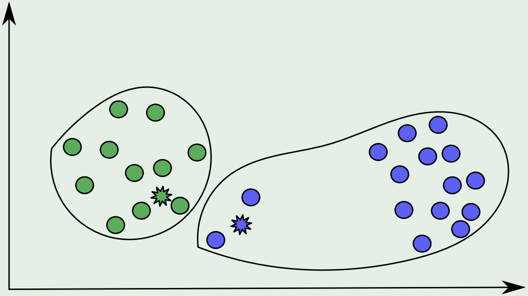
Calculate the memberships



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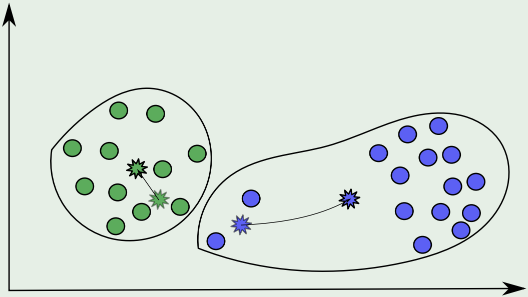
We re-calculate centroids



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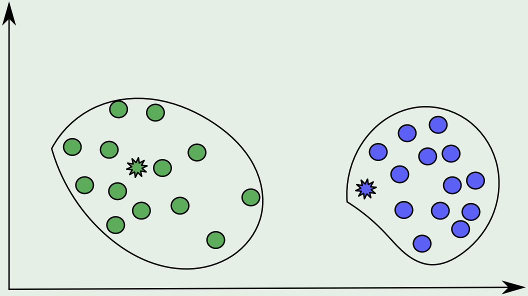

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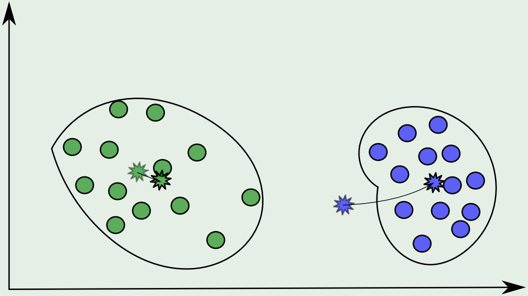
We re-calculate centroids and keep going



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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.
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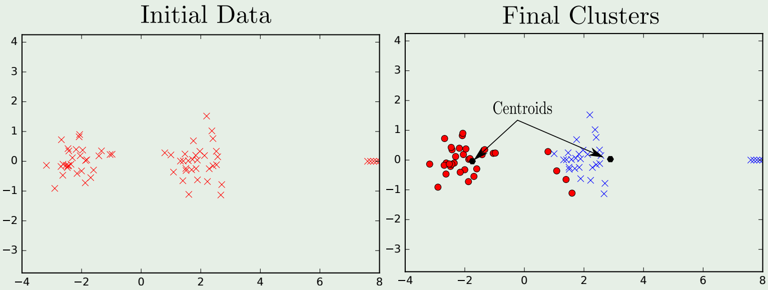
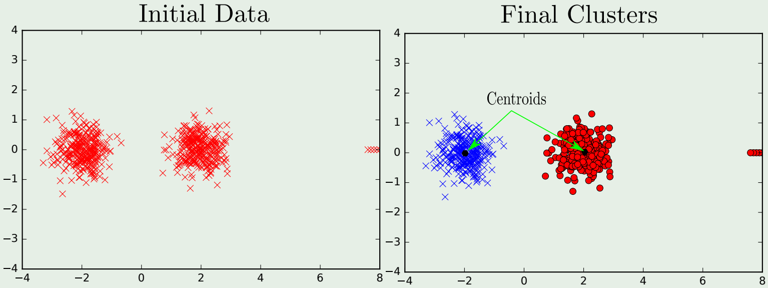
Weaknesses of K-means: Problems with outliers

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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To perform random sampling.

