Clustering under Perturbation Stability in Near-Linear Time

Pankaj K. Agarwal[†] Hsien-Chih Chang[‡] Kamesh Munagala[†]
Erin Taylor[†] Emo Welzl[§]

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Abstract

We consider the problem of center-based clustering in low-dimensional Euclidean spaces under the perturbation stability assumption. An instance is α-stable if the underlying optimal clustering continues to remain optimal even when all pairwise distances are arbitrarily perturbed by a factor of at most α. Our main contribution is in presenting efficient exact algorithms for α-stable clustering instances whose running times depend near-linearly on the size of the data set when $\alpha \geq 2+\sqrt{3}$. For k-center and k-means problems, our algorithms also achieve polynomial dependence on the number of clusters, k, when $\alpha \geq 2+\sqrt{3}+\varepsilon$ for any constant $\varepsilon > 0$ in any fixed dimension. For k-median, our algorithms have polynomial dependence on k for $\alpha > 5$ in any fixed dimension; and for $\alpha \geq 2+\sqrt{3}$ in two dimensions. Our algorithms are simple, and only require applying techniques such as local search or dynamic programming to a suitably modified metric space, combined with careful choice of data structures.

1 Introduction

Clustering is a fundamental problem in unsupervised learning and data summarization, with wide-ranging applications that span myriad areas. Typically, the data points are assumed to lie in a Euclidean space, and the goal in center-based clustering is to open a set of k centers to minimize the objective cost, usually a function over the distance from each data point to its closest center. The k-median objective minimizes the sum of distances; the k-means minimizes the sum of squares of distances; and the k-center minimizes the longest distance. In the worst case, all these objectives are NP-hard even in 2D [52, 54].

A substantial body of work has focused on developing polynomial-time approximation algorithms and analyzing natural heuristics for these problems. Given the sheer size of modern data sets, such as those generated in genomics or mapping applications, even a polynomial-time algorithm is too slow to be useful in practice—just computing all pairs of distances can be computationally burdensome. What we need is an algorithm whose running time is near-linear in the input size and polynomial in the number of clusters.

Because of NP-hardness results, we cannot hope to compute an optimal solution in polynomial time, but in the worst case an approximate clustering can be different from an optimal clustering. We focus on the case when the optimal clustering can be recovered under some reasonable assumptions on the input that hold in practice. Such methodology is termed "beyond worst-case analysis" and has been adopted by recent work [2, 10, 25]. In recent years, the notion of *stability* has emerged as a popular assumption under which polynomial-time optimal clustering algorithms have been developed. An instance of clustering is called *stable* if any "small perturbation" of input points does not change the optimal solution. This is natural in real datasets, where often, the optimal clustering is clearly demarcated, and the distances are obtained heuristically. Different notions of stability differ in how "small perturbation" is defined, though most of them are related. In this paper, we focus on the notions of stability introduced in Bilu and Linial [25] and Awasthi, Blum, and Sheffet [16]. A clustering instance is *α-perturbation*

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[†]Department of Computer Science, Duke University, USA.
[‡]Department of Computer Science, Dartmouth, USA.
[§]Department of Computer Science, ETH Zürich, Switzerland.

resilient or α-*stable* if the optimal clustering does not change when all distances are perturbed by a factor of at most α. Similarly, a clustering instance is α-*center proximal* if any point is at least a factor of α closer to its own optimal center than any other optimal center. Awasthi, Blum, and Sheffet showed that α-stability implies α-center proximity [16]. This line of work designs algorithms to recover the *exact* optimal clustering—the ground truth—in polynomial time for α-stable instances.

This paper also focuses on recovering the optimal clustering for stable clustering instances. But instead of focusing on polynomial-time algorithms and optimizing the value of α, we ask the question: *Can algorithms be designed that compute exact solutions to stable instances of Euclidean center-based clustering that run in time near-linear in the input size?* We note that an $(1+\varepsilon)$-approximation solution, for an arbitrarily small constant $\varepsilon > 0$, may differ significantly from an optimal solution (the ground truth) even for stable instances, so one cannot hope to use an approximation algorithm to recover the optimal clustering.

1.1 Our Results

In this paper, we make progress on the above question, and present near-linear time algorithms for finding optimal solutions of stable clustering instances with moderate values of α. In particular, we show the following meta-theorem:

Theorem 1.1. *Let X be a set of n points in $\mathbb{R}^d$ for some constant d, let $k \geq 1$ be an integer, and let $\alpha \geq 2+\sqrt{3}$ be a parameter. If the k-median, k-means, or k-center clustering instance for X is α-stable, then the optimal solution can be computed in $\tilde{O}(n \operatorname{poly} k + f(k))$ time.*

In the above theorem, the $\tilde{O}$ notation suppresses logarithmic terms in n and the spread of the point set. The function $f(k)$ depends on the choice of algorithm, and we present the exact dependence below. We also omit terms depending solely on the dimension, d. Furthermore, the above theorem is robust in the sense that the algorithm is not restricted to choosing the input points as centers (*discrete setting*), and can potentially choose arbitrary points in the Euclidean plane as centers (*continuous setting*, sometimes referred to as the *Steiner point setting*)—indeed, we show that these notions are identical under a reasonable assumption on stability.

At a more fine-grained level, we present several algorithms that require mild assumptions on the stability condition. In the results below, as well as throughout the paper, we present our results both for the Euclidean plane, as well as generalizations to higher (but fixed number of) dimensions.

Dynamic Programming. In Section 3, we present a dynamic programming algorithm that computes the optimal clustering in $O(nk^2 + n \operatorname{polylog} n)$ time for α-stable k-means, k-median, and k-center in any fixed dimension, provided that $\alpha \geq 2+\sqrt{3}+\varepsilon$ for any constant $\varepsilon > 0$. For $d = 2$, it suffices to assume that $\alpha \geq 2+\sqrt{3}$.

Local Search. In Sections 4 and 5, we show that the standard 1-swap local-search algorithm, which iteratively swaps out a center in the current solution for a new center as long as the resulting total cost improves, computes an optimal clustering for α-stable instances of k-median assuming $\alpha > 5$. We also show that it can be implemented in $O(nk^2 \log^3 n \log \Delta)$ for $d = 2$ and in $O(nk^{2d-1} \operatorname{polylog} n \log \Delta)$ for $d > 2$; Δ is the spread of the point set.[1]

Coresets. In the Section 6, we use multiplicative coresets to compute the optimal clustering for k-means, k-median and k-center in any fixed dimension, when $\alpha \geq 2+\sqrt{3}$. The running time is $O(nk^2 + f(k))$ where $f(k)$ is an exponential function of k.

Remark 1.2. *While the current analysis of the dynamic programming based algorithm suggests that it is better than the local-search and coreset based approaches, the latter are of independent interest—our local-search analysis is considerably simpler than the previous analysis [40], and coresets have mostly been used to compute approximate, rather than exact, solutions. We also note that our analysis of the local-search algorithm is probably not tight. Furthermore, variants of all three approaches might work for smaller values of α. We note that the value of α assumed in the above results in larger than what is known for polynomial-time algorithm (e.g. $\alpha \geq 2$ in Angelidakis et al. [12]) and that in some applications the input may not satisfy our assumption, but our results are a big first step toward developing near-linear time algorithms for stable instances. We are not aware of any previous near-linear time algorithms for computing optimal clustering even for larger values of α. We leave the problem of reducing the assumption on α as an important open question.*

[1] The *spread* of a point set is the ratio between the longest and shortest pairwise distances.

Techniques. The key difficulty with developing fast algorithms for computing the optimal clustering is that some clusters could have a very small size compared to others. This issue persists even when the instances are stable. Imagine a scenario where there are multiple small clusters, and an algorithm must decide whether to merge these into one cluster while splitting some large cluster, or keep them intact. Now imagine this situation happening recursively, so that the algorithm has multiple choices about which clusters to recursively split. The difference in cost between these options and the size of the small clusters can be small enough that any $(1+\varepsilon)$-approximation can be agnostic, while an exact solution cannot. As such, work on finding exact optima use techniques such as dynamic programming [12] or local search with large number of swaps [28, 40] in order to recover small clusters. Other work makes assumptions lower-bounding the size of the optimal clusters or the spread of their centers [36].

Our main technical insight for the first two results is simple in hindsight, yet powerful: For a stable instance, if the Euclidean metric is replaced by another metric that is a good approximation, then the optimal clustering does not change under the new metric and in fact the instance remains stable albeit with a smaller stability parameter. In particular, we replace the Euclidean metric with an appropriate *polyhedral metric*—that is, a convex distance function where each unit ball is a regular polyhedron—yielding efficient procedures for the following two primitives:

- **Cost of 1-swap.** Given a candidate set of centers S, maintain a data structure that efficiently updates the total cost if center $x \in S$ is replaced by center $y \notin S$.
- **Cost of 1-clustering.** Given a partition of the data points, maintain a data structure where the cost of 1-clustering (under any objectives) can be efficiently updated as partitions are merged.

