Exercises Learning and Intelligent Systems SS 2016

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

LAS Group, Institute for Machine Learning Dept. of Computer Science, ETH Zürich Prof. Dr. Andreas Krause Web: http://las.inf.ethz.ch/teaching/lis-s16/ Email questions to: Jens Witkowski, jensw@inf.ethz.ch

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 $1000\ {\rm two}$ dimensional points each. We want to find $4\ {\rm clusters}$ 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.

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

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

To approximate the solution, we introduce new assignment variables $z_i \in \arg \min_{j \in \{1,...,k\}} ||x_i - \mu_j||_2^2$ 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*.

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

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

- (a) Find the update steps for both z_i and for 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?