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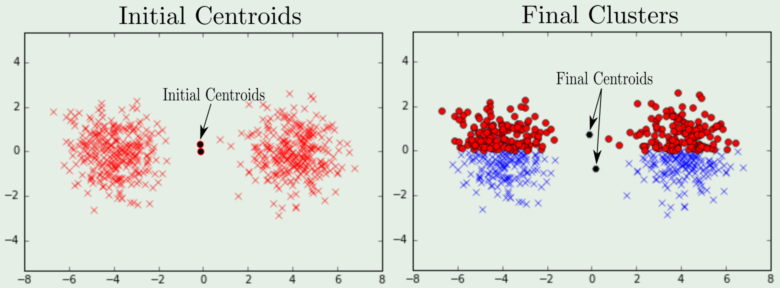
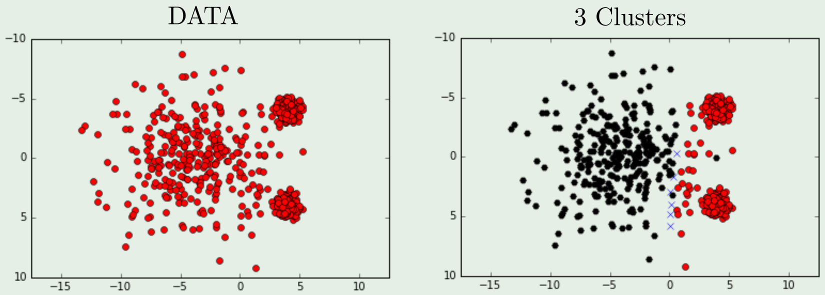
Weaknesses of K-means (cont...)

The algorithm is sensitive to initial seeds



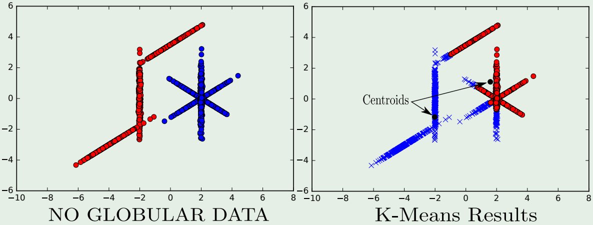
Weaknesses of K-means : Different Densities

We have three cluster nevertheless



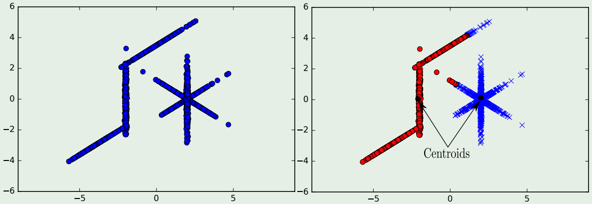
Weaknesses of K-means: Non-globular Shapes

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

Outline

Consider the following

Theorem

- Every matrix $A \in R^{m \times n}$ has an SVD.

Frobenious Matrix Norm

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Then, you have 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

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

Therefore, we have the following decomposition

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

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

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Orthogonal Projection

Therefore, we have that U is a orthogonal projection

- Given that $UU^T = I$ and $U\boldsymbol{x} = \boldsymbol{x}$

Now, we can re-write k-means

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

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Therefore, we have that U is a orthogonal projection

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Now, we can re-write k-means

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

Then

PCA can also re-write the cost function

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

Where

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

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

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Thus, using the Eckhart-Young Theorem

Assume P_k^* which contains the k optimal centers

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

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\begin{aligned}
f_{k-\text{mean}} &= \sum_{i\in[n]} \min_{j\in[k]} \left\| \boldsymbol{x}_i - \mu_j^* \right\|^2 \\
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- Where the $\widehat{S}$ and $\widehat{\mu}$ are the assignments and centers of the projected points $\boldsymbol{y}_i$:

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Steps

1. Compute the PCA of the points x_i into dimension k.
2. Solve k-means on the points y_i in dimension k.
3. Output the resulting clusters and centers.

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We have that

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

Therefore by the fact that $\boldsymbol{x}_i - \boldsymbol{y}_i$ and $\boldsymbol{y}_i - \mu_j^*$ are perpendiculars

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

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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.

We can generalize this by using a dissimilarity $D(x_i, x_{i'})$

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

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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:

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

Iterate over steps 1 and 2

- Until the assignments do not change.