We next combine the insight of changing the metrics with additional techniques. For local search, we build on the approach in [28, 33, 40] that shows local search with t-swaps for large enough constant t finds an optimal solution for stable instances in polynomial time for any fixed-dimension Euclidean space. None of the prior analysis directly extends as is to 1-swap, which is critical in achieving near-linear running time—note that even when $t = 2$ there is a quadratic number of candidate swaps per step.

For the dynamic programming algorithm, we use the following insight: In Euclidean spaces, for $\alpha \geq 2+\sqrt{3}$, the longest edge of the minimum spanning tree over the input points partitions the data set in two, such that any optimal cluster lies completely in one of the two sides of the partition. Combined with the change of metrics one can achieve near-linear running time.

1.2 Related Work

All of k-median, k-means, and k-center are widely studied from the perspective of approximation algorithms and are known to be hard to approximate [38]. Indeed, for general metric spaces, k-center is hard to approximate to within a factor of $2-\varepsilon$ [46]; k-median is hard to $(1+2/e)$-approximate [47]; and k-means is hard to $(1+8/e)$-approximate in general metrics [31], and is hard to approximate within a factor of 1.0013 in the Euclidean setting [51]. Even when the metric space is Euclidean, k-means is still NP-hard when $k = 2$ [9, 34], and there is an $n^{\Omega(k)}$ lower bound on running time for k-median and k-means in 4-dimensional Euclidean space under the exponential-time hypothesis [29].

There is a long line of work in developing $(1+\varepsilon)$-approximations for these problems in Euclidean spaces. The holy grail of this work has been the development of algorithms that are near-linear time in n, and several techniques are now known to achieve this. This includes randomly shifted quad-trees [13], coresets [4,17,39,43,44], sampling [50], and local search [28, 30, 32], among others.

There are many notions of clustering stability that have been considered in literature [1, 8, 15, 19, 20, 24, 37, 49, 56]. The exact definition of stability we study here was first introduced in Awasthi *et al.* [16]; their definition in particular resembles the one of Bilu and Linial [25] for max-cut problem, which later has been adapted to other optimization problems [11, 12, 21, 53, 55]. Building on a long line of work [16, 18, 22, 23], which gradually reduced the stability parameter, Angelidakis *et al.* [12] present a dynamic programming based polynomial-time optimal algorithm for discrete 2-stable instances for all center-based objectives.

Chekuri and Gupta [27] show that a natural LP-relaxation is integral for the 2-stable k-center problem. Recent work by Cohen-Addad [33] provides a framework for analyzing local search algorithms for stable instances. This work shows that for an α-stable instance with $\alpha > 3$, any solution is optimal if it cannot be improved by swapping $\lceil 2/(\alpha-3)\rceil$ centers. Focusing on Euclidean spaces of fixed dimensions, Friggstad *et al.* [40] show that a local-search

algorithm with $O(1)$-swaps runs in polynomial time under a $(1+\delta)$-stable assumption for any $\delta > 0$. However, none of the algorithms for stable instances of clustering so far have running time near-linear in n, even when the stability parameter α is large, points lie in $\mathbb{R}^2$, and the underlying metric is Euclidean.

On the hardness side, solving $(3-\delta)$-center proximal k-median instances in general metric spaces is NP-hard for any $\delta > 0$ [16]. When restricted to Euclidean spaces in arbitrary dimensions, Ben-David and Reyzin [24] showed that for every $\delta > 0$, solving discrete $(2-\delta)$-center proximal k-median instances is NP-hard. Similarly, the clustering problem for discrete k-center remains hard for α-stable instances when $\alpha < 2$, assuming standard complexity assumption that NP $\neq$ RP [22]. Under the same complexity assumption, discrete α-stable k-means is also hard when $\alpha < 1 + \delta_0$ for some positive constant δ_0 [40]. Deshpande *et al.* [36] showed it is NP-hard to $(1+\varepsilon)$-approximate $(2-\delta)$-center proximal k-means instances.

2 Definitions and Preliminaries

Clustering. Let $X = \{p_1, \ldots, p_n\}$ be a set of n points in $\mathbb{R}^d$, and let $\delta : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{\geq 0}$ be a distance function (not necessarily a metric satisfying triangle inequality). For a set $Y \subseteq \mathbb{R}^d$, we define $\boldsymbol{\delta(p, Y)} := \min_{y \in Y} \delta(p, y)$. A ***k*-clustering** of X is a partition of X into k non-empty **clusters** $X_1, \ldots, X_k$. We focus on center-based clusterings that are induced by a set $S := \{c_1, \ldots, c_k\}$ of k **centers**; each X_i is the subset of points of X that are closest to c_i in S under δ, that is, $X_i := \{p \in X \mid \delta(p, c_i) \leq \delta(p, c_j)\}$ (ties are broken arbitrarily). Assuming the nearest neighbor of each point of X in S is unique (under distance function δ), S defines a k-clustering of X. Sometimes it is more convenient to denote a k-clustering by its set of centers S.

The quality of a clustering S of X is defined using a cost function $\boldsymbol{\$(X, S)}$; cost function \$ depends on the distance function δ, so sometimes we may use the notation $\$_\delta$ to emphasize the underlying distance function. The goal is to compute $S^* := \arg\min_S \$(X, S)$ where the minimum is taken over all subsets $S \subset \mathbb{R}^d$ of k points. Several different cost functions have been proposed, leading to various optimization problems. We consider the following three popular variants:

- ***k*-median clustering**: the cost function is $\$(X, S) = \sum_{p \in X} \delta(p, S)$.
- ***k*-means clustering**: the cost function is $\$(X, S) = \sum_{p \in X} (\delta(p, S))^2$.
- ***k*-center clustering**: the cost function is $\$(X, S) = \max_{p \in X} \delta(p, S)$.

In some cases we wish S to be a subset of X, in which case we refer to the problem as the **discrete *k*-clustering** problem. For example, the discrete k-median problem is to compute $\arg\min_{S \subseteq X, |S|=k} \sum_{p \in X} \delta(p, S)$. The discrete k-means and discrete k-center problems are defined analogously.

Given point set X, distance function δ, and cost function \$, we refer to $(X, \delta, \$)$ as a **clustering instance**. If \$ is defined directly by the distance function δ, we use (X, δ) to denote a clustering instance. Note that a center of a set of points may not be unique (e.g. when δ is defined by the L_1-metric and \$ is the sum of distances) or it may not be easy to compute (e.g. when δ is defined by the L_2-metric and \$ is the sum of distances).

Stability. Let X be a point set in Euclidean space $\mathbb{R}^d$. For $\alpha \geq 1$, a clustering instance $(X, \delta, \$_\delta)$ is **$\boldsymbol{\alpha}$-stable** if for any *perturbed distance function* $\tilde{\delta}$ (not necessary a metric) satisfying $\delta(p, q) \leq \tilde{\delta}(p, q) \leq \alpha \cdot \delta(p, q)$ for all $p, q \in \mathbb{R}^d$, any optimal clustering of $(X, \delta, \$_\delta)$ is also an optimal clustering of $(X, \tilde{\delta}, \$_{\tilde{\delta}})$. Note that the cluster centers as well as the cost of optimal clustering may be different for the two instances. We exploit the following property of stability, which follows directly from its definition.

Lemma 2.1. *Let (X, δ) be an α-stable clustering instance with $\alpha > 1$. Then the optimal clustering O of (X, δ) is unique.*

Proof: Assume for contradiction that there are two optimal clusterings O and O'. There must be a point p in X that belongs to a cluster centered at c in O but is assigned to a different center c' in O'. Consider the perturbed distance $\tilde{\delta}$ by scaling inter-cluster distances in O by an α factor while preserving all intra-cluster distances. Then

$$\alpha \cdot \delta(p, c) \leq \alpha \cdot \delta(p, c') = \tilde{\delta}(p, c') \leq \tilde{\delta}(p, c) = \delta(p, c),$$

where the first inequality is by definition of clustering O, the second inequality is by definition of clustering O' still being optimal under $\tilde{\delta}$ by α-stability, and the two equalities are follows from how the perturbed distance is defined. This give a contradiction as long as $\alpha > 1$. □

Metric approximations. The next lemma, which we rely on heavily throughout the paper, is the observation that a change of metric preserves the optimal clustering as long as the new metric is a β-approximation of the original metric satisfying $\beta < \alpha$.

