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**A Novel Class of Globally Convergent Algorithms
For Clustering Problems**

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Abstract

The clustering problem is one of the fundamental problems in unsupervised machine learning, and arises in a wide scope of applications. It is well-known that the clustering problem is a nonconvex and nonsmooth optimization problem and therefore hard to solve. We propose two clustering center-based algorithms, each tackles a different distance function. The KPALM algorithm solves the clustering problem with the squared Euclidean distance, whereas the ε -KPALM algorithm solves the clustering problem with the standard Euclidean distance. Both algorithms are based on the classical Alternating Minimization. For fixed centers each algorithm reassigns the data points, solving a minimization subproblem, whose objective is a linear function regularized with a proximal term. For fixed partition of the data points, both algorithms update the centers of the clusters. KPALM solves the subproblem via an exact minimization, whereas ε -KPALM solves an approximated minimization subproblem performing a certain gradient step. We prove global convergence of these algorithms to a critical point of the corresponding objective function, via a new methodology which is based on the powerful Kurdyka-Łojasiewicz property. As an illustration of the theoretical results, we present numerical tests which demonstrate the effectiveness of the proposed algorithms.

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Chapter 1

Introduction

This chapter presents the importance of the clustering problem and describes the usefulness of clustering in many applications. Moreover, we describe existing types and approaches for clustering, and review the literature of the most popular clustering center-based algorithms. We outline the main contributions of the thesis which consists of: (i) the development of new algorithms, (ii) a novel methodology to prove global convergence of the proposed methods, (iii) numerical examples illustrating their performance in comparison with standard schemes.

1.1 Background and Motivation

The clustering problem is a task of grouping objects which are similar. It consists of partitioning a dataset into subsets, called clusters, such that the data points in each cluster are similar with respect to a specific criteria.

The clustering problem is a fundamental problem in the machine learning field, and it arises in a wide scope of applications, such as data mining, pattern recognition, information retrieval and many others. For example, in image segmentation, one is interested in partitioning the pixels of an image into objects, where each pixel can be described via its location in the image and its color given in RGB format. Another example is learning the probability density of some data, where the data is assumed to be drawn from a mixtures of distributions. Each partition of the data is represented by a unimodal probability density model, and a summation of all the cluster models gives a multimodal density for the entire dataset. Vector quantization is yet another example, where large sets of points are represented by their centroid point. This

approach can be used for data compression, data correction and pattern recognition.

There are several types of clustering approaches, each has a direct impact on the final clustering structure.

- (i) Hierarchical versus partitioning clustering. In partitioning clustering the dataset is divided into clusters, whereas in hierarchical clustering each cluster may have sub-clusters, thus forming a tree which leaves are single points of the dataset.
- (ii) Hard versus soft and fuzzy clustering. In hard clustering each data point is assigned to single cluster, versus a soft clustering where each point may be assigned to more than one cluster, hence clusters may overlap. In fuzzy clustering for each point there is a distribution that describes the probability of a point to be part of a certain cluster.
- (iii) Complete versus partial clustering. In complete clustering all points in the dataset are assigned to clusters, whereas in partial clustering some points may be intentionally skipped and are not being assigned to a cluster.

Finding the optimal partition of a fixed number of clusters for some given dataset is known to be an NP-hard problem (see [12]), and hence cannot be solved efficiently. Most algorithms seek to minimize certain objective function, and usually achieve local rather than global minimum solution.

In this work we focus on partitioning clustering, where the number of clusters is known in advance. Most partitioning clustering methods iteratively update the cluster centers, and hence they are often referred as center-based clustering methods.

We introduce few notations for the upcoming discussion. Let $\mathcal{A} = \{a^1, a^2, \dots, a^m\}$ be a given set of points in \mathbb{R}^n , and let $1 < k < m$ be a fixed given number of clusters. The clustering problem consists of partitioning the dataset \mathcal{A} into k subsets $\{C^1, C^2, \dots, C^k\}$, called clusters. For each $l = 1, 2, \dots, k$, the cluster C^l is represented by its center $x^l \in \mathbb{R}^n$. We describe few well-known center-based clustering algorithms.

- (i) The k-means algorithm. This algorithm is probably the most famous within the clustering scope, and dates back to Steinhaus (1956), MacQueen (1967) and Lloyd (1982) (see [20, 16, 15]). The k-means algorithm partitions the data into k sets. The solution is then a set of k centers, each of which is located at the centroid of the data for which it is the closest center. The k-means algorithm performs hard clustering, and each point is labeled according to its

closest center. This algorithm can be described as an optimization algorithm (see precise details below) which minimizes the following objective function

$$f_{KM}(x^1, x^2, \dots, x^k) = \sum_{i=1}^m \min_{1 \leq l \leq k} \|a^i - x^l\|^2.$$

The simplicity of the algorithm both in the updating rules and the implementation aspects made it very popular. There has been enormous improved techniques designed targeting a variety of applications (see [13] for a review).

- (ii) The fuzzy k-means (FKM) algorithm. The FKM algorithm is a soft clustering method. For each data point the result of the FKM algorithm is a distribution of membership over the clusters (see [6] for the original paper by Bezdek on FKM). The objective function that the FKM algorithm minimizes is

$$f_{FKM}(w^1, w^2, \dots, w^m, x^1, x^2, \dots, x^k) = \sum_{i=1}^m \sum_{l=1}^k (w_l^i)^\beta \|a^i - x^l\|^2.$$

The variable w_l^i denotes the probability that data point a^i is assigned to cluster x^l , thus it is under the constraints $\sum_{l=1}^k w_l^i = 1$ for all $1 \leq i \leq m$ and $w_l^i \geq 0$. The parameter $\beta > 1$ governs the "fuzzy partition". Setting $\beta = 1$ results in the standard k-means algorithm (see Section 2.1 for more details). The FKM algorithm is the Gauss-Seidel method applied to f_{FKM} , that is, keeping (x^1, x^2, \dots, x^k) fixed and minimizing with respect to (w^1, w^2, \dots, w^m) , and then vice-versa (see [11, p. 528]).

- (iii) The Expectation-Maximization (EM) algorithm. The EM algorithm (Dempster et al. [10]) is used extensively in statistical estimation problems for learning mixtures of distributions. It is a soft clustering algorithm. The objective function that EM maximizes is

$$f_{EM}(x^1, x^2, \dots, x^k) = \sum_{i=1}^m \log \left(\sum_{l=1}^k p(a^i | x^l) p(x^l) \right),$$

where $p(a^i | x^l)$ is the probability of a^i given that it is generated by the Gaussian distribution with center x^l and $p(x^l)$ is the prior probability of center x^l . The algorithm is guaranteed to converge to a local maximum of the likelihood function f_{EM} (see [23]).

An interesting paper of Teboulle [21] shows that these center-based clustering algorithms can be recovered from a certain proposed continuous optimization framework

which will be used in this work too (see more details below). The unified model presented in [21] provides an elegant and simple way to describe the models presented above and more. To tackle this model, Teboulle uses smoothing techniques which are based on approximation of an asymptotic convex nonlinear mean functions. The suggested center-based algorithm for soft clustering, the Smooth k-means (SKM) algorithm, generates a sequence whose each limit point is a stationary point of the approximated objective function.

We begin this work with the formulation of the clustering problem, used in [21], which consists of minimizing the sum of finite collection of min-functions. This is a nonsmooth and nonconvex optimization problem, in its most general case. The clustering problem is given by

$$\min_{x \in \mathbb{R}^{nk}} \left\{ F(x) := \sum_{i=1}^m \min_{1 \leq l \leq k} d(x^l, a^i) \right\}, \quad (1.1.1)$$

where $x = (x^1, x^2, \dots, x^k) \in \mathbb{R}^{nk}$ with $d(\cdot, \cdot)$ being a distance-like function.

We focus on two cases of distance-like functions. The first is the squared Euclidean norm, which is the standard proximity measure used in the k-means algorithm. For this case, we use an equivalent smooth optimization problem for the clustering problem presented in (1.1.1) and suggest a simple and efficient first order method for tackling it. We prove convergence result for the suggested algorithm via the methodology which was recently developed in [8] and will be discussed in great details below. The second distance-like function that we study is the Euclidean norm. In this case we present an approximation model, in order to overcome the lack of smoothness in the problem, introduced by the norm. Then we propose an algorithm to solve the approximated model which combines ideas which were used in the squared Euclidean case with a classical smoothing idea which was used in [3]. We present numerical experiments, that show the superiority of the Euclidean norm distance function for datasets in which the data points are spread relatively sparsely from their centers.

The lack of smoothness in the general model (1.1.1) can be overcome, yet the nonconvex nature of the clustering problem remains a major difficulty. Significant amount of studies have been made on convex models, even though in many cases the original optimization problem is nonconvex. To overcome the lack of convexity, one of the common approaches is usually achieved by considering a convex relaxation of the original problem. In this thesis we take a different route and consider the problem in its original nonconvex form. Very recently this complicated route became more relevant and interesting thanks to few papers (see [1, 2, 8] and the references

therein) which pave the way for dealing with nonconvex problems using sophisticated mathematical tools as will be detailed later in Section 2.2.

1.2 Outline and Contributions of The Thesis

Our main objectives and contributions in this thesis are as follows.

- To develop algorithms that address the clustering problem for two different distance-like functions and present numerical tests which demonstrate the effectiveness of the proposed algorithms.
- To demonstrate the usefulness of the Kurdyka-Łojasiewicz (KL) property and the general methodology developed in [8] to tackle the clustering problem. Specially, when the proximity function is taken to be the Euclidean norm the obtained optimization problem is completely nonsmooth (that is, all the involved functions are nonsmooth), thus in this thesis we first use this general methodology which combined with smoothing idea in the nonconvex setting.
- To prove the convergence of k-means to a critical point, and extend the result to a local minima, assuming the closest center to each data point is unique.

We outline now the contents of each chapter in this thesis.

- In Chapter 2 we transform the initial discrete formulation of the clustering problem (see (1.1.1)) into a smooth model. In addition, we recall the KL theory and the general methodology, which was developed in [8], that will be used in our analysis of the proposed algorithms.
- In Chapter 3 we tackle the clustering problem with the squared Euclidean norm distance-like function, which is the most common distance used in many other clustering algorithms. The proposed clustering algorithm (KPALM) is based on the alternating minimization method, and it is similar to the k-means algorithm. In this case the objective function is smooth and we can apply the general methodology, and prove convergence of the generated sequence to a critical point of the corresponding objective function. We show that the k-means algorithm can be recovered from the proposed KPALM algorithm by choosing specific parameters. In addition, we prove that k-means algorithm convergence to a critical point, and under additional assumption, we extend the convergence to a local minimum.

- In Chapter 4 we study the clustering problem with the Euclidean norm distance-like function and propose an iterative algorithm (ε -KPALM) to tackle a smoothed approximation model. We provide an approximation to the original objective function which overcome the lack of smoothness and then proceed with the general methodology and prove again convergence of the generated sequence to a critical point of the approximated smooth objective function.
- In Chapter 5 we illustrate the performance of the proposed algorithms, and compare them with some existing center-based clustering algorithms.

1.3 Notation and Terminology

The following notations will be used throughout this thesis

Table 1.1: Table of Notations

\mathcal{A}	dataset for clustering of size m
k	the number of clusters
x^l	center of cluster l , for each $l = 1, 2, \dots, k$; $x = (x^1, x^2, \dots, x^k)$
$\langle \cdot, \cdot \rangle$	the standard dot product in Euclidean space, that is $\langle u, v \rangle = \sum_{i=1}^d u_i v_i$
$\ \cdot\ $	Euclidean norm $\ x\ = \sqrt{\sum_{l=1}^d x_l^2}$, for any $x \in \mathbb{R}^d$
Δ	the simplex i.e., $\Delta = \left\{ u \in \mathbb{R}^d : \sum_{l=1}^d u_l = 1, u_l \geq 0 \right\}$
$\delta_S(\cdot)$	indicator function of a set $S \subset \mathbb{R}^d$, which is defined to be 0 in S and ∞ otherwise
$\text{dom}\sigma$	effective domain of the function σ , i.e., $\text{dom}\sigma := \{v \in \mathbb{R}^d : \sigma(v) < \infty\}$
$\partial\sigma$	subdifferential of the function σ (see Definition 2.2.1)
$\text{crit}\sigma$	set of all critical points of function σ , that is all vectors v such that $0 \in \partial\sigma(v)$
$\text{dist}(u, S)$	distance function, for any point $u \in \mathbb{R}^d$ and set $S \subset \mathbb{R}^d$, $\text{dist}(u, S) := \inf \{\ u - v\ : v \in S\}$
$H(w, x)$	sum of distances of x^l from each data point in \mathcal{A} , adjusted with the non-negative weights w^i , $H(w, x) = \sum_{i=1}^m \sum_{l=1}^k w_l^i d(x^l, a^i)$
$G(w)$	sum of indicator functions which constraints each w^i to be in the simplex, that is $G(w) = \sum_{i=1}^m \delta_{\Delta}(w^i)$
σ	the objective function in the clustering problem, defined by $\sigma(w, x) = H(w, x) + G(w)$

Chapter 2

Problem Reformulation and Mathematical Tools

Transforming the initial clustering problem given in (1.1.1) into a smooth form is the first main objective of this chapter. The second objective is to present the necessary mathematical background, including the general methodology developed in [8], that enables to analyze algorithms in the nonconvex and nonsmooth setting.

2.1 Reformulation of the Clustering Problem

We begin with a reformulation of the clustering problem which will be the basis for our developments in this work. The reformulation is based on the following fact:

$$\min_{1 \leq l \leq k} u_l = \min \{ \langle u, w \rangle : w \in \Delta \}, \quad (2.1.1)$$

where Δ denotes the well-known simplex defined by

$$\Delta = \left\{ w \in \mathbb{R}^k : \sum_{l=1}^k w_l = 1, w \geq 0 \right\}.$$

Note that the optimal solution, $w^* \in \Delta$, for (2.1.1) is given by

$$w_l^* = \begin{cases} 1 & u_l \text{ is the minimal component in } u, \\ 0 & \text{otherwise.} \end{cases} \quad (2.1.2)$$

Using this fact in Problem (1.1.1) and introducing new variables $w^i \in \mathbb{R}^k$, $i = 1, 2, \dots, m$, gives the equivalent reformulation of the clustering problem

$$\min_{x \in \mathbb{R}^{nk}} \sum_{i=1}^m \min_{w^i \in \Delta} \langle w^i, d^i(x) \rangle, \quad (2.1.3)$$

where

$$d^i(x) = (d(x^1, a^i), d(x^2, a^i), \dots, d(x^k, a^i)) \in \mathbb{R}^k, \quad i = 1, 2, \dots, m. \quad (2.1.4)$$

Replacing further the constraint $w^i \in \Delta$ by adding the indicator function $\delta_\Delta(\cdot)$, which is defined to be 0 in Δ and ∞ otherwise, to the objective function, results in an equivalent formulation

$$\min_{x \in \mathbb{R}^{nk}, w \in \mathbb{R}^{km}} \left\{ \sum_{i=1}^m (\langle w^i, d^i(x) \rangle + \delta_\Delta(w^i)) \right\}, \quad (2.1.5)$$

where $w = (w^1, w^2, \dots, w^m) \in \mathbb{R}^{km}$. Finally, for the simplicity of the yet to come expositions, we define the following functions

$$H(w, x) := \sum_{i=1}^m H^i(w, x) = \sum_{i=1}^m \langle w^i, d^i(x) \rangle \quad \text{and} \quad G(w) = \sum_{i=1}^m G^i(w^i) := \sum_{i=1}^m \delta_\Delta(w^i).$$

Replacing the terms in Problem (2.1.5) with the functions defined above gives a compact equivalent form of the original clustering problem

$$\min \{ \sigma(z) := H(w, x) + G(w) \mid z := (w, x) \in \mathbb{R}^{km} \times \mathbb{R}^{nk} \}. \quad (2.1.6)$$

Note in particular that when $d(\cdot)$ is smooth, then so is $H(\cdot, \cdot)$, a fact which will be exploited in Chapter 3.

2.2 Convergence Methodology

In this subsection we give a brief review of the main developments established in [8]. These developments include on one hand the proximal alternating linearized minimization (PALM) algorithm and on the other hand, a general procedure for proving global convergence of generic algorithm which will play a central role in this work. First, let us recall several definitions which are needed for the upcoming discussion.

Definition 2.2.1 (Subdifferentials). *Let $\sigma : \mathbb{R}^d \rightarrow (-\infty, +\infty]$ be a proper and lower semicontinuous function.*

- (i) For a given $x \in \text{dom } \sigma := \{x \in \mathbb{R}^d : \sigma(x) < \infty\}$, the Fréchet subdifferential of σ at x , written $\widehat{\partial}\sigma(x)$, is the set of all vectors $u \in \mathbb{R}^d$ which satisfy

$$\liminf_{y \neq x, y \rightarrow x} \frac{\sigma(y) - \sigma(x) - \langle u, y - x \rangle}{\|y - x\|} \geq 0.$$

When $x \notin \text{dom } \sigma$, we set $\widehat{\partial}\sigma(x) = \emptyset$.