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Complexity

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

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

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

- Given the new assignments

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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 $G = (V, V \times V)$.

- Such that minimize maximum distance of every point to a centroid.

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

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Therefore

We change the distance to be constrained by

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.

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.

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

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We want the following

We want to partition A into K sets labeled $C_1, C_2, ..., C_K$.

- The smallest value D for which all points in this cluster C_k are:
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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:

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

Where μ_k is the centroid for cluster C_k

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

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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

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

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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.

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

Then

Something Notable

We can think of it as a centroid.

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:

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

Thus

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

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

x_i can be a non-vector representation of the objects.

As long we can calculate

$L(x_i, x_j)$ which makes the K-center more general than the K-means.

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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

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

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

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Outline

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

Third

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

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

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For $j = 1$ to n:

1. $dist\,(\boldsymbol{x}_i) = L\,(\boldsymbol{x}_i, \boldsymbol{h}_1)$.
2. $cluster\,(\boldsymbol{x}_i)$.

- Because so far we only have one cluster, we will assign a cluster label 1 to every x_i.

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For $i = 2$ to K

1. $D = \max\limits_{\boldsymbol{x}_j : \boldsymbol{x}_j \in S - H} dist\left(\boldsymbol{x}_j\right)$
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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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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We can use the following for implementation

- The disjoint-set data structure with the following operations:
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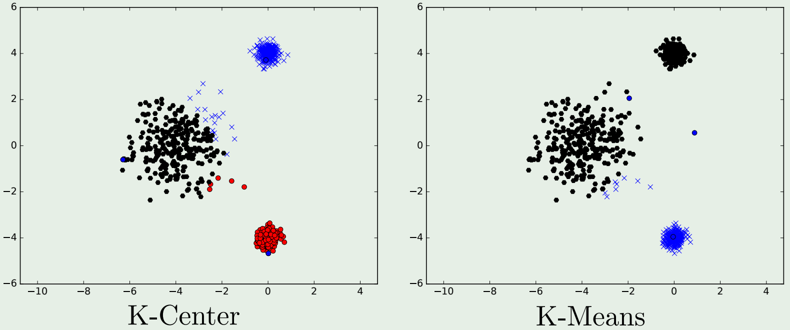
I will allow to you to think about them

Outline

Example

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



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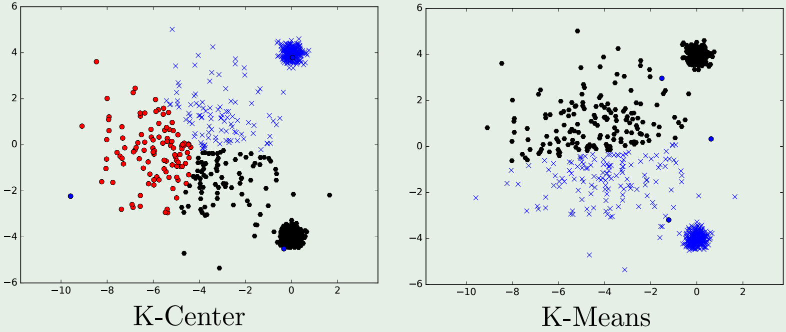
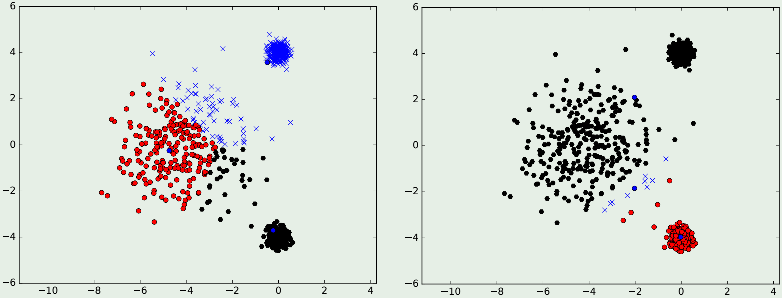
Decreasing the density of one of the clusters, we see a degradation on the clusters



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.

Why?