Lemma 2.2. *Given point set X, let δ and δ' be two metrics satisfying $\delta(p,q) \le \delta'(p,q) \le \beta \cdot \delta(p,q)$ for all p and q in X for some β. Let (X,δ) be an α-stable clustering instance with $\alpha > \beta$. Then the optimal clustering of (X,δ) is also the optimal clustering of (X,δ'), and vice versa. Furthermore, (X,δ') is an (α/β)-stable clustering instance.*

Proof: Because (X,δ) is α-stable for $\alpha > \beta$, the optimal clustering of (X,δ) is also an optimal clustering of (X,δ') by taking δ' to be the perturbed distance. Now, for an arbitrary perturbed distance $\tilde{\delta}'$ satisfying $\delta'(p,q) \le \tilde{\delta}'(p,q) \le (\alpha/\beta)\cdot\delta'(p,q)$ for all $p,q \in X$, one has

$$\delta(p,q) \le \delta'(p,q) \le \tilde{\delta}'(p,q) \le \frac{\alpha}{\beta}\cdot\delta'(p,q) \le \alpha\cdot\delta(p,q),$$

and therefore the optimal clustering O of (X,δ) and (X,δ') is must be an optimal clustering of $(X,\tilde{\delta}')$, proving that (X,δ') is (α/β)-stable. Providing $\alpha > \beta$, the optimal clustering of (X,δ') is again unique by Lemma 2.1; in other words, the optimal clustering of (X,δ') is by definition equal to the optimal clustering of (X,δ). □

Polyhedral metric. In light of the metric approximation lemma, we would like to approximate the Euclidean metric without losing too much stability, using a collection of convex distance functions generalizing the L_∞-metric in Euclidean space. Let $N \subseteq S^{d-1}$ be a centrally-symmetric set of γ unit vectors (that is, if $u \in N$ then $-u \in N$) such that for any unit vector $v \in S^{d-1}$, there is a vector $u \in N$ within angle $\arccos(1-\varepsilon) = O(\sqrt{\varepsilon})$. The number of vectors needed in N is known to be $O(\varepsilon^{-(d-1)/2})$. We define the **polyhedral metric** $\delta_N : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{\ge 0}$ to be $\boldsymbol{\delta_N(p,q)} := \max_{u\in N}\langle p-q,u\rangle$.

Since N is centrally symmetric, δ_N is symmetric and thus a metric. The unit ball under δ_N is a convex polyhedron, thus the name polyhedral metric. By construction, an easy calculation shows that for any p and q in $\mathbb{R}^d$, $\|p-q\| \ge \delta_N(p,q) \ge (1-\varepsilon)\cdot\|p-q\|$. By scaling each vector in N by a $1+\varepsilon$ factor, we can ensure that $(1+\varepsilon)\cdot\|p-q\| \ge \delta_N(p,q) \ge \|p-q\|$. By taking ε to be small enough, the optimal clustering for α-stable clustering instance $(X,\|\cdot\|,\$)$ is the same as that for $(X,\delta_N,\$)$ by Lemma 2.2, and the new instance $(X,\delta_N,\$)$ is $(1-\varepsilon)\alpha$-stable if the original instance $(X,\|\cdot\|,\$)$ is α-stable.

Center proximity. A clustering instance (X,δ) satisfies *α-center proximity property* [16] if for any distinct optimal clusters X_i and X_j with centers c_i and c_j and any point $p \in X_i$, one has $\alpha\cdot\delta(p,c_i) < \delta(p,c_j)$. Awasthi, Blum, and Sheffet showed that any α-stable instance satisfies α-center proximity [16, Fact 2.2] (also [12, Theorem 3.1] under metric perturbation). Optimal solutions of α-stable instances satisfy the following separation properties.[2]

- α-center proximity implies that $(\alpha-1)\cdot\delta(p,c_i) < \delta(p,q)$ for any $p \in X_i$ and any $q \notin X_i$. For $\alpha \ge 2$, a point is closer to its own center than to any point of another cluster.[3]
- For $\alpha \ge 2+\sqrt{3}$, α-center proximity implies that $\delta(p,p') < \delta(p,q)$ for any $p,p' \in X_i$ and any $q \notin X_i$. In other words, from any point p in X, any *intra*-cluster distance to a point p' is shorter than any *inter*-cluster distance to a point q.[3]

We make use of the following stronger intra-inter distance property on α-stable instances, which allows us to compare *any* intra-distance between two points in X_i and *any* inter-distance between a point in X_i and a point in X_j.

Lemma 2.3. *Let (X,δ) be an α-stable instance, $\alpha > 1$, and let X_1 be a cluster in an optimal clustering with $q \in X \setminus X_1$ and $p,p',p'' \in X_1$. If δ is a metric, then $\delta(p,p') \le \delta(p'',q)$ for $\alpha \ge 2+\sqrt{5}$. If δ is the Euclidean metric in $\mathbb{R}^d$, then $\delta(p,p') \le \delta(p'',q)$ for $\alpha \ge 2+\sqrt{3}$.*

Proof. See Appendix A.1.

Finally, we note that it is enough to consider the discrete version of the clustering problem for stable instances.

[2] We give an additional list of known separation properties in Appendix A.1.

[3] They are known as *weak center proximity* [22] and *strict separation property* [20,24] respectively.

Lemma 2.4. *For any α-stable instance $(X, \delta, \$_\delta)$ with $\alpha \geq 2+\sqrt{3}$, any continuous optimal k-clustering is a discrete optimal k-clustering and vice versa.*

Proof: Consider O to be an optimal solution of an arbitrary α-stable instance (X, δ) in the continuous setting; denote the centers in O as $o_1, \ldots, o_k$. Define solution O' to be the set of centers $\mathrm{nn}_1, \ldots, \mathrm{nn}_k$, where nn_i is defined to be the nearest point of o_i in X. By definition O' is a discrete solution as all centers nn_i lie in X. We now argue that O' is in fact an optimal solution of the k-clustering instance (X, δ).

First we show that nn_i must be a point that was assigned to o_i in clustering O. Assume for contradiction that nn_i was in a different cluster with center o_j. Let p be an arbitrary point in cluster O_i. By center proximity one has $\delta(p, \mathrm{nn}_i) > (\alpha-1)\cdot\delta(p, o_i)$. But then this implies $(\alpha-1)\cdot\delta(p, o_i) < \delta(p, \mathrm{nn}_i) \leq \delta(p, o_i) + \delta(o_i, \mathrm{nn}_i)$, that is, $\delta(p, o_i) \leq (\alpha-2)\cdot\delta(p, o_i) < \delta(o_i, \mathrm{nn}_i)$ given $\alpha \geq 3$, a contradiction.

Now again take an arbitrary point p in some arbitrary cluster O_i. Compare the distances $\delta(p, \mathrm{nn}_i)$ and $\delta(p, \mathrm{nn}_j)$ for any other center nn_j in O'. By [24, Theorem 8] for $\alpha > 2+\sqrt{3}$ any intra-cluster distance is smaller than any inter-cluster distance. Thus, $\delta(p, \mathrm{nn}_i) < \delta(p, \mathrm{nn}_j)$ since nn_i lies in O_i and nn_j lies in O_j. Therefore the clustering formed by the centers in O' is identical to the clustering of O, thus proving that O' is an optimal solution of (X, δ). □

3 Efficient Dynamic Programming

We now describe a simple, efficient algorithm for computing the optimal clustering for the k-means, k-center, and k-median problem assuming the given instance is α-stable for $\alpha \geq 2+\sqrt{3}$. Roughly speaking, we make the following observation: if there are at least two clusters, then the two endpoints of the longest edge of the minimum spanning tree of X belong to different clusters, and no cluster has points in both subtrees of the minimum spanning tree delimited by the longest edge. We describe the dynamic programming algorithm in Section 3.1 and then describe the procedure for computing cluster costs in Section 3.2. We summarize the results in this section by the following theorem.

Theorem 3.1. *Let X be a set with n points lying in $\mathbb{R}^d$ and $k \geq 1$ an integer. If the k-means, k-median, or k-center instance for X under the Euclidean metric is α-stable for $\alpha \geq 2+\sqrt{3}+\varepsilon$ for any constant $\varepsilon > 0$, then the optimal clustering can be computed in $O(nk^2 + n\,\mathrm{polylog}\,n)$ time. For $d = 2$ the assumption can be relaxed to $\alpha \geq 2+\sqrt{3}$.*

3.1 Fast Dynamic Programming

The following lemma is the key observation for our algorithm.