- (ii) The limiting-subdifferential, or subdifferential in short, of σ at $x \in \mathbb{R}^n$, written $\partial\sigma(x)$, is defined through the following closure process

$$\partial\sigma(x) := \left\{ u \in \mathbb{R}^d : \exists x^k \rightarrow x, \sigma(x^k) \rightarrow \sigma(x) \text{ and } u^k \in \widehat{\partial}\sigma(x^k) \text{ as } k \rightarrow \infty \right\}.$$

In the nonsmooth context, as in the smooth case, the well-known Fermat's rule remains unchanged, that is, if $x \in \mathbb{R}^d$ is a local minimizer of σ then $0 \in \partial\sigma(x)$. Points whose subdifferential contains 0 are called *critical points*, and the set of all critical points of σ is denoted by $\text{crit}\sigma$.

Now we present the Kurdyka-Łojasiewicz property, which plays a central role in the general methodology which was developed in [8]. Let $\eta \in (0, +\infty]$. Denote the following class of concave functions

$$\Phi_\eta = \left\{ \varphi \in C([0, \eta], \mathbb{R}_+) : \varphi \in C^1((0, \eta)), \varphi' > 0, \varphi(0) = 0 \right\}.$$

Definition 2.2.2 (Kurdyka-Łojasiewicz property). Let $\sigma : \mathbb{R}^d \rightarrow (-\infty, +\infty]$ be proper and lower semicontinuous.

- (i) The function σ is said to have the Kurdyka-Łojasiewicz (KL) property at $\bar{u} \in \text{dom } \partial\sigma := \{u \in \mathbb{R}^d : \partial\sigma \neq \emptyset\}$ if there exist $\eta \in (0, +\infty]$, a neighborhood U of \bar{u} and a function $\varphi \in \Phi_\eta$, such that for all

$$u \in U \cap \{x \in \mathbb{R}^d : \sigma(\bar{u}) < \sigma(x) < \sigma(\bar{u}) + \eta\},$$

the following inequality holds

$$\varphi'(\sigma(u) - \sigma(\bar{u})) \text{dist}(0, \partial\sigma(u)) \geq 1,$$

where $\text{dist}(x, S) := \inf \{\|y - x\| : y \in S\}$ denotes the distance from $x \in \mathbb{R}^d$ to $S \subset \mathbb{R}^d$.

- (ii) If σ satisfy the KL property at each point of $\text{dom } \sigma$ then σ is called a KL function.

As it can be seen from the definition above, verifying that a given function satisfies the KL property is quite involved. This can be overcome by using an important result of Bolte et al. (see [7]). Before presenting this result we will recall the definition of semi-algebraic function.

Definition 2.2.3 (Semi-algebraic sets and functions). *(i) A subset $S \subset \mathbb{R}^d$ is a real semi-algebraic set if there exists a finite number of real polynomial functions $g_{ij}, h_{ij} : \mathbb{R}^d \rightarrow \mathbb{R}$ such that*

$$S = \bigcup_{j=1}^p \bigcap_{i=1}^q \{u \in \mathbb{R}^d : g_{ij} = 0 \text{ and } h_{ij}(u) < 0\}$$

(ii) A function $h : \mathbb{R}^d \rightarrow (-\infty, +\infty]$ is called semi-algebraic if its graph

$$\{(u, t) \in \mathbb{R}^{d+1} : h(u) = t\},$$

is a semi-algebraic subset of \mathbb{R}^{d+1} .

Theorem 2.2.1. *Let $\sigma : \mathbb{R}^d \rightarrow (-\infty, +\infty]$ be a proper and lower semicontinuous function. If σ is semi-algebraic then it satisfies the KL property at any point of $\text{dom}\sigma$.*

The class of semi-algebraic functions is very broad, it includes real polynomial functions, indicator functions of semi-algebraic sets, finite sums and products of semi-algebraic functions, composition of semi-algebraic functions, and many more (see [1, 2]).

Attouch et al. [1, 2] established convergence of sequences generated by the proximal Gauss-Seidel scheme in the general nonconvex and nonsmooth setting, and by the proximal-forward-backward (aka Proximal Gradient, more on this method see [14, 22, 9]) algorithm applied to the nonconvex and nonsmooth minimization of the sum of a nonsmooth function with a smooth one. This approach assumes that the objective function to be minimized satisfies the Kurdyka-Łojasiewicz (KL) property. The convergence results were further extended in the recent work by Bolte et al. [8], to the PALM algorithm which is a novel algorithm that combines the two basic and old ideas of Alternating Minimization and Proximal Gradient (see more details below). Additional contribution of [8] is the general methodology to prove convergence of a generic algorithm in the setting of nonconvex and nonsmooth optimization problems.

Equipped with these definitions, we present the general methodology that will be used several times throughout this work. Let $\sigma : \mathbb{R}^d \rightarrow (-\infty, +\infty]$ be a proper and lower semicontinuous function which is bounded from below and consider the problem

$$(P) \quad \min \{\sigma(z) : z \in \mathbb{R}^d\}.$$

Suppose that we are given a generic algorithm \mathcal{A} which generates a sequence $\{z^k\}_{k \in \mathbb{N}}$ via the following scheme:

$$z^0 \in \mathbb{R}^d, z^{k+1} \in \mathcal{A}(z^k), \quad k = 0, 1, \dots$$

The purpose of the proposed methodology is to assure the convergence of the whole sequence $\{z^k\}_{k \in \mathbb{N}}$ to a critical point of σ . The set of all limit points is denoted by $\omega(z^0)$, and defined by

$$\{\bar{z} \in \mathbb{R}^d : \exists \text{ an increasing sequence of integers } \{k_l\}_{l \in \mathbb{N}} \text{ such that } z^{k_l} \rightarrow \bar{z} \text{ as } l \rightarrow \infty\}.$$

Definition 2.2.4. Let $\sigma : \mathbb{R}^d \rightarrow (-\infty, +\infty]$ be a proper and lower semicontinuous function. A sequence $\{z^k\}_{k \in \mathbb{N}}$ is called a *gradient-like descent sequence* for σ if for all $k \in \mathbb{N}$ the following two conditions hold:

(C1) *Sufficient decrease property:* There exists a positive scalar ρ_1 such that

$$\rho_1 \|z^{k+1} - z^k\|^2 \leq \sigma(z^k) - \sigma(z^{k+1}).$$

(C2) *A subgradient lower bound for the iterates gap:*

- $\{z^k\}_{k \in \mathbb{N}}$ is bounded.
- There exists a positive scalar ρ_2 such that

$$\|w^{k+1}\| \leq \rho_2 \|z^{k+1} - z^k\|, \quad w^{k+1} \in \partial\sigma(z^{k+1}).$$

The two conditions (C1) and (C2) defining a gradient-like descent sequence for a given σ are typical for any descent type algorithm, and provide the basic tools to prove that the limit of any convergent subsequence of $\{z^k\}_{k \in \mathbb{N}}$ is a critical point of σ . More precisely, from [8, Lemma 5, p. 476] we have the following result.

Lemma 2.2.1. If $\{z^k\}_{k \in \mathbb{N}}$ is a gradient-like descent sequence for a given function σ , which is lower semicontinuous and proper on \mathbb{R}^d , then $\omega(z^0)$ is a nonempty, compact and connected set, and we have

$$\lim_{k \rightarrow \infty} \text{dist}(z^k, \omega(z^0)) = 0.$$

This result can thus be applied to any algorithm that produces a gradient-like descent to establish convergence to accumulation points. The main goal is to establish global convergence, i.e., that the whole sequence converges to a critical point of σ . This can be achieved by imposing an additional assumption on the class of functions σ : it must satisfy the Kurdyka-Lojasiewicz property.

As proven in [8], relying on a key uniformization of the KL property it is possible to establish global convergence of any gradient-like descent sequence $\{z^k\}_{k \in \mathbb{N}}$, independently of the algorithm used. Verifying the KL property of a given function might often be a difficult task. However, thanks to a Theorem 2.2.1, any proper and lower semicontinuous function σ which is semi-algebraic satisfies the KL property at any point in $\text{dom}\sigma$. We summarize the general methodology and convergence results of [8] in the following abstract convergence result.

Theorem 2.2.2. *Let $\sigma : \mathbb{R}^d \rightarrow (-\infty, \infty]$ be a proper, lower semicontinuous and semi-algebraic function with $\inf \sigma > -\infty$, and assume that $\{z^k\}_{k \in \mathbb{N}}$ is a gradient-like descent sequence for σ . If $\omega(z^0) \subset \text{crit}(\sigma)$ then the sequence $\{z^k\}_{k \in \mathbb{N}}$ converges to a critical point z^* of σ .*

Remark 2.2.1. *Under the premises of this theorem, it is also possible to derive a rate of convergence result for the sequence $\{z^k\}_{k \in \mathbb{N}}$ of the form $\|z^k - z^*\| \leq Ck^{-\gamma}$, for some positive constant C and where $\gamma > 0$ is the so-called KL exponent, see [8].*

Finally, we present the Proximal Alternating Linearized Minimization (PALM) algorithm which solves the nonconvex and nonsmooth minimization problems of the following form

$$(M) \quad \text{minimize } \sigma(x, y) := f(x) + g(y) + H(x, y) \text{ over all } (x, y) \in \mathbb{R}^n \times \mathbb{R}^m,$$

where $f : \mathbb{R}^n \rightarrow (-\infty, +\infty]$ and $g : \mathbb{R}^m \rightarrow (-\infty, +\infty]$ are proper and lower semicontinuous functions while $H : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ is a C^1 function. In addition, partial gradients of H are Lipschitz continuous, namely, $H(\cdot, y) \in C_{L_1(y)}^{1,1}$ and $H(x, \cdot) \in C_{L_2(x)}^{1,1}$.

As mentioned in [8] the PALM algorithm is nothing but alternating the classical proximal gradient over the two blocks (x, y) . This leads towards the following approximations

$$\widehat{\sigma}(x, y^k) = \langle x - x^k, \nabla_x H(x^k, y^k) \rangle + \frac{c_k}{2} \|x - x^k\|^2 + f(x), \quad (c_k > 0),$$

and

$$\widetilde{\sigma}(x^{k+1}, y) = \langle y - y^k, \nabla_y H(x^{k+1}, y^k) \rangle + \frac{d_k}{2} \|y - y^k\|^2 + g(y), \quad (d_k > 0).$$

Thus, PALM can be summarized as follows: It generates the sequence $z^k := (x^k, y^k)$ via the iterations:

$$x^{k+1} \in \text{argmin} \{ \widehat{\sigma}(x, y^k) : x \in \mathbb{R}^n \} \quad \text{and} \quad y^{k+1} \in \text{argmin} \{ \widetilde{\sigma}(x^{k+1}, y) : y \in \mathbb{R}^m \}.$$

Assuming σ is KL function and the generated sequence by PALM, $\{(x^k, y^k)\}_{k \in \mathbb{N}}$, is bounded, Bolte et al. [8] proved that the sequence is a gradient-like descent sequence, and thus it converges to a critical point of σ .

Chapter 3

Clustering with the Squared Euclidean Norm

We develop an algorithm, called KPALM, for the clustering problem given in (2.1.6) with squared Euclidean distance-like function. We show that the acquired model is a sum of smooth and nonsmooth function, therefore it motivates us to apply the PALM idea and the convergence methodology described in Section 2.2. We prove that the generated sequence converges to a critical point of the objective function σ of the clustering problem (see (2.1.6)). We show that the k-means algorithm is a special case of KPALM algorithm and can be recovered from the developed framework, however, the convergence analysis can not be used for the k-means algorithm. Therefore, we prove the convergence of k-means to critical point, separately by using again the general methodology of Section 2.2. Assuming the uniqueness of labeling in the output of the k-means algorithm we improve the convergence result to local minimum.

3.1 Clustering with PALM

In this section we tackle the clustering problem, given in (2.1.6), for which the proximity function $d(\cdot, \cdot)$ is taken to be the classical distance function defined by $d(u, v) = \|u - v\|^2$. We devise a PALM-like algorithm, based on the discussion in the previous section. Since the clustering problem has specific structure, we are ought to exploit it in the following manner.

- (1) The function $w \mapsto H(w, x)$, for fixed x , is linear and therefore there is no need

to linearize it as suggested in the framework which was discussed in Section 2.2.

- (2) The function $x \mapsto H(w, x)$, for fixed w , is quadratic and convex. Hence, there is no need to add a proximal term as suggested in the framework of PALM.

As in the PALM algorithm, our algorithm is based on the old approach of Alternating Minimization, with the following adaptations which are motivated by the observations mentioned above. More precisely, with respect to w we suggest to regularize the first subproblem with proximal term as follows

$$w^i(t+1) = \arg \min_{w^i \in \Delta} \left\{ \langle w^i, d^i(x(t)) \rangle + \frac{\alpha_i(t)}{2} \|w^i - w^i(t)\|^2 \right\}, \quad i = 1, 2, \dots, m, \quad (3.1.1)$$

where $\alpha_i(t) > 0$ for all $i = 1, 2, \dots, m$. On the other hand, with respect to x we perform exact minimization, that is,

$$x(t+1) = \operatorname{argmin} \{ H(w(t+1), x) \mid x \in \mathbb{R}^{nk} \}. \quad (3.1.2)$$

It is easy to check that all subproblems, with respect to w^i , $i = 1, 2, \dots, m$, and x , can be rewritten explicitly (where we use P_Δ for the orthogonal projection onto the set Δ). Thus, we can present now the KPALM algorithm.

KPALM

(1) Initialization: $(w(0), x(0)) \in \Delta^m \times \mathbb{R}^{nk}$.

(2) General step ($t = 0, 1, \dots$):

(2.1) Cluster assignment: choose certain $\alpha_i(t) > 0$, $i = 1, 2, \dots, m$, and compute

$$w^i(t+1) = P_\Delta \left(w^i(t) - \frac{d^i(x(t))}{\alpha_i(t)} \right). \quad (3.1.3)$$

(2.2) Center update: for each $l = 1, 2, \dots, k$ compute

$$x^l(t+1) = \frac{\sum_{i=1}^m w_l^i(t+1) a^i}{\sum_{i=1}^m w_l^i(t+1)}. \quad (3.1.4)$$

We begin our analysis of the KPALM algorithm with the following boundedness property of the generated sequence. For simplicity, from now on, we denote $z(t) := (w(t), x(t))$, $t \in \mathbb{N}$.

Proposition 3.1.1 (Boundedness of KPALM sequence). *Let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by KPALM. Then, the following statements hold true.*

- (i) *For all $l = 1, 2, \dots, k$, the sequence $\{x^l(t)\}_{t \in \mathbb{N}}$ is contained in $\text{Conv}(\mathcal{A})$, the convex hull of \mathcal{A} , and therefore bounded by $M = \max_{1 \leq i \leq m} \|a^i\|$.*
- (ii) *The sequence $\{z(t)\}_{t \in \mathbb{N}}$ is bounded in $\mathbb{R}^{km} \times \mathbb{R}^{nk}$.*

Proof. (i) Let $1 \leq l \leq k$. We set $\lambda_i = w_l^i(t) / \sum_{j=1}^m w_l^j(t)$, $i = 1, 2, \dots, m$, then $\lambda_i \geq 0$ and $\sum_{i=1}^m \lambda_i = 1$. From (3.1.4) we have

$$x^l(t) = \frac{\sum_{i=1}^m w_l^i(t) a^i}{\sum_{i=1}^m w_l^i(t)} = \sum_{i=1}^m \left(\frac{w_l^i(t)}{\sum_{j=1}^m w_l^j(t)} \right) a^i = \sum_{i=1}^m \lambda_i a^i \in \text{Conv}(\mathcal{A}), \quad (3.1.5)$$

which proves that $x^l(t)$ is in the convex hull of \mathcal{A} , for all $l = 1, 2, \dots, k$ and $t \in \mathbb{N}$. Taking the norm of $x^l(t)$ and using (3.1.5) yields that

$$\|x^l(t)\| = \left\| \sum_{i=1}^m \lambda_i a^i \right\| \leq \sum_{i=1}^m \lambda_i \|a^i\| \leq \sum_{i=1}^m \lambda_i \max_{1 \leq i \leq m} \|a^i\| = M.$$

- (ii) The sequence $\{w(t)\}_{t \in \mathbb{N}}$ is bounded, since $w^i(t) \in \Delta$ for all $i = 1, 2, \dots, m$ and $t \in \mathbb{N}$. Combined with the previous item, the result follows. □

The following assumption will be crucial for the coming analysis.