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

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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 $\tilde{S}$ and the optimal partition be S^*, such that the cluster size of $\tilde{S}$ be $\tilde{D}$ and the one for S^* is D^*, then

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Proof

If we look only at the first j centroid

It generates a partition j with size D_j and also:

- The cluster size is the size of the biggest cluster in the current partition.
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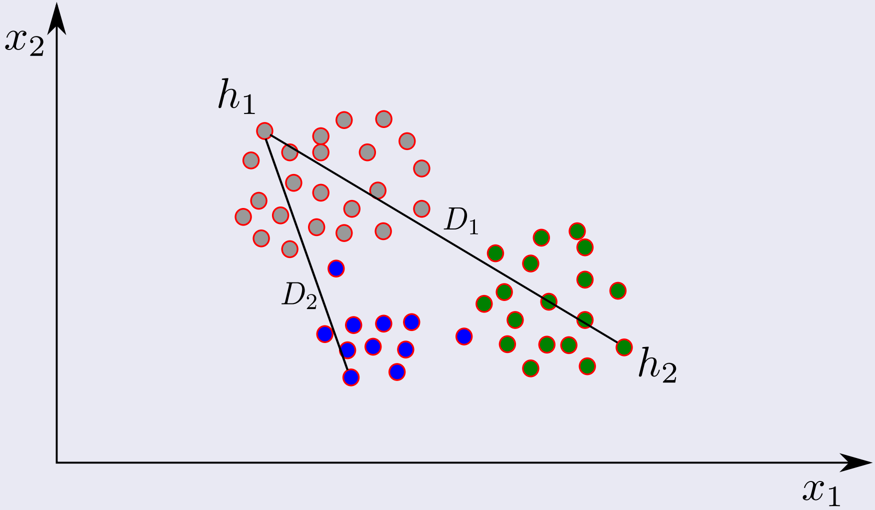
Graphically

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



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D_{j-1} is a lower bound for the distance between h_i and h_j.

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Proof of the Previous Statement

It is possible to see that

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

How?

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

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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!!!

Thus iteratively

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

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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.

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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, $\boldsymbol{h}_{K+1}$.
  - This can be done without losing generality.

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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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$1 \leq i < k < j \leq K+1 \Rightarrow$ Using the triangle inequality:

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

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Then

In addition

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

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

We define Δ as

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

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.

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

Such that

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

By definition

$$L\left(\boldsymbol{h}_{K+1}, \boldsymbol{h}_k\right) \geq \Delta, \ \forall k = 1, ..., K \tag{22}$$

Thus, we have the following sets

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

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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 $\widetilde{S} - \widetilde{H} \subset \widetilde{S} - H_j$

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L\left(\boldsymbol{h}_j, \boldsymbol{h}_i\right) &\geq \min_{\boldsymbol{h}_k : \boldsymbol{h}_k \in H_{j-1}} L\left(\boldsymbol{h}_j, \boldsymbol{h}_k\right) \\
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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.

Assume that

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

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In addition

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

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

By Triangle Inequality

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

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

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

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Outline

Some of the Fuzzy Clustering Models

Fuzzy Clustering Model

Bezdek, 1981

Possibilistic Clustering Model

Krishnapuram - Keller, 1993

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N. Pal - K. Pal - Bezdek, 1997

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Fuzzy C-Means Clustering

The input an unlabeled data set

- $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, ..., \boldsymbol{x}_N\}$.
- $\boldsymbol{x}_k \in \mathbb{R}^p$

Output

- A partition S of the X as a matrix U of $C \times N$.
- Set of cluster centers $V = \{\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_C\} \subset \mathbb{R}^p$

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What we want

Creation of the Cost Function

First:

- We can use a distance defined as:

$$\|\boldsymbol{x}_k - \boldsymbol{v}_i\| = \sqrt{(\boldsymbol{x}_k - \boldsymbol{v}_i)^T (\boldsymbol{x}_k - \boldsymbol{v}_i)} \tag{27}$$

The euclidean distance from a point k to a centroid i.
NOTE other distances based in Mahalonobis can be taken in consideration.

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Do you remember the cost function for K-means?