Lemma 3.2. *Let $(X, \delta, \$)$ be an α-stable k-clustering instance with $\alpha \geq 2+\sqrt{3}$ and $k \geq 2$, and let T be the minimum spanning tree of X under metric δ. Then (1) The two endpoints u and v of the longest edge e in T do not belong to the same cluster; (2) each cluster lies in the same connected component of $T \setminus \{e\}$.*

Proof: Assume for contradiction that the longest spanning tree edge uv belongs to the same cluster X_i in the optimal k-clustering O. Since $k > 1$, there is at least one other cluster X_j of O with a spanning tree edge xy connecting X_i to X_j. Given $\alpha \geq 2+\sqrt{3}$, $d(u, v) < d(x, y)$ by Lemma 2.3, a contradiction. The second statement follows from Angelidakis *et al.* [12, Lemma 4.1]. □

Algorithm. We fix the metric δ and the cost function $\$$. For a subset $Y \subseteq X$ and for an integer j between 1 and $k-1$, let $\boldsymbol{\mu(Y; j)}$ denote the optimal cost of an j-clustering on Y (under δ and $\$$). Recall that our definition of j-clustering required all clusters to be non-empty, so it is not defined for $|Y| < j$. For simplicity, we assume that $\mu(Y; j) = \infty$ for $|Y| < j$. Let $\boldsymbol{T}$ be the minimum spanning tree on X under δ, let uv be the longest edge in T; let X_u and X_v be the set of vertices of the two components of $T \setminus \{uv\}$. Then $\mu(X; k)$ satisfies the following recurrence relation:

$$\mu(X; k) = \begin{cases} \mu(X; 1) & \text{if } k = 1, \\ \infty & \text{if } k > |X|, \\ \min_{1 \leq i < k} \{\mu(X_u; i) + \mu(X_v; k-i)\} & \text{if } |X| > 1 \text{ and } k > 1. \end{cases} \tag{1}$$

Using recurrence (1), we compute $\mu(X;k)$ as follows. Let R be a *recursion tree*, a binary tree where each node v in R is associated with a subtree T_v of T. If v is the root of R, then $T_v = T$. Recursion tree R is defined recursively as follows. Let $X_v \subseteq X$ be the set of vertices of T in T_v. If $|X_v| = 1$, then v is a leaf. Each interior node v of T is also associated with the longest edge e_v of T_v. Removal of e_v decomposes T_v into two connected components, each of which is associated with one of the children of v. After having computed T, R can be computed in $O(n \log n)$ time by sorting the edges in decreasing order of their costs.[4]

For each node $v \in \mathsf{R}$ and for every i between 1 and $k-1$, we compute $\mu(X_v;i)$ as follows. If v is a leaf, we set $\mu(X_v;1) = 0$ and $\mu(X_v;i) = \infty$ otherwise. For all interior nodes v, we compute $\mu(X_v;1)$ using the algorithms described in Section 3.2. Finally, if v is an interior node and $i > 1$, we compute $\mu(X_v;i)$ using the recurrence relation (1). Recall that if w and z are the children of v, then $\mu(X_w;\ell)$ and $\mu(X_z;r)$ for all ℓ and r have been computed before we compute $\mu(X_v;i)$.

Let $\tau(n)$ be the time spent in computing T plus the total time spent in computing $\mu(X_v,1)$ for all nodes $v \in \mathsf{R}$. Then the overall time taken by the algorithm is $O(nk^2 + \tau(n))$. What is left is to compute the minimum spanning tree T and all $\mu(X_v,1)$ efficiently.

3.2 Efficient Implementation

In this section, we show how to obtain the minimum spanning tree and compute $\mu(X_v;1)$ efficiently for 1-mean, 1-center, and 1-median when $X \subseteq \mathbb{R}^d$. We can compute the Euclidean minimum spanning tree T in $O(n \log n)$ time in $\mathbb{R}^2$ [59]. We can then compute $\mu(X_v;1)$ efficiently either under Euclidean metric (for 1-mean), or switch to the L_1-metric and compute $\mu(X_v;1)$ efficiently using Lemma 2.2 (for 1-center and 1-median).

There are two difficulties in extending the 2D data structures to higher dimensions. No near-linear time algorithm is known for computing the Euclidean minimum spanning tree for $d \geq 3$, and we can work with the L_1-metric only if $\alpha \geq \sqrt{d}$ (Lemma 2.2). We address both of these difficulties by working with a polyhedral metric δ_N. Let $\alpha \geq 2 + \sqrt{3} + \Omega(1)$ be the stability parameter. By taking the number of vectors in N (defined by the polyhedral metric) to be large enough, we can ensure that $(1-\varepsilon)\|p-q\| \leq \delta_N(p,q) \leq \|p-q\|$ for all $p,q \in \mathbb{R}^d$. By Lemma 2.2, X is an α-stable instance under δ_N for $\alpha \geq 2+\sqrt{3}$. We first compute the minimum spanning tree of X in $O(n \operatorname{polylog} n)$ time under δ_N using the result of Callahan and Kosaraju [26], and then compute $\mu(X_v,1)$.

Data structure. We compute $\mu(X_v;1)$ in a bottom-up manner. When processing a node v of R, we maintain a dynamic data structure $\boldsymbol{\Psi_v}$ on X_v from which $\mu(X_v;1)$ can be computed quickly. The exact form of Ψ_v depends on the cost function to be described below. Before that, we analyze the running time $\tau(n)$ spent on computing every $\mu(X_v;1)$. Let w and z be the two children of v. Suppose we have Ψ_w and Ψ_z at our disposal and suppose $|X_w| \leq |X_z|$. We insert the points of X_w into Ψ_z one by one and obtain Ψ_v from which we compute $\mu(X_v;1)$. Suppose $Q(n)$ is the update time of Ψ_v as well as the time taken to compute $\mu(X_v;1)$ from Ψ_v. The total number of insert operations performed over all nodes of R is $O(n \log n)$ because we insert the points of the smaller set into the larger set at each node of R [45, 58]. Hence $\tau(n) = O(Q(n) \cdot n \log n)$. We now describe the data structure for each specific clustering problem.

1-mean. We work with the L_2-metric. Here the center of a single cluster consisting of X_v is the centroid $\sigma_v := \left(\sum_{p \in X_v} p\right)/|X_v|$, and $\mu(X_v;1) = \sum_{p \in X_v} \|p\|^2 - |X_v| \cdot \|\sigma_v\|^2$. At each node v, we maintain $\sum_{p \in X_v} p$ and $\sum_{p \in X_v} \|p\|^2$. Point insertion takes $O(1)$ time so $Q(n) = 1$.

1-center. As mentioned in the beginning of the section, we can work with the L_1-metric for $d = 2$. We wish to find the smallest L_1-disc (a diamond) that contains X_v. Let $e^+ = (1,1)$ and $e^- = (-1,1)$. Then the radius ρ_v of the smaller L_1-disc containing X_v is

$$\rho_v = \frac{1}{2} \max\left\{ \max_{p \in X_v} \langle p, e^+ \rangle - \min_{p \in X_v} \langle p, e^+ \rangle, \max_{p \in X_v} \langle p, e^- \rangle - \min_{p \in X_v} \langle p, e^- \rangle \right\}. \tag{2}$$

We maintain the four terms $\max_{p \in X_v} \langle p, e^+ \rangle$, $\min_{p \in X_v} \langle p, e^+ \rangle$, $\max_{p \in X_v} \langle p, e^- \rangle$, and $\min_{p \in X_v} \langle p, e^- \rangle$ at v. A point can be inserted in $O(1)$ time and ρ_v can be computed from these four terms in $O(1)$ time. Therefore, $Q(n) = O(1)$.

[4] Tree R is nothing but the minimum spanning tree constructed by Kruskal's algorithm.

1-center in higher dimensions For $d > 2$, we work with a polyhedral metric δ_N with $N = 2^{O(d)}$. For a node v, we need to compute the smallest ball $B(X_v)$ under δ_N that contains X_v. We need a few geometric observations to compute the smallest enclosing ball efficiently.

For each $u \in N$, let H_u be the halfspace $\langle x, u\rangle \le 1$, that is, the halfspace bounded by the hyperplane tangent to S^{d-1} at u and containing the origin. Define $Q := \bigcap_{u\in N} H_u$. A ball of radius λ centered at p under δ_N is $P + \lambda Q$. For a vector $u \in N$, let $\overline{p}_u := \arg\max_{p\in x_v}\langle p, u\rangle$ be the maximal point in direction u. Set $\overline{X}_v := \{\overline{p}_u \mid u \in N\}$. The following simple lemma is the key to computing $B(X_v)$.