Assumption 3.1.1. (i) *For all $1 \leq i \leq m$, the chosen sequence of parameters $\{\alpha_i(t)\}_{t \in \mathbb{N}}$ is bounded, that is, there exist $\underline{\alpha}_i > 0$ and $\overline{\alpha}_i < \infty$ such that*

$$\underline{\alpha}_i \leq \alpha_i(t) \leq \overline{\alpha}_i, \quad \forall t \in \mathbb{N}. \quad (3.1.6)$$

- (ii) *For all $t \in \mathbb{N}$ there exists $\underline{\beta} > 0$ such that*

$$2 \min_{1 \leq l \leq k} \sum_{i=1}^m w_l^i(t) := \beta(w(t)) \geq \underline{\beta}. \quad (3.1.7)$$

It should be noted that Assumption 3.1.1(i) is very mild since the parameters $\alpha_i(t)$, for $1 \leq i \leq m$ and $t \in \mathbb{N}$, can be chosen arbitrarily by the user and therefore it can be controlled such that the boundedness property holds true. Assumption 3.1.1(ii) is essential since if it is not true then $w_i^i(t) = 0$ for all $1 \leq i \leq m$, which means that the center x^l does not play any role in the solution process which is, of course, a meaningless situation.

Lemma 3.1.1 (Strong convexity of $H(w, x)$ in x). *The function $x \mapsto H(w, x)$ is strongly convex with parameter $\beta(w)$ which defined in (3.1.7), whenever $\beta(w) > 0$.*

Proof. Since the function $x \mapsto H(w, x) = \sum_{l=1}^k \sum_{i=1}^m w_l^i \|x^l - a^i\|^2$ is C^2 , it is strongly convex if and only if the smallest eigenvalue of the corresponding Hessian matrix is positive. Indeed, the Hessian is given by

$$\nabla_{x^j} \nabla_{x^l} H(w, x) = \begin{cases} 0 & \text{if } j \neq l, \quad 1 \leq j, l \leq k, \\ 2 \sum_{i=1}^m w_l^i & \text{if } j = l, \quad 1 \leq j, l \leq k. \end{cases}$$

Since the Hessian is a diagonal matrix, the smallest eigenvalue is $\beta(w) = 2 \min_{1 \leq l \leq k} \sum_{i=1}^m w_l^i$, and the result follows. \square

Now we are ready to prove global convergence of the sequence $\{z(t)\}_{t \in \mathbb{N}}$ generated by KPALM to a critical point of σ given in (2.1.6). We will follow here the general procedure which was discussed in Section 2.2. Therefore we need to prove that $\{z(t)\}_{t \in \mathbb{N}}$ is a gradient-like descent sequence (see Definition 2.2.4), that is, that conditions (C1) and (C2) hold. We begin by proving condition (C1).

Proposition 3.1.2 (Sufficient decrease property). *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by KPALM. Then there exists $\rho_1 > 0$ such that*

$$\rho_1 \|z(t+1) - z(t)\|^2 \leq \sigma(z(t)) - \sigma(z(t+1)), \quad \forall t \in \mathbb{N}.$$

Proof. From step (3.1.3), see also (3.1.1), we derive, for each $i = 1, 2, \dots, m$, the

following inequality

$$\begin{aligned}
H^i(w(t+1), x(t)) + \frac{\alpha_i(t)}{2} \|w^i(t+1) - w^i(t)\|^2 &= \\
&= \langle w^i(t+1), d^i(x(t)) \rangle + \frac{\alpha_i(t)}{2} \|w^i(t+1) - w^i(t)\|^2 \\
&\leq \langle w^i(t), d^i(x(t)) \rangle + \frac{\alpha_i(t)}{2} \|w^i(t) - w^i(t)\|^2 \\
&= \langle w^i(t), d^i(x(t)) \rangle \\
&= H^i(w(t), x(t)).
\end{aligned}$$

Hence, we obtain for all $t \in \mathbb{N}$, that

$$\frac{\alpha_i(t)}{2} \|w^i(t+1) - w^i(t)\|^2 \leq H^i(w(t), x(t)) - H^i(w(t+1), x(t)). \quad (3.1.8)$$

Denote $\underline{\alpha} = \min_{1 \leq i \leq m} \underline{\alpha}_i$. Summing inequality (3.1.8) over $i = 1, 2, \dots, m$ yields

$$\begin{aligned}
\frac{\underline{\alpha}}{2} \|w(t+1) - w(t)\|^2 &= \frac{\underline{\alpha}}{2} \sum_{i=1}^m \|w^i(t+1) - w^i(t)\|^2 \\
&\leq \sum_{i=1}^m \frac{\alpha_i(t)}{2} \|w^i(t+1) - w^i(t)\|^2 \\
&\leq \sum_{i=1}^m [H^i(w(t), x(t)) - H^i(w(t+1), x(t))] \\
&= H(w(t), x(t)) - H(w(t+1), x(t)), \quad (3.1.9)
\end{aligned}$$

where the first inequality follows from Assumption 3.1.1(i) and the definition of $\underline{\alpha}$.

From Assumption 3.1.1(ii) we have that $\beta(w(t)) \geq \underline{\beta}$, for all $t \in \mathbb{N}$, and from Lemma 3.1.1 it follows that the function $x \mapsto H(w(t), x)$ is strongly convex with parameter $\beta(w(t))$. Using the strong convexity of H yields

$$\begin{aligned}
H(w(t+1), x(t)) - H(w(t+1), x(t+1)) &\geq \langle \nabla_x H(w(t+1), x(t+1)), x(t) - x(t+1) \rangle \\
&\quad + \frac{\beta(w(t))}{2} \|x(t) - x(t+1)\|^2 \\
&= \frac{\beta(w(t))}{2} \|x(t+1) - x(t)\|^2 \\
&\geq \frac{\underline{\beta}}{2} \|x(t+1) - x(t)\|^2, \quad (3.1.10)
\end{aligned}$$

where the equality follows from (3.1.2), since $\nabla_x H(w(t+1), x(t+1)) = 0$. Set

$\rho_1 = \frac{1}{2} \min \{\underline{\alpha}, \underline{\beta}\}$, by combining (3.1.9) and (3.1.10), we get

$$\begin{aligned}
\rho_1 \|z(t+1) - z(t)\|^2 &= \rho_1 (\|w(t+1) - w(t)\|^2 + \|x(t+1) - x(t)\|^2) \\
&\leq [H(w(t), x(t)) - H(w(t+1), x(t))] \\
&\quad + [H(w(t+1), x(t)) - H(w(t+1), x(t+1))] \\
&= H(z(t)) - H(z(t+1)) \\
&= \sigma(z(t)) - \sigma(z(t+1)),
\end{aligned}$$

where the last equality follows from the fact that $G(w(t)) = 0$, since $w(t) \in \Delta^m$ for all $t \in \mathbb{N}$, and therefore $H(z(t)) = \sigma(z(t))$, $t \in \mathbb{N}$. This proves the desired result. \square

Now, we are focusing on proving condition (C2). For that purpose we first need the following technical result.

Lemma 3.1.2. *Let $1 \leq i \leq m$, and let $d^i : \mathbb{R}^{nk} \rightarrow \mathbb{R}^k$ be the mapping given by*

$$d^i(x) = (d(x^1, a^i), d(x^2, a^i), \dots, d(x^k, a^i)).$$

Then for any $x, y \in \mathbb{R}^{nk}$ such that $x^l, y^l \in \text{Conv}(\mathcal{A})$ for all $l = 1, 2, \dots, k$, the following inequality holds true

$$\|d^i(x) - d^i(y)\| \leq 4M \|x - y\|,$$

where $M = \max_{1 \leq i \leq m} \|a^i\|$.

Proof. Since $d(u, v) = \|u - v\|^2$, we get that

$$\begin{aligned}
\|d^i(x) - d^i(y)\| &= \left[\sum_{l=1}^k \left| \|x^l - a^i\|^2 - \|y^l - a^i\|^2 \right|^2 \right]^{\frac{1}{2}} \\
&= \left[\sum_{l=1}^k \left| \|x^l\|^2 - 2\langle x^l, a^i \rangle + \|a^i\|^2 - \|y^l\|^2 + 2\langle y^l, a^i \rangle - \|a^i\|^2 \right|^2 \right]^{\frac{1}{2}} \\
&\leq \left[\sum_{l=1}^k \left(\left| \|x^l\|^2 - \|y^l\|^2 \right| + 2|\langle y^l - x^l, a^i \rangle| \right)^2 \right]^{\frac{1}{2}} \\
&\leq \left[\sum_{l=1}^k \left((\|x^l\| - \|y^l\|) \cdot (\|x^l\| + \|y^l\|) + 2\|y^l - x^l\| \cdot \|a^i\| \right)^2 \right]^{\frac{1}{2}} \\
&\leq \left[\sum_{l=1}^k \left(\|x^l - y^l\| \cdot 2M + 2\|x^l - y^l\| \cdot M \right)^2 \right]^{\frac{1}{2}} \\
&= \left[16M^2 \sum_{l=1}^k \|x^l - y^l\|^2 \right]^{\frac{1}{2}} \\
&= 4M \|x - y\|,
\end{aligned}$$

where the last inequality follows from the fact that $x^l, y^l \in \text{Conv}(\mathcal{A})$ and hence $\|x^l\|, \|y^l\| \leq M$ for all $l = 1, 2, \dots, k$. This proves the desired result. \square

Now, using this result we can show that $\{z(t)\}_{t \in \mathbb{N}}$ satisfies condition (C2). It is important to note that in this case the boundedness of the generated sequence is obtained (see Proposition 3.1.1(ii)) and not needed to be assumed.

Proposition 3.1.3 (Subgradient lower bound for the iterates gap). *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by KPALM. For each $t \in \mathbb{N}$ define*

$$\gamma(t) := \left((d^i(x(t)) - d^i(x(t-1)) - \alpha_i(t-1)(w^i(t) - w^i(t-1)))_{i=1,2,\dots,m}, \mathbf{0} \right).$$

Then $\gamma(t) \in \partial\sigma(z(t))$ and there exists $\rho_2 > 0$ such that

$$\|\gamma(t+1)\| \leq \rho_2 \|z(t+1) - z(t)\|, \quad \forall t \in \mathbb{N}.$$

Proof. By the definition of σ (see (2.1.6)) we get

$$\partial\sigma = \nabla H + \partial G = \left((\nabla_{w^i} H^i + \partial_{w^i} \delta_\Delta)_{i=1,2,\dots,m}, \nabla_x H \right).$$

Evaluating the last relation at $z(t+1)$ yields

$$\begin{aligned} \partial\sigma(z(t+1)) &= \left((\nabla_{w^i} H^i(w(t+1), x(t+1)) + \partial_{w^i} \delta_\Delta(w^i(t+1)))_{i=1,2,\dots,m}, \right. \\ &\quad \left. \nabla_x H(w(t+1), x(t+1)) \right) \\ &= \left((d^i(x(t+1)) + \partial_{w^i} \delta_\Delta(w^i(t+1)))_{i=1,2,\dots,m}, \right. \\ &\quad \left. \nabla_x H(w(t+1), x(t+1)) \right) \\ &= \left((d^i(x(t+1)) + \partial_{w^i} \delta_\Delta(w^i(t+1)))_{i=1,2,\dots,m}, \mathbf{0} \right), \end{aligned} \quad (3.1.11)$$

where the last equality follows from (3.1.2), that is, the optimality condition of $x(t+1)$.

The optimality condition of $w^i(t+1)$ which derived from (3.1.1), yields that for all $i = 1, 2, \dots, m$ there exists $u^i(t+1) \in \partial\delta_\Delta(w^i(t+1))$ such that

$$d^i(x(t)) + \alpha_i(t) (w^i(t+1) - w^i(t)) + u^i(t+1) = \mathbf{0}. \quad (3.1.12)$$

Setting $\gamma(t+1) := \left((d^i(x(t+1)) + u^i(t+1))_{i=1,2,\dots,m}, \mathbf{0} \right)$, it follows from (3.1.11) that $\gamma(t+1) \in \partial\sigma(z(t+1))$. Using (3.1.12) we obtain

$$\gamma(t+1) = \left((d^i(x(t+1)) - d^i(x(t)) - \alpha_i(t)(w^i(t+1) - w^i(t)))_{i=1,2,\dots,m}, \mathbf{0} \right).$$

Hence, by defining $\bar{\alpha} = \max_{1 \leq i \leq m} \bar{\alpha}_i$, we obtain

$$\begin{aligned}
\|\gamma(t+1)\| &\leq \sum_{i=1}^m \|d^i(x(t+1)) - d^i(x(t)) - \alpha_i(t)(w^i(t+1) - w^i(t))\| \\
&\leq \sum_{i=1}^m \|d^i(x(t+1)) - d^i(x(t))\| + \sum_{i=1}^m \alpha_i(t) \|w^i(t+1) - w^i(t)\| \\
&\leq \sum_{i=1}^m 4M \|x(t+1) - x(t)\| + \bar{\alpha} \sqrt{m} \|w(t+1) - w(t)\| \\
&\leq (4Mm + \bar{\alpha} \sqrt{m}) \|z(t+1) - z(t)\|,
\end{aligned}$$

where the third inequality follows from Lemma 3.1.2 and the fact that $x^l(t) \in \text{Conv}(\mathcal{A})$ for all $l = 1, 2, \dots, k$ and $t \in \mathbb{N}$ (see Proposition 3.1.1). Define $\rho_2 = 4Mm + \bar{\alpha} \sqrt{m}$, and the result follows. \square

We record our main convergence result of the KPALM algorithm in the following theorem.

Theorem 3.1.1. *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by KPALM. Then, the sequence $\{z(t)\}_{t \in \mathbb{N}}$ converges to a critical point of σ .*

Proof. Due to Propositions 3.1.2 and 3.1.3 it follows that the sequence $\{z(t)\}_{t \in \mathbb{N}}$ is a gradient-like descent sequence. The function σ is clearly a semi-algebraic function, therefore in light of Theorem 2.2.2 it is sufficient to prove that $\omega(z(0)) \subset \text{crit}(\sigma)$. Indeed, let $z^* = (w^*, x^*) \in \omega(z(0))$ be a limit point of $\{z(t)\}_{t \in \mathbb{N}} = \{(w(t), x(t))\}_{t \in \mathbb{N}}$ (such a point exists since the sequence is bounded) and let $\{(w(t_k), x(t_k))\}_{t \in \mathbb{N}}$ be a subsequence such that $(w(t_k), x(t_k)) \rightarrow (w^*, x^*)$ as $k \rightarrow \infty$. Since $w(t_k) \in \Delta^m$ for all $k \in \mathbb{N}$ and due to the closedness of Δ^m it follows that $w^* \in \Delta^m$, hence $G(w^*) = 0$. Therefore, combined with the continuity of H we obtain

$$\begin{aligned}
\lim_{k \rightarrow \infty} \sigma(w(t_k), x(t_k)) &= \lim_{k \rightarrow \infty} \{H(w(t_k), x(t_k)) + G(w(t_k))\} = \lim_{k \rightarrow \infty} H(w(t_k), x(t_k)) \\
&= H(w^*, x^*) = H(w^*, x^*) + G(w^*) = \sigma(w^*, x^*)
\end{aligned}$$

Combining $\gamma(t) \in \partial\sigma(t)$ (see Proposition 3.1.3) with the gradient-like descent property of the sequence $\{z(t)\}_{t \in \mathbb{N}}$ implies that $\gamma(t) \rightarrow \mathbf{0}$ as $t \rightarrow \infty$. Indeed, from Proposition 3.1.2 we have

$$\rho_1 \|z(t+1) - z(t)\|^2 \leq \sigma(z(t)) - \sigma(z(t+1)).$$

Hence the sequence $\{\sigma(z(t))\}_{t \in \mathbb{N}}$ is decreasing and since the sequence is also bounded it converges to some real number $\underline{\sigma}$. Therefore, we deduce that $\|z(t+1) - z(t)\| \rightarrow 0$

as $t \rightarrow \infty$. Together with Proposition 3.1.3 we obtain that $\|\gamma(t)\| \rightarrow 0$ as $t \rightarrow \infty$. The closedness property of $\partial\sigma$ implies thus that $\mathbf{0} \in \partial\sigma(w^*, x^*)$. This proves that (w^*, x^*) is a critical point of σ . \square

3.2 Convergence Analysis of k-means

The well-known k-means algorithm has close relation to KPALM algorithm, and similarly k-means alternates between cluster assignment and centers update steps as well. In detail, we can write its steps in the following manner.

k-means

(1) Initialization: $x(0) \in \mathbb{R}^{nk}$.