Finding a partition S that minimizes the following function

$$\min_{S} \sum_{k=1}^{N} \sum_{k:\boldsymbol{x}_k \in C_i} \left\| \boldsymbol{x}_k - \boldsymbol{v}_i \right\|^2 \tag{28}$$

Where $\boldsymbol{v}_i = \frac{1}{N_i} \sum_{\boldsymbol{x}_k \in C_i} \boldsymbol{x}_k$

We can rewrite the previous equation as

$$\min_{S} \sum_{k=1}^{N} \sum_{i=1}^{C} I\left(\boldsymbol{x}_k \in C_i\right) \left\| \boldsymbol{x}_k - \boldsymbol{v}_i \right\|^2 \tag{29}$$

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In addition

Did you notice that the membership is always one or zero?

$$\min_{S} \sum_{k=1}^{N} \sum_{i=1}^{C} \overbrace{I\left(x_k \in C_i\right)}^{\text{Membership}} \left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2 \tag{30}$$

Outline

Thus, we can rethink the membership using something "Fuzzy"

What if we modify the cost function to something like this

$$\min_{S} \sum_{k=1}^{N} \sum_{i=1}^{C} \overbrace{\text{Fuzzy Value}}^{\text{Membership}} \left\| \boldsymbol{x}_k - \boldsymbol{v}_i \right\|^2 \tag{31}$$

This means that we think that each cluster C_i is "Fuzzy"

We can assume a fuzzy set for the cluster C_i with membership function:

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Such that we can tune it by using a power i.e. decreasing it by a m power.

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$$A_i\left(\boldsymbol{x}_k\right) \in [0,1] \;\; \forall i, k \tag{33}$$

Second

$$0 < \sum_{k=1}^{N} A_i\left(\boldsymbol{x}_k\right) < N \;\; \forall i \tag{34}$$

Third

$$\sum_{i=1}^{C} A_i\left(\boldsymbol{x}_k\right) = 1 \;\; \forall k \tag{35}$$

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$$0 < \sum_{k=1}^{N} A_i\left(\boldsymbol{x}_k\right) < N \;\forall i \tag{34}$$

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Final Cost Function

Properties

$$J_m(\mathcal{S}) = \sum_{k=1}^{N} \sum_{i=1}^{C} \left[A_i(\boldsymbol{x}_k)\right]^m \left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2 \tag{36}$$

- $\sum_{i=1}^{C} A_i(\boldsymbol{x}_k) = 1$, for $1 \leq k \leq N$
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- $A_i\left(\boldsymbol{x}_k\right)\in[0,1]$, for $1\leq k\leq N$ and $1\leq i\leq C$.
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Outline

Using the Lagrange Multipliers

New cost function

$$\bar{J}_m(\mathcal{S}) = \sum_{k=1}^{N}\sum_{i=1}^{C}\left[A_i(\boldsymbol{x}_k)\right]^m \left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2 - \sum_{k=1}^{N}\lambda_k\left[\sum_{i=1}^{C}A_i(\boldsymbol{x}_k) - 1\right] \quad (37)$$

Derive with respect to $A_i(\boldsymbol{x}_k)$

$$\frac{\partial \bar{J}_m(\mathcal{S})}{\partial A_i(\boldsymbol{x}_k)} = mA_i(\boldsymbol{x}_k)^{m-1}\left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2 - \lambda_k = 0 \quad (38)$$

Thus

$$A_i(\boldsymbol{x}_k) = \left[\frac{\lambda_k}{m\left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2}\right]^{\frac{1}{m-1}} \quad (39)$$

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Sum over all i's

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$$\lambda_k = \frac{m}{\left[\sum_{i=1}^{C}\frac{1}{\left\Vert\boldsymbol{x}_k-\boldsymbol{v}_i\right\Vert^{\frac{2}{m-1}}}\right]^{m-1}} \tag{41}$$

Plug Back on equation 38 using j instead of i

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Finally

We have that

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In a similar way we have

$$v_i = \frac{\sum_{k=1}^{N} A_i\left(x_k\right)^m x_k}{\sum_{k=1}^{N} A_i\left(x_k\right)^m} \tag{44}$$

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1. Let $t = 0$. Select an initial fuzzy pseudo-partition.
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3. Update for each x_k the membership function by
   - Case I: $\left\| x_k - v_i^{(t)} \right\|^2 > 0$ for all $i \in \{1, 2, ..., C\}$ then
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Final Output

The Matrix U

The elements of U are $U_{ik} = A_i\left(\boldsymbol{x}_k\right)$.