Lemma 3.3. *Any δ_N-ball that contains $\overline{X}_v$ also contains X_v.*

By Lemma 3.3, it suffices to compute $B(\overline{X}_v)$. The next observation is that $B(\overline{X}_v)$ has a basis of size $d+1$, i.e. there is a subset Y of $d+1$ points of X_v such that $B(Y) = B(\overline{X}_v) = B(X_v)$. One can try all possible subsets of $\overline{X}_v$ in $O(\gamma^{d+1}) = 2^{O(d^2)}$ time.[5] We note that $\overline{X}_v$ can be maintained under insertion in $O(\gamma) = 2^{O(d)}$ time, and we then re-compute $B(\overline{X}_v)$ in $2^{O(d^2)}$ time. Hence, $Q(n) = O(1)$.

1-median. Similar to 1-center, we work with the polyhedral metric. Fix a node v of T. For a point $x \in \mathbb{R}^d$, let $F_v(x) = \sum_{p\in X_v}\delta_N(x,p)$ which is a piecewise-linear function. Our goal is to compute $\xi^*_v = \arg\min_{x\in\mathbb{R}^d} F_v(x)$. Our data structure is a dynamic range-tree [3] used for orthogonal range searching that can insert a point in $O(\log n)$ time. Using multi-dimensional parametric search [5], ξ^*_v can be computed in $O(\text{poly}\log n)$ time after each update.

1-median in higher dimensions For simplicity, we describe the data structure for $d = 2$. It extends to high dimensions in a straightforward manner.

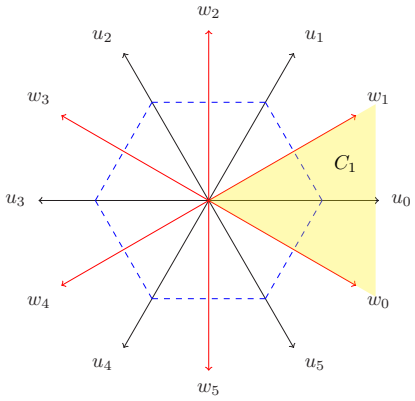

Figure 3.1. Polyhedral metric defined by $N = \{u_0, \dots u_5\}$, with C_1 corresponding to Ψ_1.

Fix a node v. We describe the data structure for maintaining ξ^*_v under insertion of points [6] Let $N = \{u_0, \dots, u_{r-1}\} \subset S^1$ be the set of unit vectors that define the metric δ_N. We partition the plane into a family $\mathcal{C} = \{C_0, \dots, C_{r-1}\}$ of r cones such that for a point $p \in C_i$, $\delta_N(p, 0) = \langle p, u_i\rangle$. C_i is defined by unit vectors w_{i-1}, w_i, where w_j is the unit vector in direction $(u_{j-1} + u_j)|_2$; see Figure 3.1. For a point $x \in \mathbb{R}^2$ and $j < r$, let $C_j(x) = C_j + x$. Then,

$$F_v(x) = \sum_{i=1}^{r-1}\sum_{p\in C_i(x)\cap X_v}\delta_N(p,x) = \sum_{i=0}^{r-1}\sum_{p\in C_i(x)\cap X_v}\langle p - x, u_i\rangle$$
$$= \sum_{i=0}^{r-1}\sum_{p\in C_i(x)\cap X_v}\langle p, u_i\rangle - \sum_{i=0}^{r}|C_i(x)\cap X_v|\cdot\langle x, u_i\rangle.$$

[5] A more complex algorithm can compute $B(\overline{X}_v)$ in $\gamma\cdot 2^{O(d)} = 2^{O(d)}$ time, but we ignore this improvement.

[6] We note that ξ^*_v may not be unique. The minimum may be realized of a convex polygon.

We note that $F_v(x)$ is a piecewise-linear convex function. We construct a separate data structure Ψ_i for each i so that for any $x \in \mathbb{R}^2$, Ψ_i computes $\alpha_i(x) = \sum_{p \in C_i(x) \cap X_v} \langle p, u_i \rangle$ and $\beta_i(x) = |C_i(x) \cap X_v|$. Ψ_i is basically a dynamic $2D$ range tree in which the coordinates of a point are described with w_{i-1}, w_i as the coordinate axes; see [35]. Ψ_i requires $O(n \log n)$ space, a query can be answered in $O(\log^2 n)$ time, and a point can be inserted in $O(\log^2 n)$ amortized time. Hence, the overall query and update time is $O(r \log^2 n)$. We note that α_i, β_i for $i < r$ can be used to compute the linear function $L_{v,x}$ that represents x (recall that F_v is piecewise linear). Let $\Psi = (\Psi_0, \ldots, \Psi_{r-1})$ denote the overall data structure, and let $Q_0(x)$ be the above query procedure on Ψ.

Using $\Psi, Q_0(\cdot)$, and multi-dimensional parametric search, we compute ξ^*_v as follows. For a line ℓ in $\mathbb{R}^2$, let $\xi^*_{v,\ell} = \arg\min_{x \in \ell} F_v(x)$. We first describe how to compute $\xi^*_{v,\ell}$. Let q be a point on ℓ. By invoking $Q_0(q)$ on Ψ, we can compute $F_v(q)$ as well as $L_{v,q}$. Using $L_{v,q}$, we can determine whether $q = \xi^*_{v,l}$, q lies to left of $\xi^*_{v,l}$, or q lies to the right of $\xi^*_{v,l}$. We refer to this as the "decision" procedure. In order to compute ξ^*_v, we simulate Q_0 generically on $\xi^*_{v,l}$ without knowing its value and using Q_0 on known points as the decision procedure at each step of this generic procedure. More precisely, at each step, a Ψ_i compares the w_{i-1} or w_i-coordinate, say w_i-coordinate $\xi_{v,x}$, with a real value Δ. Let q be the intersection point of ℓ and the line $w_i = \Delta$. By invoking $Q_0(q)$ on Ψ, we can determine in $O(r \log^2 n)$ time whether q lies to the left or right of ξ^*_v, which in turn determines whether the w_i-coordinate of $\xi^*_{v,\ell}$ is smaller or greater than Δ. (If $q = \xi^*_{x,\ell}$, then we have found $\xi^*_{x,\ell}$). Hence, each step of the decision procedure can be determined in $O(r \log^2 n)$ time. The total time taken by the generic procedure is $O(r^2 \log^4 n)$. The parametric search technique ensures that the generic procedure will query with $\xi^*_{v,\ell}$ as one of the steps, so the decision procedure will detect this and return $\xi^*_{v,\ell}$.

Let $Q_1(\ell)$ denote the above procedure to compute $\xi^*_{v,\ell}$. By simulating Q_0 on ξ^*_v generically but now using Q_1 as the decision procedure, we can compute ξ^*_v in $O(r^3 \log^6 n)$ time. Hence, we can maintain ξ^*_v in $O(\log^6 n)$ time under insertion of a point. In higher dimensions, Q_0 takes $O(\log^d n)$ time in $\mathbb{R}^d$. So the parametric search will take $O(\log^{d(d+1)} n)$ time to compute ξ^*_v.

4 k-Median: Single-Swap Local Search

We customize the standard local-search framework for the k-clustering problem [32, 33, 41]. In order to recover the optimal solution, we must define near-optimality more carefully. Let (X, δ) be an instance of α-stable k-median in $\mathbb{R}^2$ for $\alpha > 5$. By Lemma 2.4, it suffices to consider the *discrete* k-median problem In Section 4, we describe a simple local-search algorithm for finding the optimal clustering of (X, δ). In Section 4 we show that the algorithm terminates within $O(k \log(n\Delta))$ iterations. We obtain the following.

Theorem 4.1. *Let (X, δ) be an α-stable instance of the k-median problem for some $\alpha > 5$ where X is a set of n points in $\mathbb{R}^2$ equipped with L_p-metric δ. The 1-swap local search algorithm terminates with the optimal clustering in $O(k \log(n\Delta))$ iterations.*

Local-search algorithm. The local-search algorithm maintains a k-clustering induced by a set S of k cluster centers. At each step, it finds a pair of points $x \in X$ and $y \in S$ such that $\$(X, S + x - y)$ is minimized. If $\$(X, S + x - y) \geq \$(X, S)$, it stops and returns the k-clustering induced by S. Otherwise it replaces S with $S + x - y$ and repeats the above step. The pair (x, y) will be referred to as a **1-swap**.

