Exercises
Learning and Intelligent Systems
SS 2016

Series 4, April 19th, 2016 (Clustering and K-means)

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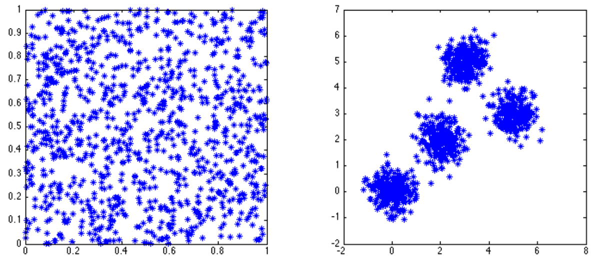
It is not mandatory to submit solutions and sample solutions will be published in two weeks. If you choose to submit your solution, please send an e-mail from your `ethz.ch` **address with subject** `Exercise4` **containing a PDF (LaTeX or scan) to** `lis2016@lists.inf.ethz.ch` **until Sunday, May 1st 2016.**

Problem 1 (K-means initialization):

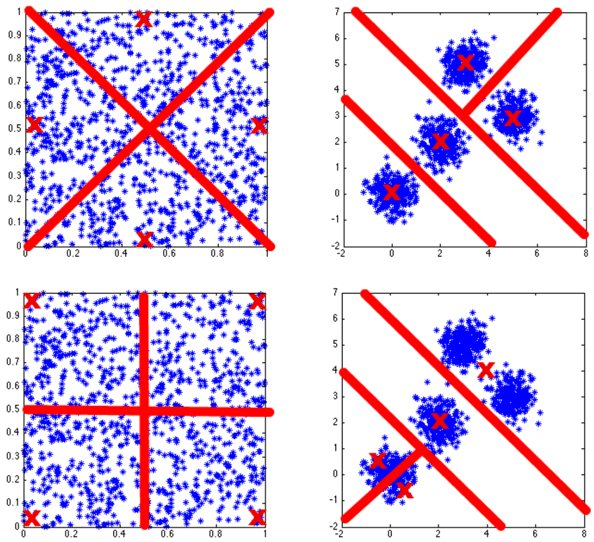
You are given two example datasets consisting of 1000 two dimensional points each. We want to find 4 clusters in each of them.



We know that K-means is not robust to initialization. Can you provide two different initializations for each of the datasets that would result in qualitatively different clusters? Sketch initializations and resulting clusters.

Solution 1:

In the plot below, you can see two possible initializations with all the resulting separating hyperplanes for each of the datasets.



This is just a sketch, but it is clearly visible that the clusters obtained with different initializations can differ a lot.

Problem 2 (K-means convergence):

In the K-means clustering algorithm, you are given a set of n points $x_i \in \mathbb{R}^d$, $i \in \{1, \ldots, n\}$ and you want to find the centers of k clusters $\mu = (\mu_1, \ldots, \mu_k)$ by minimizing the average distance from the points to the closest cluster center. Formally, you want to minimize the following loss function

$$L(\mu) = \sum_{i=1}^{n} \min_{j \in \{1,\ldots,k\}} \|x_i - \mu_j\|_2^2.$$

To approximate the solution, we introduce new assignment variables $z_i \in \arg\min_{j\in\{1,\ldots,k\}} \|x_i - \mu_j\|_2^2$ for each data point x_i. The K-means algorithm iterates between updating the variables z_i (*assignment step*) and updating the centers $\mu_j = \frac{1}{|\{i:z_i=j\}|} \sum_{i:z_i=j} x_i$ (*refitting step*). The algorithm stops when no change occurs during the *assignment step*.

Show that K-means is guaranteed to converge (to a local optimum). *Hint:* You need to prove that the loss function is guaranteed to decrease monotonically in each iteration until convergence. Prove this separately for the *assignment step* and the *refitting step* .

Solution 2:

To prove convergence of the K-means algorithm, we show that the loss function is guaranteed to decrease monotonically in each iteration until convergence for the *assignment step* and for the *refitting step*. Since the loss function is non-negative, the algorithm will eventually converge when the loss function reaches its (local) minimum.

Let $z = (z_1, \ldots, z_n)$ denote the cluster assignments for the n points.

(i) *Assignment step*
We can write down the original loss function $L(\mu)$ as follows:

$$L(\mu, z) = \sum_{i=1}^{n} \|x_i - \mu_{z_i}\|_2^2$$

Let us consider a data point x_i, and let z_i be the assignment from the previous iteration and z_i^* be the new assignment obtained as:

$$z_i^* \in \arg \min_{j\in\{1,\ldots,k\}} \|x_i - \mu_j\|_2^2$$

Let z^* denote the new cluster assignments for all the n points. The change in loss function after this assignment step is then given by:

$$L(\mu, z^*) - L(\mu, z) = \sum_{i=1}^{n} \left(\|x_i - \mu_{z_i^*}\|_2^2 - \|x_i - \mu_{z_i}\|_2^2 \right) \leq 0$$

The inequality holds by the rule z_i^* is determined, i.e. to assign x_i to the nearest cluster.