The centroids

$V = \{\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_C\}$

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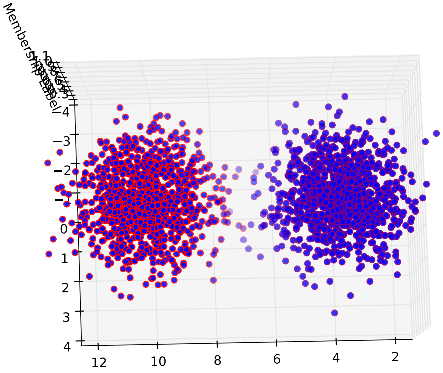
Outline

Example

Here the clustering of two Gaussian Clusters with $\mu_1 = (4,0)^T$, $\mu_2 = (10,0)^T$ and variance 1.0



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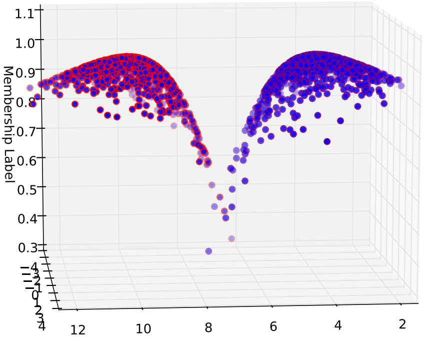

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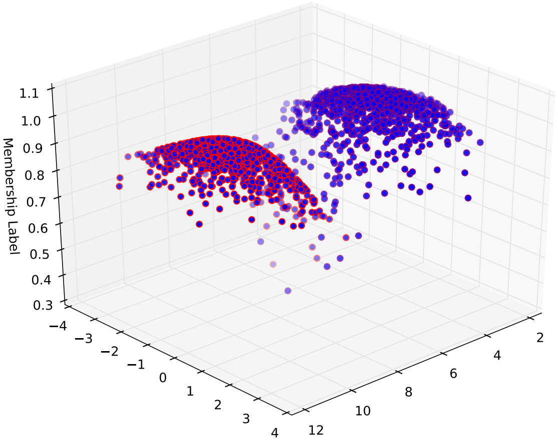

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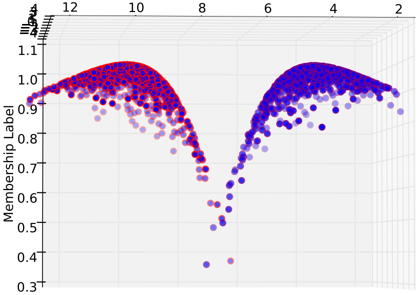

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Pros and Cons of Fuzzy C-Means

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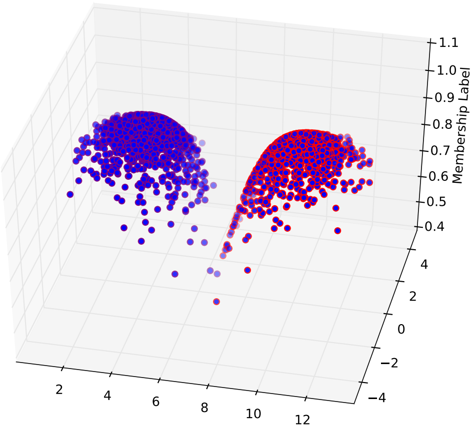
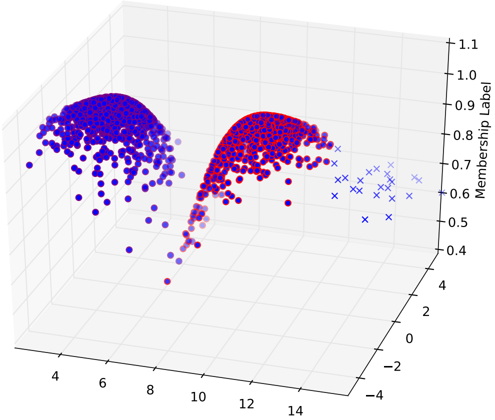
Outliers, Disadvantage of FCM