Local-search analysis. The high-level structure of our analysis follows Friggstad *et al.* [41], however new ideas are needed for 1-swap. In this subsection, we denote a k-clustering by the set of its cluster centers. Let S be a fixed k-clustering, and let O be the optimal clustering. For a subset $Y \subseteq X$, we use $\mathbf{\$(Y)}$ and $\mathbf{\$^*(Y)}$ to denote $\$(Y, S)$ and $\$(Y, O)$, respectively. Similarly, for a point $p \in X$, we use $\mathbf{nn(p)}$ and $\mathbf{nn^*(p)}$ to denote the nearest neighbor of p in S and in O, respectively; define $\boldsymbol{\delta(p)}$ to be $\delta(p, S)$ and $\boldsymbol{\delta^*(p)}$ to be $\delta(p, O)$. We partition X into four subsets as follows:

- $\boldsymbol{X_{00}} := \{p \in X \mid \mathrm{nn}(p) \in S \setminus O, \mathrm{nn}^*(p) \in O \setminus S\}$;
- $\boldsymbol{X_{01}} := \{p \in X \mid \mathrm{nn}(p) \in S \setminus O, \mathrm{nn}^*(p) \in S \cap O\}$;
- $\boldsymbol{X_{10}} := \{p \in X \mid \mathrm{nn}(p) \in S \cap O, \mathrm{nn}^*(p) \in O \setminus S\}$;

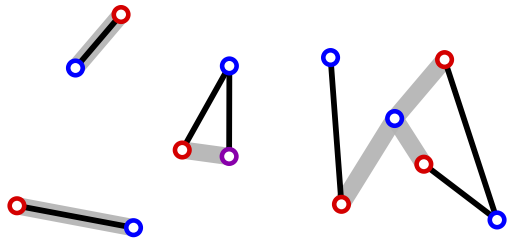

Figure 4.1. Illustration of candidate swaps $\mathscr{S}$ in $\mathbb{R}^2$. The blue dots belong to set S, the red dots belong to set O; the only purple dot is in $S \cap O$. The thick gray segments indicate pairs inside the stars; each star has exact one blue dot as its center. The black pairs are the candidate swaps. Notice that the partitions of S and O form connected components.

- $\boldsymbol{X_{11}} \coloneqq \left\{p \in X \mid \mathrm{nn}(p) \in S \cap O, \mathrm{nn}^*(p) \in S \cap O\right\}$.

Observe that for any point p in X_{11}, $\mathrm{nn}(p) = \mathrm{nn}^*(p)$ and $\$(p) = \$^*(p)$; for any point p in X_{01}, one has $\$(p) \le \$^*(p)$; and for any point p in X_{10}, one has $\$(p) \ge \$^*(p)$. Costs $\delta(p)$ and $\delta^*(p)$ are not directly comparable for point p in X_{00}. A k-clustering S is **C-good** for some parameter $C \ge 0$ if $\$(X) \le \$^*(X) + C \cdot \$^*(X_{00})$.

Lemma 4.2. *Any C-good clustering S for an α-stable clustering instance $(X, \delta, \$)$ must be optimal for $\alpha \ge C + 1$.*

Proof: Define a perturbed distance function $\tilde{\boldsymbol{\delta}} : X \times X \to \mathbb{R}_{\ge 0}$ with respect to the given clustering S as follows:

$$\tilde{\delta}(p', p) \coloneqq \begin{cases} \alpha \cdot \delta(p', p) & \text{if } p \ne \mathrm{nn}(p'), \\ \delta(p', p) & \text{otherwise.} \end{cases}$$

Note that $\tilde{\delta}$ is not symmetric. Let $\tilde{\boldsymbol{\$}}\boldsymbol{(\cdot,\cdot)}$ denote the cost function under the perturbed distance function $\tilde{\delta}$. The optimal clustering under perturbed cost function is the same as the original optimal clustering O by the stability assumption. Since $\mathrm{nn}(p) = \mathrm{nn}^*(p)$ if and only if $p \in X_{11}$, the cost of O under the perturbed cost can be written as:

$$\tilde{\$}(X, O) = \alpha \cdot \$(X_{00}, O) + \alpha \cdot \$(X_{01}, O) + \alpha \cdot \$(X_{10}, O) + \$(X_{11}, O).$$

By definition of perturbed distance $\tilde{\delta}$, $\tilde{\$}(X, S) = \$(X, S)$. Now, by the assumption that clustering S is C-good,

$$\begin{aligned} \tilde{\$}(X, S) = \$(X, S) &\le \$(X, O) + C \cdot \$(X_{00}, O) \\ &\le (C+1) \cdot \$(X_{00}, O) + \$(X_{01}, O) + \$(X_{10}, O) + \$(X_{11}, O) \\ &\le \tilde{\$}(X, O); \end{aligned}$$

the last inequality follows by taking $\alpha \ge C + 1$. This implies that S is an optimal clustering for $(X, \tilde{\delta})$, and thus is equal to O. □

Next, we prove a lower bound on the improvement in the cost of a clustering that is not C-good after performing a 1-swap. Following Arya *et al.* [14], define the set of **candidate swaps** $\mathscr{S}$ as follows: For each center i in S, consider the **star $\boldsymbol{\Sigma_i}$** centered at i defined as the collection of pairs $\Sigma_i \coloneqq \{(i, j) \in S \times O \mid \mathrm{nn}(j) = i\}$. Denote **center($\boldsymbol{j}$)** to be the center of the star where j belongs; in other words, $\mathrm{center}(j) = i$ if j belongs to Σ_i.

For $i \in S$, let $\boldsymbol{O_i} \coloneqq \{j \in O \mid \mathrm{center}(j) = i\}$ be the set of centers of O in star Σ_i. If $|O_i| = 1$, then we add the only pair $(i, j) \in \Sigma_i$ to the candidate set $\mathscr{S}$. Let $\boldsymbol{S_\varnothing} \coloneqq \{i \in S \mid O_i = \varnothing\}$. Let $\boldsymbol{O_{>1}}$ contain centers in O that belong to a star of size greater than 1. We pick $|O_{>1}|$ pairs from $S_\varnothing \times O_{>1}$ such that each point of $O_{>1}$ is matched only once and each point of $S_\varnothing$ is matched at most twice and add them to $\mathscr{S}$; this is feasible because $|S_\varnothing| \ge |O_{>1}|/2$. Since each center in O belongs to exactly one pair of $\mathscr{S}$, $|\mathscr{S}| = k$. By construction, if $|\Sigma_i| \ge 2$, then i does not belong to any candidate swap. See Figure 4.1.

Lemma 4.3. *For each point p in X_{01}, X_{10}, or X_{11}, the set of candidate swaps $\mathscr{S}$ satisfies*

$$\sum_{(i,j) \in \mathscr{S}} (\delta(p) - \delta'(p)) \ge \delta(p) - \delta^*(p); \tag{3}$$

and for each point p in X_{00}, the set of candidate swaps $\mathscr{S}$ satisfies

$$\sum_{(i,j)\in\mathscr{S}} (\delta(p)-\delta'(p)) \geq (\delta(p)-\delta^*(p))-4\delta^*(p), \tag{4}$$

where $\$'$ is the cost function on X defined with respect to $S' := S-i+j$, and $\delta'(p)$ is the distance between p and its nearest neighbor in S'.

Proof: For point p in X_{11}, both $\mathrm{nn}(p)$ and $\mathrm{nn}^*(p)$ are in S', so $\delta'(p)=\delta(p)=\delta^*(p)$. For point p in X_{01}, $\delta(p)\leq\delta^*(p)$; when $\mathrm{nn}(p)$ is being swapped out by some in 1-swap S', $\mathrm{nn}^*(p)$ must be in S'. For point p in X_{10}, $\delta(p)\geq\delta^*(p)$; center $\mathrm{nn}(p)$ will never be swapped out by any 1-swap in $\mathscr{S}$, so $\delta'(p)\leq\delta(p)$. By construction of $\mathscr{S}$, there is exactly one choice of S' that swaps $\mathrm{nn}^*(p)$ in; for that particular swap we have $\delta'(p)=\delta^*(p)$. In all three cases one has inequality (3). Our final goal is to prove inequality (4). Consider a swap (i,j) in $\mathscr{S}$. There are three cases to consider:

- $j=\mathrm{nn}^*(p)$. There is exactly one swap for which $j=\mathrm{nn}^*(p)$. In this case $\delta(p)\leq\delta^*(p)$, therefore $\delta(p)-\delta'(p)\geq\delta(p)-\delta^*(p)$.
- $j\neq\mathrm{nn}^*(p)$ *and* $i\neq\mathrm{nn}(p)$. Since $\mathrm{nn}(p)\in S'$, $\delta'(p)\leq\delta(p)$. Therefore $\delta(p)-\delta'(p)\geq 0$.
- $j\neq\mathrm{nn}^*(p)$ *and* $i=\mathrm{nn}(p)$. By construction, there are most two swaps in $\mathscr{S}$ that may swap out $\mathrm{nn}(p)$. We claim that $i\neq\mathrm{center}(\mathrm{nn}^*(p))$. Indeed, if $i=\mathrm{center}(\mathrm{nn}^*(p))$, then by construction, $\Sigma_i=\{(i,\mathrm{nn}^*(p))\}$ because the center of star of size greater than one is never added to a candidate swap. But this contradicts the assumption that $j\neq\mathrm{nn}^*(p)$. The claim implies that $\mathrm{center}(\mathrm{nn}^*(p))\in S'$ and thus $\delta'(p)\leq\delta(p,\mathrm{center}(\mathrm{nn}^*(p)))$. We obtain a bound on $\delta(p,\mathrm{center}(\mathrm{nn}^*(p)))$ as follows:

$$\begin{aligned}\delta(p,\mathrm{center}(\mathrm{nn}^*(p))) &\leq \delta(p,\mathrm{nn}^*(p))+\delta(\mathrm{nn}^*(p),\mathrm{center}(\mathrm{nn}^*(p)))\\ &\leq \delta^*(p)+\delta(\mathrm{nn}^*(p),\mathrm{nn}(p)) \leq \delta^*(p)+(\delta^*(p)+\delta(p))=\delta(p)+2\delta^*(p).\end{aligned}$$