(ii) *Refitting step*
We can write down the original loss function $L(\mu)$ as follows:

$$L(\mu, z) = \sum_{j=1}^{k} \Big(\sum_{i:z_i=j} \|x_i - \mu_j\|_2^2 \Big)$$

Let us consider the j^{th} cluster, and let μ_j be the cluster center from the previous iteration and μ_j^* be the new cluster center obtained as:

$$\mu_j^* = \frac{1}{|\{i : z_i = j\}|} \sum_{i:z_i=j} x_i$$

Let μ^* denote the new cluster centers for all the k clusters. The change in loss function after this refitting step is then given by:

$$L(\mu^*, z) - L(\mu, z) = \sum_{j=1}^{k} \Big(\big(\sum_{i:z_i=j} \|x_i - \mu_j^*\|_2^2 \big) - \big(\sum_{i:z_i=j} \|x_i - \mu_j\|_2^2 \big) \Big) \leq 0$$

The inequality holds because the update rule of μ_j^* essentially minimizes this quantity.

Problem 3 (K-medians clustering):

In this exercise, you are asked to derive a new clustering algorithm that would use a different loss function given by

$$L(\mu) = \sum_{i=1}^{n} \min_{j \in \{1,\ldots,k\}} \|x_i - \mu_j\|_1.$$

(a) Find the update steps both for z_i and μ_j in this case.

(b) What can you say about the convergence of your algorithm?

(c) In which situation would you prefer to use K-medians clustering instead of K-means clustering?

Solution 3:

(a) As in the K-means algorithm, let's again introduce hidden variables $z_i = \arg\min_{j \in 1,\ldots,k} ||x_i - \mu_j||_1$ for each data point x_i. Then the initial problem

$$\mu = \arg\min_{\mu} \sum_{i=1}^{n} \min_{j \in 1,\ldots,k} ||x_i - \mu_j||_1$$

can be rewritten in a different form (because we know where exactly the minimum is achieved):

$$\mu = \arg\min_{\mu} \sum_{i=1}^{n} ||x_i - \mu_{z_i}||_1$$

In order to find the solution with respect to μ_j with fixed z_i, let's leave only the data points that correspond to the j^{th} component:

$$\mu_j = \arg\min_{\mu_j} \sum_{i:z_i=j} ||x_i - \mu_j||_1$$

$$\mu_j = \arg\min_{\mu_j} \sum_{i:z_i=j} \sum_{q=1}^{d} |x_{i,q} - \mu_{j,q}|$$

This can again be separated component-wise:

$$\mu_{j,q} = \arg\min_{\mu_{j,q}} \sum_{i:z_i=j} |x_{i,q} - \mu_{j,q}|$$

Again, as in the K-means algorithm, we proceed by finding the derivative of the functional and setting it to zero. In order to get rid of the L_1 norm, we also separate the functional into the sum over those $x_{i,q}$ that are smaller than $\mu_{j,q}$ and those that are larger:

$$\sum_{i:z_i=j,x_{i,q}\leq\mu_{j,q}} |x_{i,q}-\mu_{j,q}| + \sum_{i:z_i=j,x_{i,q}>\mu_{j,q}} |x_{i,q}-\mu_{j,q}| = \sum_{i:z_i=j,x_{i,q}\leq\mu_{j,q}} (\mu_{j,q}-x_{i,q}) + \sum_{i:z_i=j,x_{i,q}>\mu_{j,q}} (x_{i,q}-\mu_{j,q})$$

The derivative of every bracket in the sum is either $+1$ or -1, and the number of $+1$'s is exactly $|\{i : z_i = j, x_{i,q} \leq \mu_{j,q}\}|$. Therefore, we need to set

$$|\{i : z_i = j, x_{i,q} \leq \mu_{j,q}\}| - |\{i : z_i = j, x_{i,q} > \mu_{j,q}\}| = 0$$

This means that $\mu_{j,q}$ is nothing but the *median* of all the numbers $x_{i,q}$, $i : z_i = j$.

The resulting algorithm then iterates between two steps:

- $z_i = \arg\min_{j\in 1,\ldots,k} ||x_i - \mu_j||_1$
- $\mu_{j,q} = \text{median}(x_{i,q}, i : z_i = j), \forall j = 1, \ldots, k; \forall q = 1, \ldots, d.$

(b) You can prove the same convergence properties for K-medians as for K-means.

(c) In comparison with K-means, K-medians clustering is particularly robust to outliers. Thus, if we expect out input data to have many outliers, it is preferable to use K-medians clustering.