After running without outliers



Outliers, Disadvantage of FCM

Now add outliers (Shown in blue $x's$) and their high memberships



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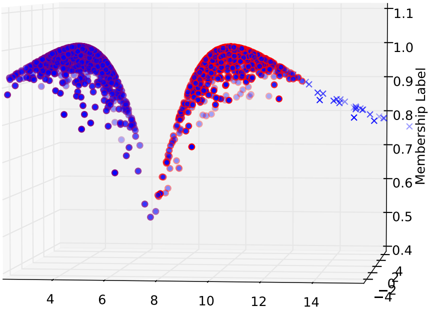

Outline

Krinshapuram and Keller

Following Zadeh

They took in consideration that each class prototype as defining an elastic constraint.

What?

Giving the $t_i(x_k)$ as degree of compatibility of sample x_k with cluster C_i.

We do the following

If we consider the C_i as fuzzy sets over the set of samples $X = \{x_1, x_2, ..., x_N\}$

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Here is the Catch!!!

We should not use the old membership

$$\sum_{i=1}^{C} A_i\left(\boldsymbol{x}_k\right) = 1 \tag{45}$$

Because

This is quite probabilistic... which is not what we want!!!

Thus

We only ask for membership, now using the possibilistic notation of $t_i\left(\boldsymbol{x}_k\right)$ (This is known as **typicality** value), to be in the interval $[0, 1]$.

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New Constraints

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Outline

We have the following cost function

Cost Function

$$\sum_{k=1}^{N} \sum_{i=1}^{C} \left[t_i\left(\boldsymbol{x}_k\right)\right]^m \left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2 \tag{49}$$

Problem

Unconstrained optimization of first term will lead to the trivial solution $t_i\left(\boldsymbol{x}_k\right) = 0$ for all i, k.

Thus, we can introduce the following constraint

$$t_i\left(\boldsymbol{x}_k\right) \to 1 \tag{50}$$

- Roughly it means to make the typicality values as large as possible.

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By putting all them together in

$$\sum_{k=1}^{N} \left(1 - t_i\left(\boldsymbol{x}_k\right)\right)^m \tag{51}$$

With m to control the tendency of $t_i\left(\boldsymbol{x}_k\right) \rightarrow 1$

We can also run this tendency over all the cluster using a suitable $w_i > 0$ per cluster

$$\sum_{i=1}^{C} w_i \sum_{k=1}^{N} \left(1 - t_i\left(\boldsymbol{x}_k\right)\right)^m \tag{52}$$

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Possibilistic C-Mean Clustering (PCM)

The final Cost Function

$$J_m(\mathcal{S}) = \sum_{k=1}^{N} \sum_{i=1}^{C} [t_i(\boldsymbol{x}_k)]^m \|\boldsymbol{x}_k - \boldsymbol{v}_i\|^2 + \sum_{i=1}^{C} w_i \sum_{k=1}^{N} (1 - t_i(\boldsymbol{x}_k))^m \quad (53)$$

Where

- $t_i(\boldsymbol{x}_k)$ are **typicality** values.
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It demands that the distance from feature vector to prototypes be as small as possible!!!