  Therefore, $\delta(p)-\delta'(p)\geq\delta(p)-\delta(p,\mathrm{center}(\mathrm{nn}^*(p)))$. Putting everything together, we obtain:

$$\sum_{S'\in\mathscr{S}}(\delta(p)-\delta'(p)) \geq (\delta(p)-\delta^*(p))+0+2(\delta(p)-\delta(p)-2\delta^*(p))=\delta(p)-5\delta^*(p).$$

□

Using Lemma 4.3, we can prove the following.

Lemma 4.4. *Let S be a k-clustering of (X,δ) that is not C-good for some fixed constant $C>4+\varepsilon$ with arbitrarily small $\varepsilon>0$. There is always a 1-swap S' such that $\$'(X)-\$^*(X)\leq(1-\varepsilon/(1+\varepsilon)k)\cdot(\$(X)-\$^*(X))$, where $\$'$ is the cost function defined with respect to S'.*

Proof: By Lemma 4.3 one has $\$(X)-\$'(X)\geq(\$(X)-\$^*(X)-\Psi(X_{00}))/k$ for some 1-swap S' and its corresponding cost function $\$'(\cdot)$. Since S is not C-good, $\$(X)-\$^*(X)>C\cdot\$^*(X_{00})$. Rearranging and plugging the definition of $\Psi(\cdot)$, we have

$$\begin{aligned}\$'(X)-\$^*(X) &\leq \$(X)-\$^*(X)-(\$(X)-\$^*(X)-\Psi(X_{00}))/k\\ &\leq \$(X)-\$^*(X)-(\$(X)-\$^*(X)-4\cdot\$^*(X_{00}))/k\\ &\leq \$(X)-\$^*(X)-(\$(X)-\$^*(X)+(M-1)\cdot(\$(X)-\$^*(X))-4M\cdot\$^*(X_{00}))/Mk\\ &\leq \left(1-\frac{\varepsilon}{(1+\varepsilon)k}\right)\cdot(\$(X)-\$^*(X)),\end{aligned}$$

where the last inequality holds by taking M to be arbitrarily large (say $M>1+1/\varepsilon$). □

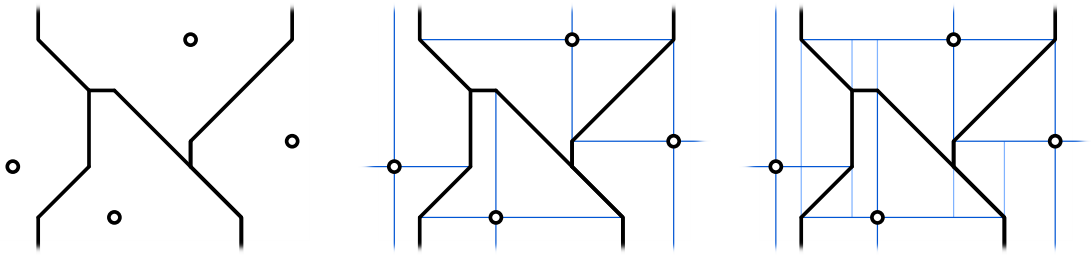

Figure 5.1. L_1 Voronoi diagram V, quadrant decomposition $\tilde{V}$, and trapezoid decomposition $V^{\parallel}$.

5 Efficient Implementation of Local Search

We describe an efficient implementation of each step of the local-search algorithm in this section. By Lemma 2.2, it suffices to implement the algorithm using a polyhedral metric δ_N. We show that each step of 1-swap can be implemented in $O(nk^{2d-1}\operatorname{polylog} n)$ time under the assumption that $\alpha > 5$. We obtain the following:

Theorem 5.1. *Let (X,δ) be an α-stable instance of the k-median problem where $X \subset \mathbb{R}^d$ and δ is the Euclidean metric. For $\alpha > 5$, the 1-swap local search algorithm computes the optimal k-clustering of (X,δ) in $O(nk^{2d-1}\operatorname{polylog} n)$ time.*

For simplicity, we present a slightly weaker result for $d = 2$ using the L_1-metric, as it is straightforward to implement and more intuitive. Using the L_1-metric requires $\alpha > 5\sqrt{2}$. The extension to higher dimensional Euclidean space using the polyhedral works for $\alpha > 5$.

Voronoi diagram under $\mathbf{L_1}$ norm. First, we fix a point $x \in X \setminus S$ to insert and a center $y \in S$ to drop. Define $S' := S + x - y$. We build the L_1 Voronoi diagram V of S'. The cells of V may not be convex, but they are *star-shaped*: for any $c \in S'$ and for any point $x \in \mathrm{Vor}(c)$, the segment cx lies completely in $\mathrm{Vor}(c)$. Furthermore, all line segments on the cell boundaries of V must have slopes belonging to one of the four possible values: vertical, horizontal, diagonal, or antidiagonal.

Next, decompose each Voronoi cell $\mathrm{Vor}(c)$ into four *quadrants* centered at c. Denote the resulting subdivision of V as $\tilde{V}$. We compute a *trapezoidal decomposition* $V^{\parallel}$ of the diagram $\tilde{V}$ by drawing a vertical segment from each vertex of $\tilde{V}$ in both directions until it meets an edge of V; $V^{\parallel}$ has $O(k)$ trapezoids, see Figure 5.1. For each trapezoid $\tau \in V^{\parallel}$, let $X_\tau := X \cap \tau$. The cost of the new clustering S' can be computed as $\$(X,S') = \sum_{\tau \in V^{\parallel}} \$(X_\tau, S')$.

Range-sum queries. Now we discuss how to compute $\$(X_\tau, S')$. Each trapezoid τ in cells $\mathrm{Vor}(c)$ is associated with a vector $u(\tau) \in \{\pm 1\}^2$, depending on which of the four quadrants τ belongs to with respect to the axis-parallel segments drawn passing through the center c of the cell. If τ lies in the top-right quadrant then $u(\tau) = (1,1)$. Similarly if τ lies in the top-left (resp. bottom-left, bottom-right) then $u(\tau) = (-1,1)$ (resp. $(-1,-1)$, $(1,-1)$).

$$\$(X_\tau, S') = \sum_{x \in X_\tau} \|x - c\|_1 = \sum_{x \in X_\tau} \langle x - c, u(\tau)\rangle = \sum_{x \in X_\tau} \langle x, u(\tau)\rangle - |X_\tau| \cdot \langle c, u(\tau)\rangle. \tag{5}$$

We preprocess X into a data structure that answers the following query:

- TRAPEZOIDSUM(τ, u): Given a trapezoid τ and a vector $u \in \{\pm 1\}^2$, return $|X \cap \tau|$ as well as $\sum_{x \in X \cap \tau} \langle x, u\rangle$.

The above query can be viewed as a 3-oriented polygonal range query [35]. We construct a 3-level range tree Ψ on X. Omitting the details (which can be found in [35]), Ψ can be constructed in $O(n \log^2 n)$ time and uses $O(n \log^2 n)$ space. Each node ξ at the third level of Ψ is associated with a subset $X_\xi \subseteq X$. We store $w(\xi, u) := \sum_{x \in X_\xi} \langle x, u\rangle$ for each $u \in \{\pm 1\}^2$ and $|X_\xi|$ at ξ. For a trapezoid τ, the query procedure identifies in $O(\log^3 n)$ time a set Ξ_τ of $O(\log^3 n)$ third-level nodes such that $X \cap \tau = \cup_{\xi \in \Xi_\tau} X_\xi$ and each point of $X \cap \tau$ appears as exactly one node of Ξ_τ. Then $\sum_{x \in X_\tau} \langle x, u\rangle = \sum_{\xi \in \Xi_\tau} w(\xi, u)$ and $|X_\tau| = \sum_{\xi \in \Xi_\tau} |X_\xi|$.