(2) General step ($t = 0, 1, \dots$):

(2.1) Cluster assignment: for $i = 1, 2, \dots, m$ compute

$$w^i(t+1) = \arg \min_{w^i \in \Delta} \{ \langle w^i, d^i(x(t)) \rangle \}. \quad (3.2.13)$$

(2.2) Center update: for $l = 1, 2, \dots, k$ compute

$$x^l(t+1) = \frac{\sum_{i=1}^m w_l^i(t+1) a^i}{\sum_{i=1}^m w_l^i(t+1)}. \quad (3.2.14)$$

It is easy to see that if we take in (3.1.1), $\alpha_i(t) = 0$ for all $1 \leq i \leq m$ and $t \in \mathbb{N}$, then KPALM becomes k-means. In this case, it is clear that Assumption 3.1.1(i) does not hold and therefore we can not use the convergence analysis presented before for the KPALM algorithm. We aim to use the theory described in Section 2.2 once again and show that the sequence generated by k-means converges to a critical point of σ , as defined in (2.1.6). The proof of sufficient decrease property (see Proposition 3.1.2) collapses in this case, since it is based on Assumption 3.1.1(i), that is, $\alpha_i(t) > \underline{\alpha}_i > 0$, for all $t \in \mathbb{N}$ and $i = 1, 2, \dots, m$. However, the proof of the subgradient lower bound for the iterates gap property (see Proposition 3.1.3) follows through as is. Now we will prove a sufficient decrease property for k-means. To this end we will first need the following result.

Lemma 3.2.1. *Let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by k-means. Then, there exists $c > 0$ such that*

$$\|w^i(t+1) - w^i(t)\| \leq c\|x(t+1) - x(t)\|, \quad \forall i = 1, 2, \dots, m, t \in \mathbb{N}.$$

Proof. If $x(t+1) = x(t)$ for some $t \in \mathbb{N}$ then the result is true since $w(t+1) = w(t)$. Indeed, since we are dealing with hard clustering it means that each data point a^i , $i = 1, 2, \dots, m$, is assigned to a single cluster and therefore if the centers didn't change then it implies that the clusters didn't change. Assume that $x(t+1) \neq x(t)$ at each $t \in \mathbb{N}$. At each iteration (with respect to w), k-means partitions the set \mathcal{A} into k clusters, and the center of each cluster is its mean. Since the number of the obtained partitions is finite, there exists a finite set of possible centers for all clusters. Denote by $\mathcal{C} = \{c^1, c^2, \dots, c^N\} \subset \mathbb{R}^{nk}$, the set of all different possible centers. From the center update rule (see step (3.2.14)) it is clear that $x(t) \in \mathcal{C}$ for all $t \in \mathbb{N}$. In addition, since \mathcal{C} contains N different points we can define

$$r := \min_{1 \leq i < j \leq N} \|c^i - c^j\|,$$

and obviously $r \neq 0$. By the definition of step (3.2.13) and (2.1.2) it follows that for all $t \in \mathbb{N}$ there is exactly one nonzero entry in $w^i(t)$ which equals 1. Thus, it is clear that

$$\|w^i(t+1) - w^i(t)\| \leq \sqrt{2}.$$

Since $x(t) \in \mathcal{C}$ for all $t \in \mathbb{N}$ it follows that $\|x(t+1) - x(t)\| \geq r$ and therefore

$$\|w^i(t+1) - w^i(t)\| \leq \frac{\sqrt{2}}{r} \|x(t+1) - x(t)\|,$$

and the result follows. \square

Equipped with the last lemma we can prove the sufficient decrease property of k-means.

Proposition 3.2.1 (Sufficient decrease property for k-means sequence). *Suppose that Assumption 3.1.1(ii) holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by k-means. Then, there exists $\rho_1 > 0$ such that*

$$\rho_1 \|z(t+1) - z(t)\|^2 \leq \sigma(z(t)) - \sigma(z(t+1)), \quad \forall t \in \mathbb{N}.$$

Proof. The function $x \mapsto H(w(t), x)$ remains strongly convex with parameter $\beta(w(t))$ (see (3.1.10)), hence, as obtained in Proposition 3.1.2, we have a sufficient decrease in the x variable, namely,

$$\frac{\beta}{2} \|x(t+1) - x(t)\|^2 \leq H(w(t), x(t)) - H(w(t+1), x(t+1)). \quad (3.2.15)$$

Setting $\rho_1 = \underline{\beta}(m/r^2 + 0.5)$, we can write

$$\begin{aligned}
\rho_1 \|z(t+1) - z(t)\|^2 &= \rho_1 \sum_{i=1}^m \|w^i(t+1) - w^i(t)\|^2 + \rho_1 \|x(t+1) - x(t)\|^2 \\
&\leq \rho_1 \left(1 + m \frac{2}{r^2}\right) \|x(t+1) - x(t)\|^2 \\
&\leq H(w(t), x(t)) - H(w(t+1), x(t+1)) \\
&= \sigma(z(t)) - \sigma(z(t+1))
\end{aligned}$$

where the first inequality follows from Lemma 3.2.1, the second follows from (3.2.15), and the last equality follows from the fact that $G(w(t)) = 0$, for all $t \in \mathbb{N}$. \square

In light of the preceding discussion we deduce the following convergence result.

Theorem 3.2.1 (k-means converges to critical point). *Suppose that Assumption 3.1.1(ii) holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by k-means. Then, the sequence $\{z(t)\}_{t \in \mathbb{N}}$ converges to a critical point of σ .*

Proof. Due to Propositions 3.1.3 and 3.2.1 it follows that the sequence $\{z(t)\}_{t \in \mathbb{N}}$ is a gradient-like descent sequence. The function σ is clearly a semi-algebraic function, and the proof that $\omega(z(0)) \subset \text{crit}(\sigma)$ is analogous to the one given in Theorem 3.1.1, hence Theorem 2.2.2 implies the desired result. \square

3.3 Convergence to Local Minima of k-means

In this section we present a simple and direct proof that k-means converges to local minima. We start with rewriting the k-means algorithm, in its most familiar form. It should be noted that the algorithm stops whenever all clusters do not change, i.e., $C^l(t+1) = C^l(t)$ for some $t \in \mathbb{N}$ and all $1 \leq l \leq k$.

k-means

(1) Initialization: $x(0) \in \mathbb{R}^{nk}$.

(2) General step ($t = 0, 1, \dots$):

(2.1) Cluster assignment: for $l = 1, 2, \dots, k$ compute

$$C^l(t+1) = \{a \in \mathcal{A} : \|a - x^l(t)\| \leq \|a - x^j(t)\|, \forall 1 \leq j \leq k\}. \quad (3.3.16)$$

(2.2) Center update: for $l = 1, 2, \dots, k$ compute

$$x^l(t+1) = \frac{1}{|C^l(t+1)|} \sum_{a \in C^l(t+1)} a. \quad (3.3.17)$$

As in KPALM, k-means needs Assumption 3.1.1(ii) for step (3.3.17) to be well defined. In order to prove the convergence of k-means to local minimum, we will need the additional assumption.

Assumption 3.3.1. *Suppose that k-means stops after $\tilde{t} \in \mathbb{N}$ iterations, then each $a \in \mathcal{A}$ belongs exclusively to single cluster $C^l(\tilde{t})$.*

For any $x \in \mathbb{R}^{nk}$ we denote the super-partition of \mathcal{A} with respect to x by $\overline{C}^l(x) = \{a \in \mathcal{A} \mid \|a - x^l\| \leq \|a - x^j\|, \forall j \neq l\}$, for all $1 \leq l \leq k$, and the sub-partition of \mathcal{A} by $\underline{C}^l(x) = \{a \in \mathcal{A} \mid \|a - x^l\| < \|a - x^j\|, \forall j \neq l\}$. Moreover, denote $R_{lj}(t) = \min_{a \in C^l(t)} \{\|a - x^j(t)\| - \|a - x^l(t)\|\}$ for all $1 \leq l, j \leq k$, and $r(t) = \min_{l \neq j} R_{lj}(t)$.

Due to Assumption 3.3.1 we have that $\overline{C}^l(x(\tilde{t})) = \underline{C}^l(x(\tilde{t})) = C^l(\tilde{t} + 1)$, for all $1 \leq l \leq k$, we also have that $r(\tilde{t}) > 0$.

Proposition 3.3.1. *Let $(C(\tilde{t}), x(\tilde{t}))$ be the clusters and centers k-means returns. Denote by $U = B\left(x^1(\tilde{t}), \frac{r(\tilde{t})}{2}\right) \times B\left(x^2(\tilde{t}), \frac{r(\tilde{t})}{2}\right) \times \dots \times B\left(x^k(\tilde{t}), \frac{r(\tilde{t})}{2}\right)$ an open neighbourhood of $x(\tilde{t})$. Then for any $x \in U$ we have $C^l(\tilde{t}) = \underline{C}^l(x)$ for all $1 \leq l \leq k$.*

Proof. Pick some $a \in C^l(\tilde{t})$, then $x^l(\tilde{t} - 1)$ is the closest center among the centers of $x(\tilde{t} - 1)$. Since k-means stops after \tilde{t} iterations it is clear that $x(\tilde{t}) = x(\tilde{t} - 1)$, thus $x^l(\tilde{t})$ is the closest center to a among the centers of $x(\tilde{t})$. Further we have

$$r(\tilde{t}) \leq \|x^j(\tilde{t}) - a\| - \|x^l(\tilde{t}) - a\|, \quad \forall j \neq l. \quad (3.3.18)$$

Next, we show that $a \in \underline{C}^l(x)$, indeed

$$\begin{aligned}
\|a - x^l\| - \|a - x^j\| &\leq \|a - x^l(\tilde{t})\| + \|x^l(\tilde{t}) - x^l\| - (\|a - x^j(\tilde{t})\| - \|x^j(\tilde{t}) - x^j\|) \\
&= \|a - x^l\| - \|a - x^j(\tilde{t})\| + \|x^l(\tilde{t}) - x^l\| + \|x^j(\tilde{t}) - x^j\| \\
&< \|a - x^l\| - \|a - x^j(\tilde{t})\| + r(\tilde{t}) \\
&\leq -r(\tilde{t}) + r(\tilde{t}) = 0,
\end{aligned}$$

where the second inequality holds since $x^l \in B\left(x^l(\tilde{t}), \frac{r(\tilde{t})}{2}\right)$ and $x^j \in B\left(x^j(\tilde{t}), \frac{r(\tilde{t})}{2}\right)$, and the third inequality follows from (3.3.18). This proves that $a \in C^l(x)$ and therefore $C^l(\tilde{t}) \subseteq \underline{C}^l(x)$ for all $l = 1, 2, \dots, k$. By the definition of $\underline{C}^l(x)$ we have for any $l \neq j$ that $\underline{C}^l(x) \cap \underline{C}^j(x) = \emptyset$. Now, since $C(\tilde{t})$ is a partition of \mathcal{A} , and $\underline{C}^l(x) \subset \mathcal{A}$ for all $1 \leq l \leq k$ it must hold that $C^l(\tilde{t}) = \underline{C}^l(x)$ for all $1 \leq l \leq k$. \square

Proposition 3.3.2 (k-means converges to local minimum). *Let $(C(\tilde{t}), x(\tilde{t}))$ be the clusters and centers k-means returns. Then $x(\tilde{t})$ is local minimum of F (see (1.1.1)) on $U = B\left(x^1(\tilde{t}), \frac{r(\tilde{t})}{2}\right) \times B\left(x^2(\tilde{t}), \frac{r(\tilde{t})}{2}\right) \times \dots \times B\left(x^k(\tilde{t}), \frac{r(\tilde{t})}{2}\right) \subset \mathbb{R}^{nk}$.*

Proof. The minimum of F in U is

$$\min_{x \in U} F(x) = \min_{x \in U} \sum_{l=1}^k \sum_{a \in \underline{C}^l(x)} \|a - x^l\|^2 = \min_{x \in U} \sum_{l=1}^k \sum_{a \in C^l(\tilde{t})} \|a - x^l\|^2,$$

where the last equality follows from Proposition 3.3.1.

The function $x \mapsto \sum_{l=1}^k \sum_{a \in C^l(\tilde{t})} \|a - x^l\|^2$ is strictly convex, separable in x^l for all $1 \leq l \leq k$, and reaches its minimum at $\frac{1}{|C^l(\tilde{t})|} \sum_{a \in C^l(\tilde{t})} a = x^l(\tilde{t})$, and the result follows. \square

Chapter 4

Clustering with the Euclidean Norm

We develop an algorithm for the clustering problem given in (2.1.6) with the Euclidean distance-like function. Due to the lack of smoothness in the obtained model, we can not apply directly the general methodology of Section 2.2. Therefore, we approximate the coupling function H in the objective function with a smooth function H_ε and replace the original objective function of the clustering problem, σ , with its approximation σ_ε . The proposed algorithm ε -KPALM, still performs alternation between cluster assignment and center update steps. The cluster assignment step is equivalent to the same step as in KPALM, whereas for the center update step it performs a certain gradient step with respect to H_ε . We prove that the sequence which is generated by ε -KPALM globally converges to a critical point of σ_ε .

4.1 A Smoothed Clustering Problem

In Section 2.1 (see (2.1.6)) we have formulated the clustering problem in the following equivalent form

$$\min \left\{ \sigma(z) := H(w, x) + G(w) \mid z := (w, x) \in \mathbb{R}^{km} \times \mathbb{R}^{nk} \right\},$$

where, in this setting, the involved functions are

$$H(w, x) = \sum_{i=1}^m \langle w^i, d^i(x) \rangle = \sum_{i=1}^m \sum_{l=1}^k w_l^i \|x^l - a^i\| \quad \text{and} \quad G(w) = \sum_{i=1}^m \delta_\Delta(w^i).$$

In order to be able to use the idea of PALM and the theory mentioned in Section 2.2, the coupling function $H(w, x)$ should be smooth, which is not the case here.

Therefore, for any $\varepsilon > 0$, it leads us to consider the following smoothed form of the clustering problem (motivated by [5])

$$\min \{ \sigma_\varepsilon(z) := H_\varepsilon(w, x) + G(w) \mid z := (w, x) \in \mathbb{R}^{km} \times \mathbb{R}^{nk} \}, \quad (4.1.1)$$

where

$$H_\varepsilon(w, x) = \sum_{l=1}^k H_\varepsilon^l(w, x) = \sum_{l=1}^k \sum_{i=1}^m w_l^i (\|x^l - a^i\|^2 + \varepsilon^2)^{1/2}, \quad (4.1.2)$$

and for all $i = 1, 2, \dots, m$,

$$d_\varepsilon^i(x) = \left((\|x^1 - a^i\|^2 + \varepsilon^2)^{1/2}, (\|x^2 - a^i\|^2 + \varepsilon^2)^{1/2}, \dots, (\|x^k - a^i\|^2 + \varepsilon^2)^{1/2} \right) \in \mathbb{R}^k. \quad (4.1.3)$$

Note that $\sigma_\varepsilon(z)$ is a perturbed form of $\sigma(z)$ for a small $\varepsilon > 0$, and obviously $\sigma_0(z) = \sigma(z)$. The following lemma shows that the smoothed function $H_\varepsilon(w, x)$ indeed approximates $H(w, x)$.

Lemma 4.1.1 (Closeness of smooth). *For any $(w, x) \in \Delta^m \times \mathbb{R}^{nk}$ and $\varepsilon > 0$ the following relations hold true*

$$H(w, x) \leq H_\varepsilon(w, x) \leq H(w, x) + m\varepsilon.$$

Proof. It is clear that for all $\lambda \geq 0$ we have

$$\lambda \leq \sqrt{\lambda^2 + \varepsilon^2} \leq \lambda + \varepsilon.$$

Applying this inequality with $\lambda = \|x^l - a^i\|$, yields

$$\|x^l - a^i\| \leq (\|x^l - a^i\|^2 + \varepsilon^2)^{1/2} \leq \|x^l - a^i\| + \varepsilon,$$

for all $l = 1, 2, \dots, k$ and $i = 1, 2, \dots, m$. Multiplying each inequality by w_l^i and summing over $l = 1, 2, \dots, k$ and $i = 1, 2, \dots, m$ yields

$$H(w, x) \leq H_\varepsilon(w, x) \leq H(w, x) + \sum_{i=1}^m \sum_{l=1}^k w_l^i \varepsilon.$$

Since for all $i = 1, 2, \dots, m$, $w^i \in \Delta$, the result follows. \square

Now we would like to develop an algorithm which is based on the idea of PALM (see Section 2.2) to solve Problem (4.1.1). It is easy to see that with respect to w , the objective function σ_ε keeps on the same structure as σ and therefore we apply the same step as in KPALM. More precisely, for all $i = 1, 2, \dots, m$, we have

$$\begin{aligned} w^i(t+1) &= \arg \min_{w^i \in \Delta} \left\{ \langle w^i, d_\varepsilon^i(x(t)) \rangle + \frac{\alpha_i(t)}{2} \|w^i - w^i(t)\|^2 \right\} \\ &= P_\Delta \left(w^i(t) - \frac{d_\varepsilon^i(x(t))}{\alpha_i(t)} \right), \quad \forall t \in \mathbb{N}, \end{aligned}$$

where $\alpha_i(t)$, $i = 1, 2, \dots, m$, is arbitrarily chosen. On the other hand, with respect to x we tackle the subproblem differently than in KPALM. Here we don't solve it exactly but use an approximation as in PALM, that is, linearizing the function $x \rightarrow H(w, \cdot)$, for fixed w , and adding a regularizing term

$$x^l(t+1) = \operatorname{argmin}_{x^l} \left\{ \langle x^l - x^l(t), \nabla_{x^l} H_\varepsilon(w(t+1), x(t)) \rangle + \frac{L_\varepsilon^l(w(t+1), x(t))}{2} \|x^l - x^l(t)\|^2 \right\},$$

where

$$L_\varepsilon^l(w(t+1), x(t)) := \sum_{i=1}^m \frac{w_i^l(t+1)}{(\|x^l(t) - a^i\|^2 + \varepsilon^2)^{1/2}}, \quad \forall l = 1, 2, \dots, k. \quad (4.1.4)$$

The motivation to use this specific regularizing parameter (see (4.1.4)) will be discussed later.