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Final Updating Equations

Typicality Values

$$t_i\left(\boldsymbol{x}_k\right) = \frac{1}{1 + \left(\frac{\left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2}{w_i}\right)^{\frac{1}{m-1}}},\ \forall i, k \tag{56}$$

Cluster Centers

$$v_i = \frac{\sum_{k=1}^{N} t_i\left(\boldsymbol{x}_k\right)^m \boldsymbol{x}_k}{\sum_{k=1}^{n} t_i\left(\boldsymbol{x}_k\right)^m} \tag{57}$$

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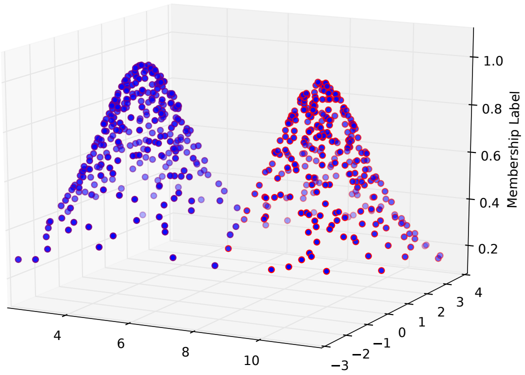
$$w_i = M \frac{\sum_{k=1}^{N} \left[t_i\left(\boldsymbol{x}_k\right)\right]^m \left\|\boldsymbol{x}_k - \boldsymbol{v}_i\right\|^2}{\sum_{k=1}^{n} \left[t_i\left(\boldsymbol{x}_k\right)\right]^m}, \tag{58}$$

with $M > 0$.

Possibilistic can deal with outliers

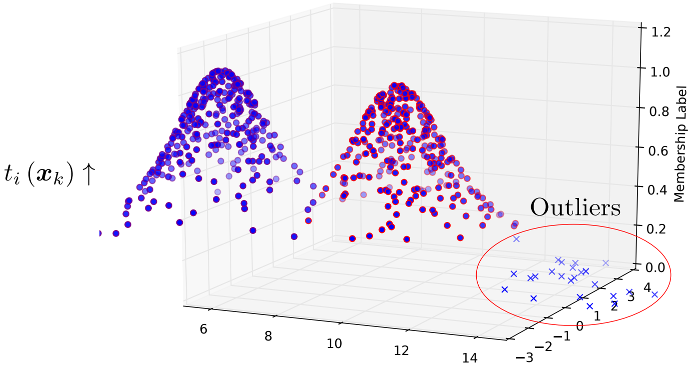
Two Gaussian Clusters with $\mu_1 = (4,0)^T$, $\mu_2 = (10,0)^T$ and $\sigma^2 = 1.0$

$t_i(\boldsymbol{x}_k) \uparrow$



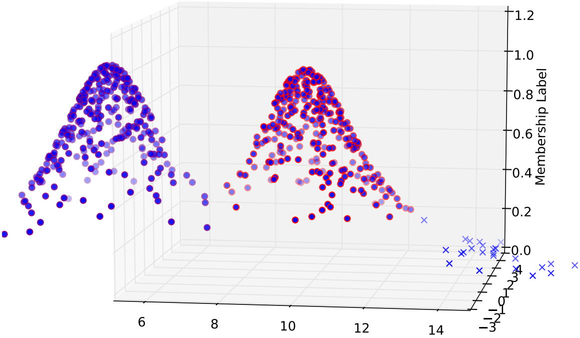
Possibilistic can deal with outliers

Now add outliers



Possibilistic can deal with outliers

Another Angle



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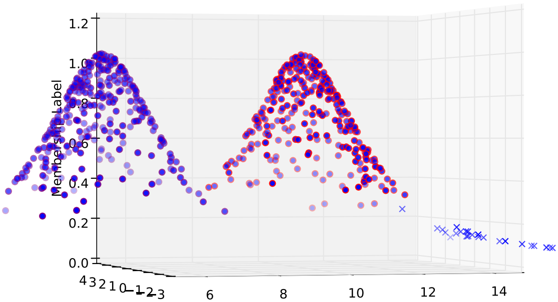

Pros and Cons of Fuzzy C-Means

Advantages

Clustering noisy data samples.

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- Very sensitive to good initialization.
- For example, I needed to run fuzzy C-means to obtain good initial typicalities

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Nevertheless

There are more advanced clustering methods based on the possibilistic and fuzzy idea

Pal, N.R.; Pal, K.; Keller, J.M.; Bezdek, J.C., "A Possibilistic Fuzzy c-Means Clustering Algorithm," Fuzzy Systems, IEEE Transactions on , vol.13, no.4, pp.517,530, Aug. 2005.