Now we present our algorithm for solving Problem (4.1.1), we call it ε -KPALM. The algorithm alternates between cluster assignment step, similar to KPALM, and centers update step that is based on a certain gradient step.

ε -KPALM

(1) Initialization: $(w(0), x(0)) \in \Delta^m \times \mathbb{R}^{nk}$.

(2) General step ($t = 0, 1, \dots$):

(2.1) Cluster assignment: choose certain $\alpha_i(t) > 0$, $i = 1, 2, \dots, m$, and compute

$$w^i(t+1) = P_\Delta \left(w^i(t) - \frac{d_\varepsilon^i(x(t))}{\alpha_i(t)} \right). \quad (4.1.5)$$

(2.2) Center update: for each $l = 1, 2, \dots, k$ compute

$$x^l(t+1) = x^l(t) - \frac{1}{L_\varepsilon^l(w(t+1), x(t))} \nabla_{x^l} H_\varepsilon(w(t+1), x(t)). \quad (4.1.6)$$

Remark 4.1.1. Similarly to the KPALM algorithm, the sequence generated by the ε -KPALM is also bounded, since here we also have that

$$\begin{aligned} x^l(t+1) &= x^l(t) - \frac{1}{L_\varepsilon^l(w(t+1), x(t))} \nabla_{x^l} H(w(t+1), x(t)) \\ &= x^l(t) - \frac{1}{L_\varepsilon^l(w(t+1), x(t))} \sum_{i=1}^m w_i^l(t+1) \cdot \frac{x^l(t) - a^i}{(\|x^l(t) - a^i\|^2 + \varepsilon^2)^{1/2}} \\ &= \frac{1}{L_\varepsilon^l(w(t+1), x(t))} \sum_{i=1}^m \left(\frac{w_i^l(t+1)}{(\|x^l(t) - a^i\|^2 + \varepsilon^2)^{1/2}} \right) a^i \in \operatorname{Conv}(\mathcal{A}). \end{aligned}$$

Before we will be able to analyze the algorithm and to prove the properties (see Section 2.2) needed for global convergence of the sequence $\{z(t)\}_{t \in \mathbb{N}}$ generated by ε -KPALM, we will need several auxiliary results which are motivated by the recent paper [3] (see also [4]). For the simplicity of the expositions we define the function $f_\varepsilon : \mathbb{R}^n \rightarrow \mathbb{R}$ by

$$f_\varepsilon(x) = \sum_{i=1}^m v_i (\|x - a^i\|^2 + \varepsilon^2)^{1/2}, \quad (4.1.7)$$

for fixed non-negative numbers (not all zero) $v_1, v_2, \dots, v_m \in \mathbb{R}$ and $a^i \in \mathbb{R}^n$, $i = 1, 2, \dots, m$. We also need the following auxiliary function $h_\varepsilon : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ given by

$$h_\varepsilon(x, y) = \sum_{i=1}^m \frac{v_i (\|x - a^i\|^2 + \varepsilon^2)}{(\|y - a^i\|^2 + \varepsilon^2)^{1/2}}.$$

Then it easily seen that

$$\nabla_x h_\varepsilon(y, y) = 2\nabla f_\varepsilon(y), \quad (4.1.8)$$

with

$$\nabla f_\varepsilon(y) = \sum_{i=1}^m v_i \frac{y - a^i}{(\|y - a^i\|^2 + \varepsilon^2)^{1/2}}.$$

Finally we introduce the following modulus, $L_\varepsilon : \mathbb{R}^n \rightarrow \mathbb{R}$ defined by

$$L_\varepsilon(x) = \sum_{i=1}^m \frac{v_i}{(\|x - a^i\|^2 + \varepsilon^2)^{1/2}}.$$

Lemma 4.1.2 (Properties of the auxiliary function h_ε). *The following properties of h_ε hold.*

(i) For any $y \in \mathbb{R}^n$,

$$h_\varepsilon(y, y) = f_\varepsilon(y).$$

(ii) For any $x, y \in \mathbb{R}^n$,

$$h_\varepsilon(x, y) \geq 2f_\varepsilon(x) - f_\varepsilon(y).$$

(iii) For any $x, y \in \mathbb{R}^n$,

$$f_\varepsilon(x) \leq f_\varepsilon(y) + \langle \nabla f_\varepsilon(y), x - y \rangle + \frac{L_\varepsilon(y)}{2} \|x - y\|^2.$$

Proof. (i) Follows by substituting $x = y$ in $h_\varepsilon(x, y)$.

(ii) For any two numbers $a \in \mathbb{R}$ and $b > 0$ the inequality

$$\frac{a^2}{b} \geq 2a - b,$$

holds true. Thus, for every $i = 1, 2, \dots, m$, we have that

$$\frac{\|x - a^i\|^2 + \varepsilon^2}{(\|y - a^i\|^2 + \varepsilon^2)^{1/2}} \geq 2(\|x - a^i\|^2 + \varepsilon^2)^{1/2} - (\|y - a^i\|^2 + \varepsilon^2)^{1/2}.$$

Multiplying the last inequality by v_i and summing over $i = 1, 2, \dots, m$, the results follows.

- (iii) The function $x \mapsto h_\varepsilon(x, y)$ is quadratic with associated matrix $L_\varepsilon(y)\mathbf{I}$. Therefore, its second-order Taylor expansion around y leads to the following identity

$$h_\varepsilon(x, y) = h_\varepsilon(y, y) + \langle \nabla_x h_\varepsilon(y, y), x - y \rangle + L_\varepsilon(y)\|x - y\|^2.$$

Using (i) and (ii), and the fact (cf. (4.1.8)) that $\nabla_x h_\varepsilon(y, y) = 2\nabla f_\varepsilon(y)$ yields the desired result. \square

Now we get back to the ε -KPALM algorithm and prove two technical results about the involved functions which are based on the properties obtained above.

Proposition 4.1.1 (Bounds for L_ε^l). *Let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. Then, the following two statements hold true.*

- (i) *For all $t \in \mathbb{N}$ and $l = 1, 2, \dots, k$ we have*

$$L_\varepsilon^l(w(t+1), x(t)) \geq \frac{\underline{\beta}}{(d_{\mathcal{A}}^2 + \varepsilon^2)^{1/2}},$$

where $d_{\mathcal{A}} = \text{diam}(\text{Conv}(\mathcal{A}))$ is the diameter of $\text{Conv}(\mathcal{A})$ and $\underline{\beta}$ is given in (3.1.7) (see Assumption 3.1.1(ii)).

- (ii) *For all $t \in \mathbb{N}$ and $l = 1, 2, \dots, k$ we have*

$$L_\varepsilon^l(w(t+1), x(t)) \leq \frac{m}{\varepsilon}.$$

Proof. (i) From Assumption 3.1.1(ii) and the fact that $x^l(t) \in \text{Conv}(\mathcal{A})$ for all $1 \leq l \leq k$, it follows that

$$L_\varepsilon^l(w(t+1), x(t)) = \sum_{i=1}^m \frac{w_i^l(t+1)}{(\|x^l(t) - a^i\|^2 + \varepsilon^2)^{1/2}} \geq \frac{\sum_{i=1}^m w_i^l(t+1)}{(d_{\mathcal{A}}^2 + \varepsilon^2)^{1/2}} \geq \frac{\underline{\beta}}{(d_{\mathcal{A}}^2 + \varepsilon^2)^{1/2}},$$

where the first inequality follows from the fact that $\|x^l(t) - a^i\| \leq d_{\mathcal{A}}$, for all $1 \leq l \leq k$.

(ii) Since $w(t+1) \in \Delta^m$ we have

$$L_\varepsilon^l(w(t+1), x(t)) = \sum_{i=1}^m \frac{w_l^i(t+1)}{(\|x^l(t) - a^i\|^2 + \varepsilon^2)^{1/2}} \leq \sum_{i=1}^m \frac{1}{\varepsilon} = \frac{m}{\varepsilon},$$

as asserted. □

Now we prove the following result.

Proposition 4.1.2. *Let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. Then, for all $t \in \mathbb{N}$, we have*

$$\begin{aligned} H_\varepsilon(w(t+1), x(t+1)) &\leq H_\varepsilon(w(t+1), x(t)) + \langle \nabla_x H_\varepsilon(w(t+1), x(t)), x(t+1) - x(t) \rangle \\ &\quad + \sum_{l=1}^k \frac{L_\varepsilon^l(w(t+1), x(t))}{2} \|x^l(t+1) - x^l(t)\|^2. \end{aligned}$$

Proof. By definition (see (4.1.2)) we have, for $i = 1, 2, \dots, m$, that

$$H_\varepsilon^l(w(t+1), x(t)) = f_\varepsilon(x^l(t)),$$

where in (4.1.7) we set $v_i = w_l^i(t+1)$, $i = 1, 2, \dots, m$. Therefore, by applying Lemma 4.1.2(iii) with $x = x^l(t+1)$ and $y = x^l(t)$, we get

$$\begin{aligned} H_\varepsilon^l(w(t+1), x(t+1)) &\leq H_\varepsilon^l(w(t+1), x(t)) + \langle \nabla_{x^l} H_\varepsilon^l(w(t+1), x(t)), x(t+1) - x(t) \rangle \\ &\quad + \frac{L_\varepsilon^l(w(t+1), x(t))}{2} \|x^l(t+1) - x^l(t)\|^2. \end{aligned}$$

Summing the last inequality over $l = 1, 2, \dots, k$, yields

$$\begin{aligned} H_\varepsilon(w(t+1), x(t+1)) &\leq H_\varepsilon(w(t+1), x(t)) + \sum_{l=1}^k \frac{L_\varepsilon^l(w(t+1), x(t))}{2} \|x^l(t+1) - x^l(t)\|^2 \\ &\quad + \sum_{l=1}^k \langle \nabla_{x^l} H_\varepsilon(w(t+1), x(t)), x^l(t+1) - x^l(t) \rangle. \end{aligned}$$

Replacing the last term with the following compact form

$$\sum_{l=1}^k \langle \nabla_{x^l} H_\varepsilon(w(t+1), x(t)), x^l(t+1) - x^l(t) \rangle = \langle \nabla_x H_\varepsilon(w(t+1), x(t)), x(t+1) - x(t) \rangle,$$

the result follows. □

Now we are finally ready to prove that the sequence $\{z(t)\}_{t \in \mathbb{N}}$ is a gradient-like descent sequence (see Definition 2.2.4), and that conditions (C1) and (C2) hold. This will be the main step in proving that the sequence $\{z(t)\}_{t \in \mathbb{N}}$ which is generated by ε -KPALM converges to a critical point of σ_ε .

Proposition 4.1.3 (Sufficient decrease property). *Suppose that Assumption 3.1.1 and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. Then, there exists $\rho_1 > 0$ such that*

$$\rho_1 \|z(t+1) - z(t)\|^2 \leq \sigma_\varepsilon(z(t)) - \sigma_\varepsilon(z(t+1)), \quad \forall t \in \mathbb{N}.$$

Proof. As we already mentioned, the step with respect to w of KPALM and ε -KPALM are similar in nature and therefore following the same arguments given at the beginning of the proof of Proposition 3.1.2 we can also obtain here that

$$\frac{\underline{\alpha}}{2} \|w(t+1) - w(t)\|^2 \leq H_\varepsilon(w(t), x(t)) - H_\varepsilon(w(t+1), x(t)), \quad (4.1.9)$$

where $\underline{\alpha} = \min_{1 \leq i \leq m} \alpha_i$. Applying Proposition 4.1.2 and using (4.1.6) we get for all $t \in \mathbb{N}$ that

$$\begin{aligned} H_\varepsilon(w(t+1), x(t)) - H_\varepsilon(w(t+1), x(t+1)) &\geq \\ &\geq \sum_{l=1}^k \frac{L_\varepsilon^l(w(t+1), x(t))}{2} \|x^l(t+1) - x^l(t)\|^2 \\ &\geq \frac{\underline{\beta}}{(d_{\mathcal{A}}^2 + \varepsilon^2)^{1/2}} \sum_{l=1}^k \|x^l(t+1) - x^l(t)\|^2 \\ &\geq \frac{\underline{\beta}}{(d_{\mathcal{A}}^2 + \varepsilon^2)^{1/2}} \|x(t+1) - x(t)\|^2, \end{aligned} \quad (4.1.10)$$

where the second inequality follows from Proposition 4.1.1(i).

Set $\rho_1 = \frac{1}{2} \min \left\{ \underline{\alpha}, \underline{\beta} / (d_{\mathcal{A}}^2 + \varepsilon^2)^{1/2} \right\}$. Summing (4.1.9) and (4.1.10) yields

$$\begin{aligned} \rho_1 \|z(t+1) - z(t)\|^2 &= \rho_1 (\|w(t+1) - w(t)\|^2 + \|x(t+1) - x(t)\|^2) \\ &\leq [H_\varepsilon(w(t), x(t)) - H_\varepsilon(w(t+1), x(t))] \\ &\quad + [H_\varepsilon(w(t+1), x(t)) - H_\varepsilon(w(t+1), x(t+1))] \\ &= H_\varepsilon(z(t)) - H_\varepsilon(z(t+1)) \\ &= \sigma_\varepsilon(z(t)) - \sigma_\varepsilon(z(t+1)), \end{aligned}$$

where the last equality follows from the fact that $G(w(t)) = 0$, since $w(t) \in \Delta^m$ for all $t \in \mathbb{N}$. This proves the desired result. \square

The next two lemmas will be useful in proving condition (C2), which means that there exists a subgradient of σ_ε which is bounded from above by the iterates gap of the sequence generated by ε -KPALM. The proof is motivated by the proof of [17, Theorem 2.1.5, p. 56].

Lemma 4.1.3. *For all $y, z \in \mathbb{R}^n$ the following statement holds true*

$$\|\nabla f_\varepsilon(y) - \nabla f_\varepsilon(z)\| \leq \frac{2L_\varepsilon(z)L_\varepsilon(y)}{L_\varepsilon(z) + L_\varepsilon(y)}\|z - y\|.$$

Proof. Let $z \in \mathbb{R}^n$ be a fixed vector. Define the following function

$$\tilde{f}_\varepsilon(y) = f_\varepsilon(y) - \langle \nabla f_\varepsilon(z), y \rangle,$$

hence,

$$f_\varepsilon(y) = \tilde{f}_\varepsilon(y) + \langle \nabla f_\varepsilon(z), y \rangle. \quad (4.1.11)$$

Substituting (4.1.11) into Lemma 4.1.2(iii) yields

$$\tilde{f}_\varepsilon(x) \leq \tilde{f}_\varepsilon(y) + \left\langle \nabla \tilde{f}_\varepsilon(y), x - y \right\rangle + \frac{L_\varepsilon(y)}{2}\|x - y\|^2. \quad (4.1.12)$$

It is clear that the optimal point of \tilde{f}_ε is z since $\nabla \tilde{f}_\varepsilon(z) = 0$, therefore using (4.1.12) with $x = y - (1/L_\varepsilon(y)) \nabla \tilde{f}_\varepsilon(y)$ yields

$$\begin{aligned} \tilde{f}_\varepsilon(z) &\leq \tilde{f}_\varepsilon\left(y - \frac{1}{L_\varepsilon(y)} \nabla \tilde{f}_\varepsilon(y)\right) \\ &\leq \tilde{f}_\varepsilon(y) + \left\langle \nabla \tilde{f}_\varepsilon(y), -\frac{1}{L_\varepsilon(y)} \nabla \tilde{f}_\varepsilon(y) \right\rangle + \frac{L_\varepsilon(y)}{2} \left\| \frac{1}{L_\varepsilon(y)} \nabla \tilde{f}_\varepsilon(y) \right\|^2 \\ &= \tilde{f}_\varepsilon(y) - \frac{1}{2L_\varepsilon(y)} \left\| \nabla \tilde{f}_\varepsilon(y) \right\|^2. \end{aligned}$$

Thus, using the definition of \tilde{f}_ε and the fact that $\nabla \tilde{f}_\varepsilon(y) = \nabla f_\varepsilon(y) - \nabla f_\varepsilon(z)$, yields that

$$f_\varepsilon(z) \leq f_\varepsilon(y) + \langle \nabla f_\varepsilon(z), z - y \rangle - \frac{1}{2L_\varepsilon(y)} \|\nabla f_\varepsilon(y) - \nabla f_\varepsilon(z)\|^2.$$

Now, following the same arguments we can show that

$$f_\varepsilon(y) \leq f_\varepsilon(z) + \langle \nabla f_\varepsilon(y), y - z \rangle - \frac{1}{2L_\varepsilon(z)} \|\nabla f_\varepsilon(z) - \nabla f_\varepsilon(y)\|^2.$$

Combining the last two inequalities yields that

$$\left(\frac{1}{2L_\varepsilon(z)} + \frac{1}{2L_\varepsilon(y)} \right) \|\nabla f_\varepsilon(y) - \nabla f_\varepsilon(z)\|^2 \leq \langle \nabla f_\varepsilon(z) - \nabla f_\varepsilon(y), z - y \rangle,$$

which implies,

$$\|\nabla f_\varepsilon(y) - \nabla f_\varepsilon(z)\| \leq \frac{2L_\varepsilon(z)L_\varepsilon(y)}{L_\varepsilon(z) + L_\varepsilon(y)}\|z - y\|,$$

for all $z, y \in \mathbb{R}^n$. This proves the desired result. \square

Lemma 4.1.4. *For any $x, y \in \mathbb{R}^{nk}$ such that $x^l, y^l \in \text{Conv}(\mathcal{A})$ for all $1 \leq l \leq k$ the following inequality holds*

$$\|d_\varepsilon^i(x) - d_\varepsilon^i(y)\| \leq \frac{d_{\mathcal{A}}}{\varepsilon} \|x - y\|, \quad \forall i = 1, 2, \dots, m,$$

with $d_{\mathcal{A}} = \text{diam}(\text{Conv}(\mathcal{A}))$ and $d_\varepsilon^i(\cdot)$ is defined in (4.1.3).

Proof. Define $\psi(t) = \sqrt{t + \varepsilon^2}$, for $t \geq 0$. Using the Lagrange mean value theorem over $a > b \geq 0$ yields

$$\frac{\psi(a) - \psi(b)}{a - b} = \psi'(c) = \frac{1}{2\sqrt{c + \varepsilon^2}} \leq \frac{1}{2\varepsilon},$$

where $c \in (b, a)$. Therefore, for all $i = 1, 2, \dots, m$ and $l = 1, 2, \dots, k$ we have

$$\begin{aligned} \left| (\|x^l - a^i\|^2 + \varepsilon^2)^{1/2} - (\|y^l - a^i\|^2 + \varepsilon^2)^{1/2} \right| &\leq \frac{1}{2\varepsilon} \left| \|x^l - a^i\|^2 + \varepsilon^2 - (\|y^l - a^i\|^2 + \varepsilon^2) \right| \\ &= \frac{1}{2\varepsilon} \left| \|x^l - a^i\|^2 - \|y^l - a^i\|^2 \right| \\ &= \frac{1}{2\varepsilon} \left| \|x^l - a^i\| + \|y^l - a^i\| \right| \cdot \left| \|x^l - a^i\| - \|y^l - a^i\| \right| \\ &\leq \frac{1}{\varepsilon} d_{\mathcal{A}} \|x^l - y^l\|, \end{aligned}$$

where the last inequality follows from $\|x^l - a^i\|, \|y^l - a^i\| \leq d_{\mathcal{A}}$ and the reverse triangle inequality. Therefore,

$$\begin{aligned} \|d_\varepsilon^i(x) - d_\varepsilon^i(y)\| &= \left[\sum_{l=1}^k \left| (\|x - a^i\|^2 + \varepsilon^2)^{1/2} - (\|y - a^i\|^2 + \varepsilon^2)^{1/2} \right|^2 \right]^{\frac{1}{2}} \\ &\leq \left[\sum_{l=1}^k \left(\frac{1}{\varepsilon} d_{\mathcal{A}} \|x^l - y^l\| \right)^2 \right]^{\frac{1}{2}} \\ &= \frac{d_{\mathcal{A}}}{\varepsilon} \|x - y\|, \end{aligned}$$

as asserted. □

Now we can prove condition (C2). Similarly to the case of KPLAM, also here we don't need to assume any boundedness of the generated sequence and it is obtained from the algorithm itself (see Remark 4.1.1).

Proposition 4.1.4 (Subgradient lower bound for the iterates gap). *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. For each $t \in \mathbb{N}$ define*

$$\gamma(t) := \left((d^i(x(t)) - d^i(x(t-1)) - \alpha_i(t-1)(w^i(t) - w^i(t-1)))_{i=1,2,\dots,m}, \nabla_x H_\varepsilon(z(t)) \right).$$

Then $\gamma(t) \in \partial\sigma_\varepsilon(z(t))$ and there exists $\rho_2 > 0$ such that

$$\|\gamma(t+1)\| \leq \rho_2 \|z(t+1) - z(t)\|, \quad \forall t \in \mathbb{N}.$$

Proof. Repeating the steps of the proof in the case of KPALM (see Proposition 3.1.3) yields that

$$\begin{aligned} \gamma(t+1) &:= \left((d_\varepsilon^i(x(t+1)) + u^i(t+1))_{i=1,\dots,m}, \nabla_x H_\varepsilon(w(t+1), x(t+1)) \right) \\ &\in \partial\sigma_\varepsilon(z(t+1)), \end{aligned} \quad (4.1.13)$$

where $u^i(t+1) \in \partial\delta_\Delta(w^i(t+1))$, $i = 1, 2, \dots, m$. Now, writing the optimality condition of step (4.1.5), yields that

$$d_\varepsilon^i(x(t)) + \alpha_i(t) (w^i(t+1) - w^i(t)) + u^i(t+1) = \mathbf{0}. \quad (4.1.14)$$

Plugging (4.1.14) into (4.1.13), and taking the norm yields

$$\begin{aligned} \|\gamma(t+1)\| &\leq \sum_{i=1}^m \|d_\varepsilon^i(x(t+1)) - d_\varepsilon^i(x(t)) - \alpha_i(t) (w^i(t+1) - w^i(t))\| \\ &\quad + \|\nabla_x H_\varepsilon(w(t+1), x(t+1))\| \\ &\leq \sum_{i=1}^m \|d_\varepsilon^i(x(t+1)) - d_\varepsilon^i(x(t))\| + \sum_{i=1}^m \alpha_i(t) \|w^i(t+1) - w^i(t)\| \\ &\quad + \|\nabla_x H_\varepsilon(w(t+1), x(t+1))\| \\ &\leq \frac{md_A}{\varepsilon} \|x(t+1) - x(t)\| + \bar{\alpha}\sqrt{m} \|w(t+1) - w(t)\| \\ &\quad + \|\nabla_x H_\varepsilon(w(t+1), x(t+1))\|, \end{aligned}$$

where the last inequality follows from Lemma 4.1.4 and the fact that $\bar{\alpha} = \max_{1 \leq i \leq m} \bar{\alpha}_i$. Next we will show that $\|\nabla_x H_\varepsilon(w(t+1), x(t+1))\| \leq c \|x(t+1) - x(t)\|$, for some constant $c > 0$. First, note that for fixed $w \in \Delta^m$ and any $x \in \mathbb{R}^{nk}$ the following relation holds (where the fixed $v \equiv w$ in (4.1.7))

$$\nabla_{x^l} H_\varepsilon(w, x) = \nabla f_\varepsilon(x^l), \quad \forall l = 1, 2, \dots, k. \quad (4.1.15)$$

Now, for all $l = 1, 2, \dots, k$, we have

$$\begin{aligned} \nabla_{x^l} H_\varepsilon(w(t+1), x(t+1)) &= \nabla_{x^l} H_\varepsilon(w(t+1), x(t+1)) - \nabla_{x^l} H_\varepsilon(w(t+1), x(t)) \\ &\quad + \nabla_{x^l} H_\varepsilon(w(t+1), x(t)) \\ &= \nabla_{x^l} H_\varepsilon(w(t+1), x(t+1)) - \nabla_{x^l} H_\varepsilon(w(t+1), x(t)) \\ &\quad + L_\varepsilon^l(w(t+1), x(t)) (x^l(t) - x^l(t+1)), \end{aligned} \quad (4.1.16)$$

where the last equality follows from (4.1.6). Therefore,

$$\begin{aligned}
\|\nabla_x H_\varepsilon(w(t+1), x(t+1))\| &\leq \sum_{l=1}^k \|\nabla_{x^l} H_\varepsilon(w(t+1), x(t+1))\| \\
&\leq \sum_{l=1}^k L_\varepsilon^l(w(t+1), x(t)) \|x^l(t+1) - x^l(t)\| \\
&\quad + \sum_{l=1}^k \|\nabla_{x^l} H_\varepsilon(w(t+1), x(t+1)) - \nabla_{x^l} H_\varepsilon(w(t+1), x(t))\| \\
&\leq \frac{m}{\varepsilon} \sum_{l=1}^k \|x^l(t+1) - x^l(t)\| \\
&\quad + \sum_{l=1}^k \gamma^l(t) \|x^l(t+1) - x^l(t)\|, \tag{4.1.17}
\end{aligned}$$

where the last inequality follows from Proposition 4.1.1(ii) and Lemma 4.1.3 combined with the (4.1.15) observation using

$$\gamma^l(t) = \frac{2L_\varepsilon^l(w(t+1), x(t))L_\varepsilon^l(w(t+1), x(t+1))}{L_\varepsilon^l(w(t+1), x(t)) + L_\varepsilon^l(w(t+1), x(t+1))}, \quad l = 1, 2, \dots, k.$$

From Proposition 4.1.1(ii) we obtain that

$$\gamma^l(t) = \frac{2}{\frac{1}{L_\varepsilon^l(w(t+1), x(t))} + \frac{1}{L_\varepsilon^l(w(t+1), x(t+1))}} \leq \frac{2}{\frac{\varepsilon}{m} + \frac{\varepsilon}{m}} = \frac{m}{\varepsilon}.$$

Hence, from (4.1.17), we have

$$\begin{aligned}
\|\nabla_x H_\varepsilon(w(t+1), x(t+1))\| &\leq \frac{2m}{\varepsilon} \sum_{l=1}^k \|x^l(t+1) - x^l(t)\| \\
&\leq \frac{2m\sqrt{k}}{\varepsilon} \|x(t+1) - x(t)\|. \tag{4.1.18}
\end{aligned}$$

Therefore, setting $\rho_2 = \frac{md_A}{\varepsilon} + \bar{\alpha}\sqrt{m} + \frac{2m\sqrt{k}}{\varepsilon}$, yields the result. \square

We conclude our main convergence result of the ε -KPALM algorithm in the following theorem.

Theorem 4.1.1. *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. Then, the sequence $\{z(t)\}_{t \in \mathbb{N}}$ converges to a critical point of σ_ε .*

Proof. Due to Propositions 4.1.3 and 4.1.4 it follows that the sequence $\{z(t)\}_{t \in \mathbb{N}}$ is a gradient-like descent sequence. The function σ_ε is clearly a semi-algebraic function, and the proof that $\omega(z(0)) \subset \text{crit}(\sigma_\varepsilon)$ is analogous to the one given in Theorem 3.1.1 (even though it is a different objective function, the same arguments can apply here), hence Theorem 2.2.2 implies the desired result. \square

4.2 A Different Approach Towards Solving the Smoothed H_ε

In this section we describe a different approach towards solving the smoothed clustering problem given in (4.1.1). Using the Arithmetic-Geometric inequality we derive the following simple observation

$$\frac{1}{2} \min_{s \geq 0} \left\{ s\lambda + \frac{1}{\lambda} \right\} \geq \min_{s \geq 0} \left\{ \sqrt{s\lambda \cdot \frac{1}{s}} \right\} = \sqrt{\lambda}, \quad \forall \lambda \geq 0,$$

and the unique minimizer is given by $s^* = 1/\sqrt{\lambda}$. Using this fact we can write

$$\sqrt{\|u\|^2 + \varepsilon^2} = \frac{1}{2} \min_{v \geq 0} \left\{ v (\|u\|^2 + \varepsilon^2) + \frac{1}{v} \right\}, \quad (4.2.19)$$

with $v^* = 1/\sqrt{\|u\|^2 + \varepsilon^2}$. Thus, instead of solving problem (4.1.1) with $H_\varepsilon(\cdot, \cdot)$, as defined in (4.1.2), we replace it with the following function

$$B_\varepsilon(v, w, x) = \frac{1}{2} \sum_{i=1}^m \sum_{l=1}^k \left\{ v_l^i w_l^i (\|x^l - a^i\|^2 + \varepsilon^2) + \frac{w_l^i}{v_l^i} \right\}, \quad (4.2.20)$$

where $v = (v^1, v^2, \dots, v^m)$. Then problem (4.1.1) can be written equivalently as

$$\min_{x, v, w} \{ B_\varepsilon(v, w, x) + G(w) : v \geq 0 \}.$$

For all $i = 1, 2, \dots, m$ we define $b_\varepsilon^i : \mathbb{R}^{mk} \times \mathbb{R}^{nk} \rightarrow \mathbb{R}^k$ by

$$b_\varepsilon^i(v, x) = \left(\frac{1}{2} v_l^i (\|x^l - a^i\|^2 + \varepsilon^2) + \frac{1}{2v_l^i} \right)_{l=1,2,\dots,k} \in \mathbb{R}^k,$$

and we have that

$$B_\varepsilon(v, w, x) = \sum_{i=1}^m \langle w^i, b_\varepsilon^i(v, x) \rangle. \quad (4.2.21)$$

Now the situation is similar to that of Section 3.1, namely

- (1) The function $w \mapsto B_\varepsilon(v, w, x)$, for fixed v and x , is linear.
- (2) The function $x \mapsto B_\varepsilon(v, w, x)$, for fixed v and w , is quadratic and convex.

Hence we can tackle these two steps as in KPALM.

Equipped with these observations we proceed with a PALM-like algorithm, which is based on three steps alternating minimization. More precisely, with respect to v we perform exact minimization

$$v(t+1) = \operatorname{argmin} \{ B_\varepsilon(v, w(t), x(t)) : v \geq 0 \}.$$

It should be noted that this problem can be written equivalently by

$$v(t+1) = \operatorname{argmin} \{ B_\varepsilon(v, w(t), x(t)) : v \in I^{mk} \},$$

where $I := [1/\kappa, 1/\varepsilon]$ and $\kappa = \sqrt{d_{\mathcal{A}}^2 + \varepsilon^2}$. With respect to w , as in the KPALM case, for each $i = 1, 2, \dots, m$, we need to solve the subproblem given by

$$w^i(t+1) = \operatorname{argmin}_{w^i \in \Delta} \left\{ \langle w^i, b_\varepsilon^i(v(t+1), x(t)) \rangle + \frac{\alpha_i(t)}{2} \|w^i - w^i(t)\|^2 \right\}, \quad (4.2.22)$$

where $\alpha_i(t) > 0$, $i = 1, 2, \dots, m$, is arbitrarily chosen. With respect to x , again as in the KPALM case, we perform exact minimization

$$x(t+1) = \operatorname{argmin}_{x \in \mathbb{R}^{nk}} B_\varepsilon(v(t+1), w(t+1), x). \quad (4.2.23)$$

It is easy to check that all three subproblems have explicit solutions which are given by

$$v_l^i(t+1) = \frac{1}{\left(\|x^l(t) - a^i\|^2 + \varepsilon^2 \right)^{1/2}}, \quad i = 1, 2, \dots, m, \quad l = 1, 2, \dots, k, \quad (4.2.24)$$

$$w^i(t+1) = P_\Delta \left(w^i(t) - \frac{b_\varepsilon^i(v(t+1), x(t))}{\alpha_i(t)} \right), \quad i = 1, 2, \dots, m, \quad (4.2.25)$$

and

$$x^l(t+1) = \frac{\sum_{i=1}^m w_l^i(t+1) v_l^i(t+1) a^i}{\sum_{i=1}^m w_l^i(t+1) v_l^i(t+1)}, \quad l = 1, 2, \dots, k. \quad (4.2.26)$$

From the subproblem for v and the observation given in (4.2.19), we derive the following three relations

$$B_\varepsilon(v(t+1), w, x(t)) = H_\varepsilon(w, x(t)), \quad \forall t \in \mathbb{N}, \forall w \in \Delta^m, \quad (4.2.27)$$

$$b_\varepsilon^i(v(t+1), x(t)) = d_\varepsilon^i(x(t)), \quad \forall t \in \mathbb{N}, i = 1, 2, \dots, m, \quad (4.2.28)$$

where d_ε^i is defined in (4.1.3), and

$$B_\varepsilon(v, w, x) \geq H_\varepsilon(w, x), \quad \forall (v, w, x) \in I^{mk} \times \Delta^m \times \mathbb{R}^{nk}. \quad (4.2.29)$$

Substituting (4.2.28) into (4.2.25) yields

$$w^i(t+1) = P_\Delta \left(w^i(t) - \frac{d_\varepsilon^i(x(t))}{\alpha_i(t)} \right), \quad i = 1, 2, \dots, m.$$

Moreover, substituting (4.2.24) into (4.2.26) yields

$$x^l(t+1) = \frac{1}{L_\varepsilon^l(w(t+1), x(t))} \sum_{i=1}^m \left(\frac{w_l^i(t+1)}{(\|x^l(t) - a^i\|^2 + \varepsilon^2)^{1/2}} \right) a^i, \quad l = 1, 2, \dots, k,$$

where L_ε^l is defined in (4.1.4). Thus, we recover the ε -KPALM algorithm, which means these two different approaches lead to the same iterative algorithm. However, with the current approach we can swiftly prove that conditions (C1) and (C2) hold true, which are needed to obtain that $\{z(t)\}_{t \in \mathbb{N}}$ is a gradient-like sequence (see Definition 2.2.4) and the global convergence of $\{z(t)\}_{t \in \mathbb{N}}$ which generated by ε -KPALM.

Proposition 4.2.1 (Sufficient decrease property). *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. Then, there exists $\rho_1 > 0$ such that*

$$\rho_1 \|z(t+1) - z(t)\|^2 \leq \sigma_\varepsilon(z(t)) - \sigma_\varepsilon(z(t+1)), \quad \forall t \in \mathbb{N}.$$

Proof. From (4.2.22) we have

$$\langle w^i(t+1), b_\varepsilon^i(v(t+1), x(t)) \rangle + \frac{\alpha_i(t)}{2} \|w^i(t+1) - w^i(t)\|^2 \leq \langle w^i(t), b_\varepsilon^i(v(t+1), x(t)) \rangle.$$

Summing the last inequality over $i = 1, 2, \dots, m$ and applying (4.2.21) yields

$$B_\varepsilon(v(t+1), w(t+1), x(t)) + \sum_{i=1}^m \frac{\alpha_i(t)}{2} \|w^i(t+1) - w^i(t)\|^2 \leq B_\varepsilon(v(t+1), w(t), x(t)).$$

Using Assumption 3.1.1(i) we derive

$$\begin{aligned} \frac{\alpha}{2} \|w(t+1) - w(t)\|^2 &\leq B_\varepsilon(v(t+1), w(t), x(t)) - B_\varepsilon(v(t+1), w(t+1), x(t)) \\ &\leq H_\varepsilon(w(t), x(t)) - H_\varepsilon(w(t+1), x(t)), \end{aligned} \quad (4.2.30)$$

where the last inequality follows from (4.2.27) and (4.2.29).

Since the function $x \mapsto B_\varepsilon(v, w, x)$ is C^2 , and

$$\nabla_{x^j} \nabla_{x^l} B_\varepsilon(v, w, x) = \begin{cases} 0 & \text{if } j \neq l, \quad 1 \leq j, l \leq k, \\ \sum_{i=1}^m w_l^i v_l^i & \text{if } j = l, \quad 1 \leq j, l \leq k, \end{cases}$$

it follows that, the function $x \mapsto B_\varepsilon(v(t+1), w(t), x)$ is strongly convex with parameter $\underline{\beta}/2\kappa$, for all $t \in \mathbb{N}$. Indeed,

$$\nabla_{x^l}^2 B_\varepsilon(v(t+1), w(t), x) = \sum_{i=1}^m w_l^i(t) v_l^i(t+1) \geq \frac{1}{\kappa} \sum_{i=1}^m w_l^i(t) \geq \frac{\beta(w^i(t))}{2\kappa} > \frac{\underline{\beta}}{2\kappa} > 0,$$

where the first inequality follows from the fact that $v_l^i(t) \in I$ for all $t \in \mathbb{N}$, $\beta(\cdot)$ is defined in (3.1.7), and the second inequality is due to Assumption 3.1.1(ii). Using

the strong convexity property we deduce the sufficient decrease in x , as follows,

$$\begin{aligned}
\frac{\beta}{4\kappa} \|x(t+1) - x(t)\|^2 &= \langle \nabla_x B_\varepsilon(z(t+1)), x(t) - x(t+1) \rangle + \frac{\beta}{4\kappa} \|x(t+1) - x(t)\|^2 \\
&\leq B_\varepsilon(w(t+1), x(t)) - B_\varepsilon(z(t+1)) \\
&\leq H_\varepsilon(w(t+1), x(t)) - H_\varepsilon(w(t+1), x(t+1)), \tag{4.2.31}
\end{aligned}$$

where the first equality follows from (4.2.23), the second inequality follows from the strong convexity, and the last inequality is due to (4.2.27) and (4.2.29). Set $\rho_1 = \min\{\underline{\alpha}/2, \underline{\beta}/4\kappa\}$. Summing (4.2.30) and (4.2.31), we get

$$\begin{aligned}
\rho_1 \|z(t+1) - z(t)\|^2 &= \rho_1 (\|w(t+1) - w(t)\|^2 + \|x(t+1) - x(t)\|^2) \\
&\leq [H_\varepsilon(z(t)) - H_\varepsilon(w(t+1), x(t))] \\
&\quad + [H_\varepsilon(w(t+1), x(t)) - H_\varepsilon(z(t+1))] \\
&= H_\varepsilon(z(t)) - H_\varepsilon(z(t+1)) \\
&= \sigma_\varepsilon(z(t)) - \sigma_\varepsilon(z(t+1)),
\end{aligned}$$

where the last equality follows from the fact that $G(w(t)) = 0$, since $w(t) \in \Delta^m$ for all $t \in \mathbb{N}$. This proves the desired result. \square

Proposition 4.2.2 (Subgradient lower bound for the iterates gap). *Suppose that Assumption 3.1.1 holds true and let $\{z(t)\}_{t \in \mathbb{N}}$ be the sequence generated by ε -KPALM. For each $t \in \mathbb{N}$ define*

$$\gamma(t) := \left((d^i(x(t)) - d^i(x(t-1)) - \alpha_i(t-1)(w^i(t) - w^i(t-1)))_{i=1,2,\dots,m}, \nabla_x H_\varepsilon(z(t)) \right).$$

Then $\gamma(t) \in \partial \sigma_\varepsilon(z(t))$ and there exists $\rho_2 > 0$ such that

$$\|\gamma(t+1)\| \leq \rho_2 \|z(t+1) - z(t)\|, \quad \forall t \in \mathbb{N}.$$

Proof. By the definition of σ_ε (see (4.1.1)) we get

$$\sigma_\varepsilon(w, x) = H_\varepsilon(w, x) + \sum_{i=1}^m \delta_\Delta(w^i). \tag{4.2.32}$$

Differentiating (4.2.32) with respect to x and evaluating it in $z(t+1)$ yields

$$\partial_x \sigma_\varepsilon(z(t+1)) = \nabla_x H_\varepsilon(z(t+1)). \tag{4.2.33}$$

Similarly, differentiating (4.2.32) with respect to w^i and evaluating it in $z(t+1)$ yields

$$\partial_{w^i} \sigma_\varepsilon(z(t+1)) = d_\varepsilon^i(x(t+1)) + \partial_{w^i} \delta_\Delta(w^i(t+1)). \tag{4.2.34}$$

The optimality condition of $w^i(t+1)$ which derived from (4.2.22), yields that for all $i = 1, 2, \dots, m$ there exists $u^i(t+1) \in \partial\delta_\Delta(w^i(t+1))$ such that

$$\begin{aligned} \mathbf{0} &= b_\varepsilon^i(v(t+1), x(t)) + \alpha_i(t) (w^i(t+1) - w^i(t)) + u^i(t+1) \\ &= d_\varepsilon^i(x(t)) + \alpha_i(t) (w^i(t+1) - w^i(t)) + u^i(t+1), \end{aligned} \quad (4.2.35)$$

where the last equality follows from (4.2.28). Substituting (4.2.35) into (4.2.34) and combining with (4.2.33) we deduce that

$$\begin{aligned} \gamma(t+1) &:= \left((d^i(x(t+1)) - d^i(x(t)) - \alpha_i(t)(w^i(t+1) - w^i(t)))_{i=1,2,\dots,m}, \nabla_x H_\varepsilon(z(t+1)) \right) \\ &\in \partial\sigma_\varepsilon(z(t+1)). \end{aligned}$$

Therefore,

$$\begin{aligned} \|\gamma(t+1)\| &\leq \sum_{i=1}^m \|d^i(x(t+1)) - d^i(x(t)) - \alpha_i(t)(w^i(t+1) - w^i(t))\| + \|\nabla_x H_\varepsilon(z(t+1))\| \\ &\leq \sum_{i=1}^m \|d^i(x(t+1)) - d^i(x(t))\| + \bar{\alpha} \sum_{i=1}^m \|w^i(t+1) - w^i(t)\| \\ &\quad + \frac{2m\sqrt{k}}{\varepsilon} \|x(t+1) - x(t)\| \\ &\leq \sum_{i=1}^m \frac{d_A}{\varepsilon} \|x(t+1) - x(t)\| + \bar{\alpha}\sqrt{m} \|w(t+1) - w(t)\| \\ &\quad + \frac{2m\sqrt{k}}{\varepsilon} \|x(t+1) - x(t)\| \\ &\leq \left(\frac{md_A}{\varepsilon} + \bar{\alpha}\sqrt{m} + \frac{2m\sqrt{k}}{\varepsilon} \right) \|z(t+1) - z(t)\|, \end{aligned}$$

where the second inequality was established in Proposition 4.1.4 (see (4.1.18)) and the third inequality follows from Lemma 4.1.4. Define $\rho_2 = \frac{md_A}{\varepsilon} + \bar{\alpha}\sqrt{m} + \frac{2m\sqrt{k}}{\varepsilon}$, and the result follows. \square

Once again, Propositions 4.2.1 and 4.2.2 set the foundations for proving that the sequence $\{z(t)\}_{t \in \mathbb{N}}$, generated by ε -KPALM, converges to a critical point of σ_ε as stated in Theorem 4.1.1.

Chapter 5

Numerical Results

In this chapter we present the numerical results and compare the algorithms presented in this work with other center-based algorithms that are commonly used to address the clustering problem. We describe in detail the setting used in each comparison. We compare the commonly used parameters, such as function objective values and number of iterations until a certain precision is achieved. In addition to these parameters, we use several different types of clustering metrics to compare the final clusterings obtained by the discussed algorithms.

Most of the existing clustering methods are sensitive to the starting point, namely choosing different starting point result in significant differences in the final clustering. There are plethora of heuristic initialization methods. One such initialization method is to choose k random data points as staring centers, assuming uniform distribution or some other prior distribution on the data. Another popular initialization method is to label at random each data point, assuming uniform distribution over the labels for each point.

The initialization points used within the implementation of the compared algorithms are as follows. k-means staring point is constructed by randomly choosing k different points from the dataset. The same technique is employed in the cases of KPALM and ε -KPALM, for the $x(0)$ variable. Whereas for the $w(0)$ variable, it is chosen at random from Δ^m . k-means++ takes also part in our comparison, and it is basically the same as k-means, with the exception of its starting point that is constructed in the following manner. The first center $x^1(0)$ is chosen randomly from the dataset \mathcal{A} . Suppose that $1 \leq l < k$ centers have already been chosen, set $x^{l+1}(0)$ to be the point in the dataset that is the furthest from its closest center.

Since it is impractical to compare the function values achieved with the algorithms

which solve the squared Euclidean clustering problem with that of the algorithms which solve the Euclidean clustering problem, we used some criteria devised to compare clustering partitions. Criteria such as *variation of information (VI)*, *Mirkin metric*, and *Van Dongen metric*, are few examples for metrics that measure the difference between two clustering partitions (see [18]). With these metrics we compared the similarity of the partition achieved with each algorithm to the desired partition of each dataset. The goal is to decrease the value of the metrics.

5.1 Iris Dataset

We used the famous Iris dataset to test the performance of the KPALM algorithm. It is important to note that choosing the parameter α is left to the user, and as presented below, has a significant effect on the convergence rate and the quality of the achieved clustering, namely the value of the objective function over the generated series. All the plots in this section are made by averaging over 100 trials, each trial with random starting point. Figure 5.1 shows that dynamic values of the parameter α which

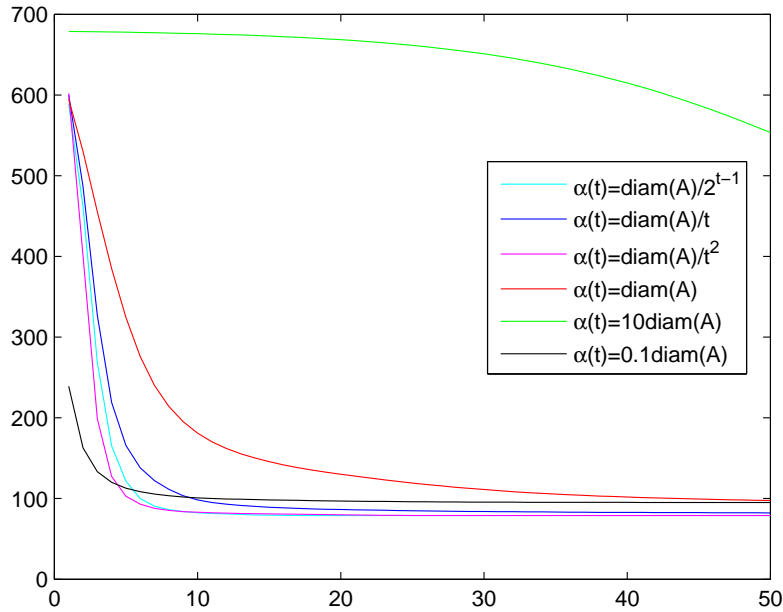


Figure 5.1: Comparison of the objective values for different values of α .

decreases fast, such as $\alpha_i(t) = \frac{\text{diam}(\mathcal{A})}{2^{t-1}}$, achieve smaller function values. Similarly to Figure 5.1, in Figure 5.2 we can see a comparison of the objective values of σ_ε for different function values. The value of ε is set to be $1e-5$.

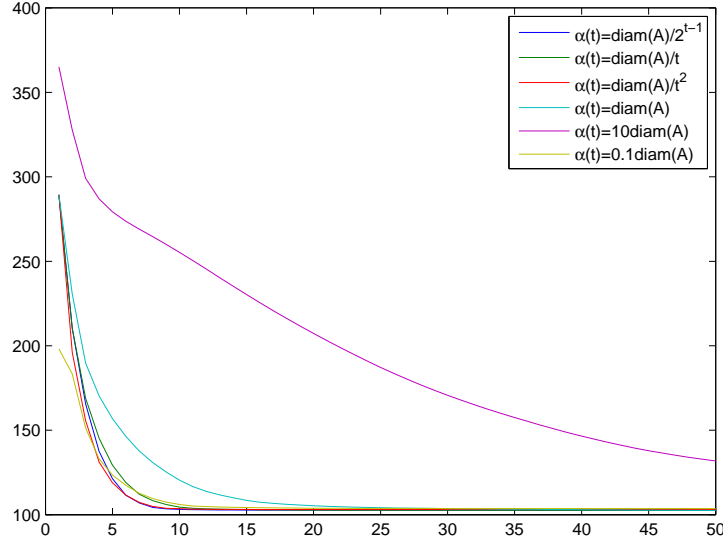
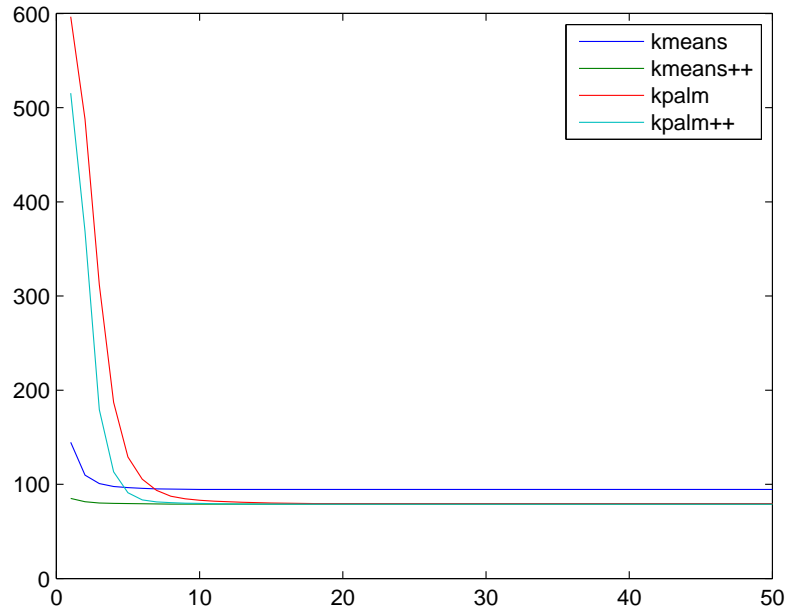
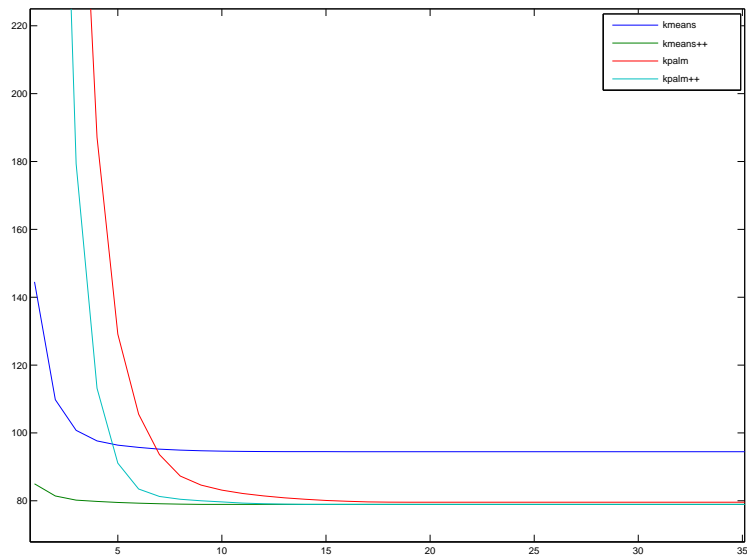


Figure 5.2: Comparison of the objective values for different values of α .

In Figure 5.3 we made a comparison between KPALM with dynamic rule for choosing the parameter α , that is $\alpha_i(t) = \frac{\text{diam}(\mathcal{A})}{2^{t-1}}$, with k-means and k-means++. It demonstrates that KPALM can reach lower objective function values than k-means, and these are similar to the values achieved with KMEAN++. In addition, the KPALM++ are the objective function values achieved with KPALM when the x variable is initialized as in k-means++. Unlike k-means, the objective function values KPALM converge to are more stable and less sensitive to its starting point. Figure 5.4 shows the number of iteration needed to reach precision of $1e-3$ between consecutive objective function values.

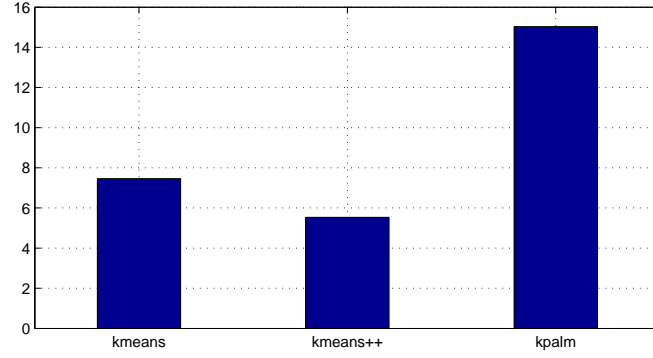


(a) Comparison of objective function values.

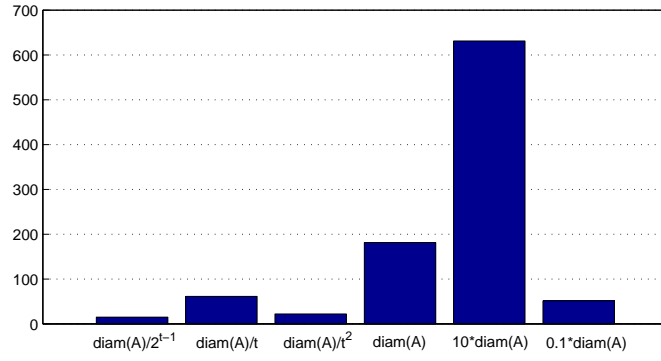


(b) Zoom of Figure 5.3a.

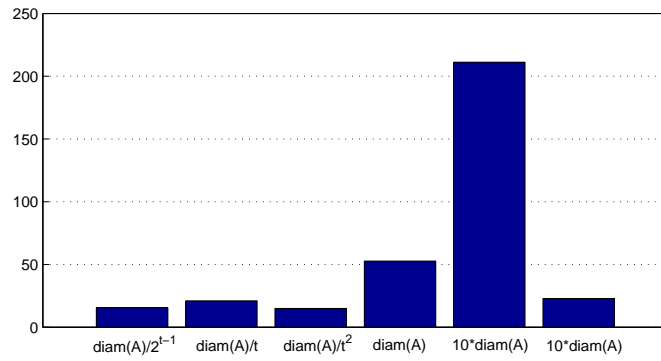
Figure 5.3: Comparison of objective function values for k-means, k-means++, KPALM and KPALM++.



(a) Number of iterations of k-means, k-means++ and KPALM with $\alpha(t) = \text{diam}(\mathcal{A})/2^{t-1}$.



(b) Number of iterations of KPALM with different updates of $\alpha(t)$.

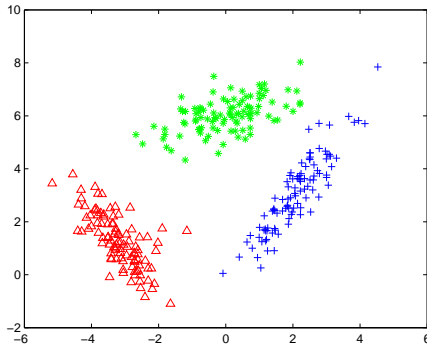


(c) Number of iterations of ε -KPALM with different updates of $\alpha(t)$.

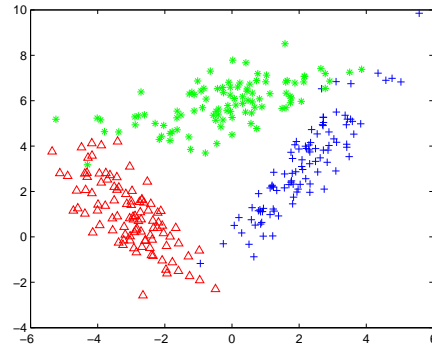
Figure 5.4: Comparison of number of iterations needed to reach $1e-3$ precision of σ .

5.2 Synthetic Dataset

In this section we show that ε -KPALM is less sensitive to outliers in the data verses algorithms that suit the squared Euclidean norm (e.g., k-means, k-means++ and KPALM). We generated two synthetic datasets, each contains 300 points in the plane, by sampling three two-dimensional Gaussian, 100 samples each. In Figure 5.5(5.5a) the clusters are denser than in Figure 5.5(5.5b). Then we run the clustering algorithms and compared their clustering results, namely, how many points were clustered correctly. From Figure 5.6(5.6a) it is evident that k-means is superior to other algorithms in the dense case and ε -KPALM is quite sensitive. Whereas, in the sparse case in Figure 5.6(5.6b), ε -KPALM is superior, and less sensitive to outliers. In Figure 5.7 we compare the distance of clusterings achieved with different algorithms to the desired clustering, where kpalm1 , kpalm2 and kpalm3 match using $\alpha(t) = \text{diam}(\mathcal{A})/2^{t-1}$, $\alpha(t) = \text{diam}(\mathcal{A})/t^2$ and $\alpha(t) = \text{diam}(\mathcal{A})$ respectively, and similarly for $\varepsilon\text{-kpalm}i$, $i \in \{1, 2, 3\}$. In Figure 5.7(5.7a) we witness that for dense dataset, the resulting clusterings of squared Euclidean algorithms, namely, k-means, k-means++ and KPALM, are superior to the clustering ε -KPALM, where KPALM with $\alpha(t) = \text{diam}(\mathcal{A})/2^{t-1}$ gives the best result, that is, the clustering in this setting is the closest to the desired clustering. Whereas in the sparse dataset, the clustering achieved with ε -KPALM with $\alpha(t) = \text{diam}(\mathcal{A})/t^2$ is the closest to the desired clustering, as reflected from Figure 5.7(5.7b).

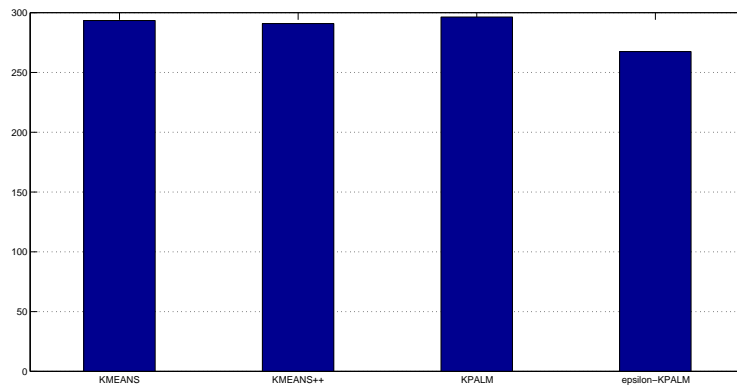


(a) Dense Gaussians.

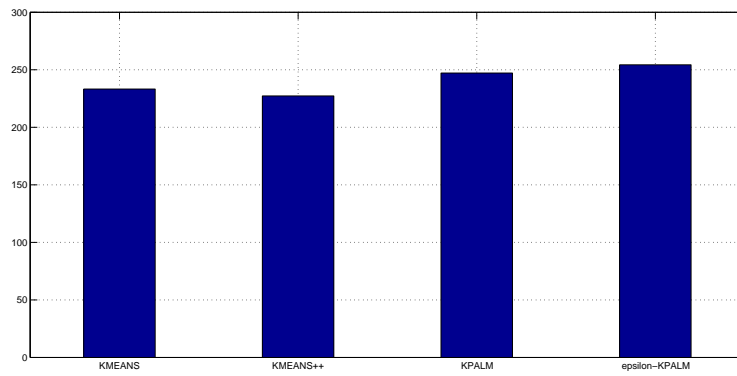


(b) Sparse Gaussians.

Figure 5.5: Two datasets, each 300 points.

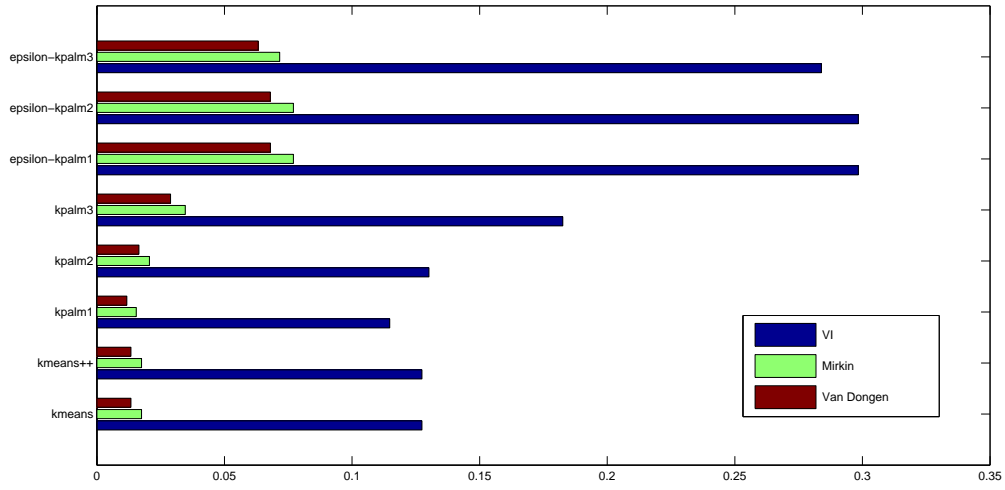


(a) Dense Gaussians clustering.

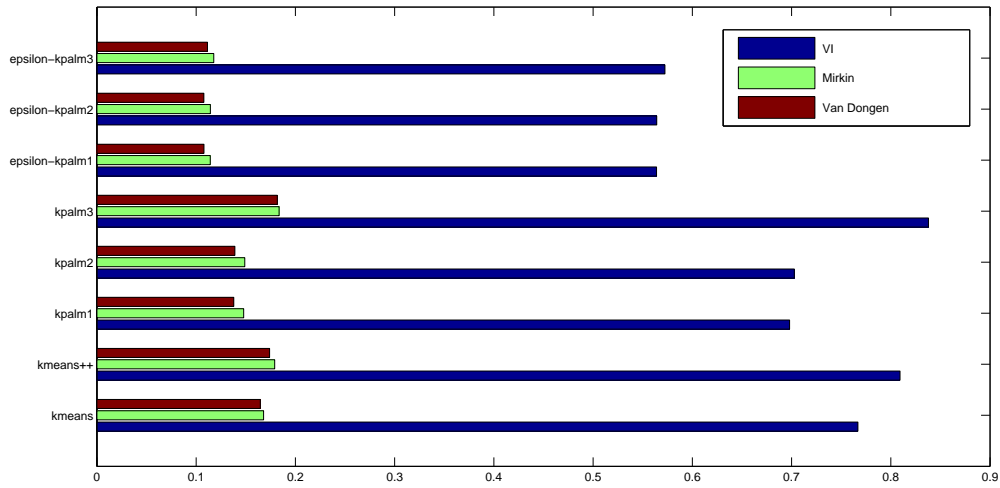


(b) Sparse Gaussians clustering.

Figure 5.6: Results of clustering algorithms for dense and sparse datasets.



(a) Dense Gaussians metrics comparison.



(b) Sparse Gaussians metrics comparison.

Figure 5.7: Comparison of metrics between clusterings for dense and sparse datasets.

5.3 Summary of Numerical Results

From the conducted numerical experiments we deduce the following:

- In the squared Euclidean setting, KPALM achieves lower objective function values than k-means. When using a more sophisticated initialization step, such as the one in k-means++, then k-means++ and KPALM++ achieve similar objective function values.
- k-means needs less number of iterations than KPALM to reach a certain precision.
- It is preferable to use dynamic update of $\alpha(t)$ parameter to achieve a faster convergence, both in KPALM and ϵ -KPALM. Example for suitable choices can be $\alpha(t) = \text{diam}(\mathcal{A})/t$ and $\alpha(t) = \text{diam}(\mathcal{A})/2^t$.
- When the convex hulls of the desired clusters are mutually exclusive, algorithms which solve the clustering problem with the squared Euclidean distance are preferable to ϵ -KPALM. This can be witnessed from the dense Gaussians example in Figure 5.5(5.5a), and the comparison made in Figure 5.7(5.7a), which shows that clusterings obtained with squared Euclidean algorithm are more similar to the desired clustering, and have lower distance in terms of clustering metrics, than the clustering obtained with ϵ -KPALM.
- In datasets with outliers, the clustering obtained with ϵ -KPALM is more similar to the desired clustering, in terms of clustering metrics, than the clusterings obtained via the squared Euclidean algorithms. This is witnessed from the sparse Gaussians example in Figure 5.5(5.5b), and the comparison made in Figure 5.7(5.7b). Therefore, as expected, for data with outliers, the choice of a norm instead of the squared norm is a more natural choice, and the ϵ -KPALM algorithm appears to be a promising algorithm to handle such data.

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תקציר

בעיית החלוקה לאשכולות הינה בעיה בסיסית ומרכזית בתחום הלמידה החישובית הבלתי מונחית, והיא שימושית במגוון רחב של יישומים. בעיית החלוקה לאשכולות היא בעיה לא קמורה ולא חלקה ולפיכך היא קשה לפתירה. בעבודה זו מוצעים שני אלגוריתמים עבור בעיית החלוקה לאשכולות מבוססי מרכזים, כל אלגוריתם פותר את הבעיה עבור פונקצית מרחק שונה. אלגוריתם KPALM פותר את הבעיה כאשר פונקצית המרחק היא המרחק האוקלידי בריבוע, בעוד שאלגוריתם ε -KPALM פותר את הבעיה כאשר פונקצית המרחק היא המרחק האוקלידי הסטנדרטי. שני האלגוריתמים מבוססים על השיטה הקלאסית של מינימיזציה משוחלפת (Alternating Minimization). בשלב חלוקת המדגם, כל אחד משני האלגוריתמים משייך לכל מרכז את הנקודות המתאימות מהמדגם ע"י מציאת מינימום של תת בעיה, שפונקצית המטרה שלה היא ליניארית בתוספת גורם רגולריזציה. בשלב עדכון המרכזים, אלגוריתם KPALM פותר בעיית מינימיזציה בצורה מדויקת, בעוד שאלגוריתם ε -KPALM מוצא פתרון מקורב לבעיית המינימיזציה ע"י ביצוע צעד גרדיאנט. בעבודה מופיעה הוכחת התכנסות גלובלית של האלגוריתמים הנ"ל לנקודה קריטית, הנעשית ע"י שימוש במתודולוגיה חדשנית המבוססת על תכונת Kurdyka-Łojasiewicz. בנוסף לתוצאות התיאורטיות, אנחנו מציגים תוצאות נומריות המדגימות את האפקטיביות של האלגוריתמים המוצעים.

אוניברסיטת תל אביב
הפקולטה למדעים מדויקים ע"ש ריימונד וברלי סאקלר

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מאת סרגיי וולדמן

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