1-SWAP(X,S):
input: Point set X and centers S
for each point $x \in X \setminus S$ and center $y \in S$:
$S' \leftarrow S + x - y$
$V \leftarrow L_1$ Voronoi diagram of S'
$\tilde{V} \leftarrow$ decompose each cell Vor(c) into four quadrants centered at c
$V^{\parallel} \leftarrow$ trapezoidal decomposition of $\tilde{V}$
for each trapezoid $\tau \in V^{\parallel}$:
$\$(X_\tau, S') \leftarrow$ TRAPEZOIDSUM$(\tau, u(\tau))$
$\$(X,S') \leftarrow \sum_{\tau \in V^{\parallel}} \$(X_\tau, S')$
return (x,y) with the lowest $\$(X, S+x-y)$

Figure 5.2. Efficient implementation of 1-swap under 1-norm.

With the information stored at the nodes in Ξ_τ, TRAPEZOIDSUM(τ,u) query can be answered in $O(\log^3 n)$ time. By performing TRAPEZOIDSUM$(\tau,u(\tau))$ query for all $\tau \in V^{\parallel}$, $\$(X_\tau,S')$ can be computed in $O(k\log^3 n)$ time since $V^{\parallel}$ has a total of $O(k)$ trapezoids.

We summarize the implementation of 1-swap algorithm in Figure 5.2. The 1-swap procedure considers at most nk different k-clusterings. Therefore we obtain the following.

Lemma 5.2. *Let $(X,\delta,\$)$ be a given clustering instance where δ is the L_1 metric, and let S be a given k-clustering. After $O(n\log n)$ time preprocessing, we find a k-clustering $S' := S + x - y$ minimizing $\$(X,S')$ among all choices of (x,y) in $O(nk^2\log^3 n)$ time.*

5.1 Cost of 1-swap in higher dimensions

The 1-SWAP algorithm can be extended to higher dimensions using the theory of geometric arrangements [6,7,57]. The details are rather technical, so we only sketch the proofs here. As in Section 3.2, instead of working with the L_1 metric, we work with a polyhedral metric. Let the centrally-symmetric set $N \subseteq S^{d-1}$ and the convex polyhedron Q be defined as in Section 3.2. The set N partitions $\mathbb{R}^d$ into a set of $O(1)$ polyhedral cones denoted by $\mathscr{C} := \{C_1,\ldots,C_\gamma\}$, each with 0 as its apex so that all points (when viewed as vectors) in a cone have the same vector u of N as the nearest neighbor under the cosine distance, i.e. the polyhedral distance $\delta_N(0,u)$ is realized by u. The total complexity of $\mathscr{C}$ is $O(\gamma) = O(1)$.

We show that X can be preprocessed into a data structure so that $\$(X,S)$, the cost of the k-clustering induced by any k-point subset S of X under δ_N can be computed in $O(k^{2d}\,\mathrm{polylog}(n))$ time.

Let $S \subset X$ be a set of k points. We compute the Voronoi diagram VD(S) of S under the distance function δ_N. More precisely, for a point $c \in S$, let $f_c\colon \mathbb{R}^d \to \mathbb{R}_{\geq 0}$ be the function $f_c(x) := \delta_N(c,x)$. The graph of f_c is a polyhedral cone in $\mathbb{R}^{d+1}$ whose level set for the value λ is the *homothet* copy of Q, $c + \lambda Q$. Voronoi diagram VD(S) is the minimization diagram of function f_c over every point c in S; that is, the projection of the lower envelope $f(x) := \min_c f_c(x)$ onto the hyperplane $X_{d+1} = 0$ (identified with $\mathbb{R}^d$). We further decompose each Voronoi cell Vor(c) of VD(S) by drawing the family of cones in $\mathscr{C}$ from c; put it differently, by drawing the cone $c + C_j$ for $1 \leq j \leq k$, within the cell Vor(c). Each cell τ in the refined subdivision of Vor(c) has the property that for all points $x \in \tau$, $\delta_N(x,c)$ is realized by the vector of N—by u_j if $x \in c + C_j$. Let $\tilde{V}$ denote the resulting refinement of VD(S).

Finally, we compute the vertical decomposition of each cell in $\tilde{V}$, which is the extension of the trapezoidal decomposition to higher dimensions; see [48,57] for details. Let $V^{\parallel}$ denote the resulting convex subdivision of $\mathbb{R}^d$. It is known that $V^{\parallel}$ has $O(k^{2d-2})$ cells, that it can be computed in $O(k^{2d-2})$ time, and that each cell of $V^{\parallel}$ is convex and bounded by at most $2d$ facets, namely it is the intersection of at most $2d$ halfspaces. Using the same structure of the distance function δ_N, we can show that there is a set U of $O(\gamma^d) = O(1)$ unit vectors such that each facet of a cell in $V^{\parallel}$ is normal to a vector in U, and that U depends only on N and not on S.

With these observations at hand, we preprocess X into a data structure as follows: we fix a $2d$-tuple $\bar{u} := (u_1,\ldots,u_{2d}) \in U^{2d}$. Let $R_{\bar{u}}$ be the set of all convex polyhedra formed by the intersection of at most $2d$ halfspaces each of which is normal to a vector in $\bar{u}$. Using a multi-level range tree (consisting of $2d$ levels), we preprocess X in $O(n\log^{2d} n)$ time into a data structure $\Psi_{\bar{u}}$ of size $O(n\log^{2d-1} n)$ for each $\bar{u}$, so that for a query cell $\tau \in R_{\bar{u}}$ and for a vector $u \in N$, we can quickly compute the total weight $w(\tau,u) = \sum_{p \in X\cap\tau}\langle p,u\rangle$ in $O(\log^{2d} n)$ time.

For a given S, we compute the cost $\$(X,S)$ as follows. We first compute $\mathrm{VD}(S)$ and $V^{\parallel}(S)$. For each cell $\tau \in V^{\parallel}(S)$ lying in $\mathrm{Vor}(c)$, let $u(\tau) \in N$ be the vector u_j such that $\tau \subseteq c + C_j$. As in the 2d case,

$$\$(X,S) = \sum_c \sum_{p \in \mathrm{Vor}(c)} \delta_N(p,c) = \sum_c \sum_{\tau \in V^{\parallel}(S) \cap \mathrm{Vor}(c)} \sum_{p \in X \cap \tau} \langle p - c, u(\tau) \rangle$$
$$= \sum_c \sum_{\tau \in V^{\parallel}(S) \cap \mathrm{Vor}(c)} \left(\sum_{p \in X \cap \tau} \langle p, u(\tau) \rangle - |X \cap \tau| \cdot \langle c, u(\tau) \rangle \right).$$

Fix a cell $\tau \in V^{\parallel}(S) \cap \mathrm{Vor}(c)$. Suppose $\tau \in R_{\bar{u}}$. Then by querying the data structure $\Psi_{\bar{u}}$ with τ and $u(\tau)$, we can compute $w(\tau,u) = \sum_{p \in X \cap \tau} \langle p, u(\tau) \rangle$ in $O(\log^d n)$ time. Repeating this procedure over all cells of $V^{\parallel}(S)$, $\$(X,S)$ can be computed in $O(k^{2d-1} \log^{2d} n)$ time, after an initial preprocessing of $O(n \log^{2d} n)$ time.

6 Coresets and an Alternative Linear Time Algorithm

In this section we provide an alternative way to compute the optimal k-clustering, where the objective can be any of k-center, k-means, or k-median. Here we are aiming for a running time linear in n, but potentially with exponential dependence on k. With such a goal we can further relax the stability requirement using the idea of *coresets*. When there is strict separation between clusters (when $\alpha \geq 2 + \sqrt{3}$), we can recover the optimal clustering. We note that this provides a significant improvement to the stability parameter needed for k-median over the local search approach, albeit with worse running time dependence on k.

Coresets. Let (X,δ) be a clustering instance. The **radius** of a cluster X_i is the maximum distance between its center and any point in X_i. Let S be a given k-clustering of (X,δ), with clusters $X_1,\ldots,X_k$, centers $c_1,\ldots,c_k$, and radius $r_1,\ldots,r_k$, respectively. Let O be the optimal k-clustering of (X,δ), with clusters $X_1^*,\ldots,X_k^*$, centers $c_1^*,\ldots,c_k^*$ and radius $r_1^*,\ldots,r_k^*$, respectively. Let $B(c,r)$ denote the ball centered at c with radius r under δ.

A point set $Q \subseteq X$ is a **multiplicative ε-coreset** of X if every k-clustering S of Q satisfies

$$X \subseteq \bigcup_i B\left(c_i, (1+\varepsilon) \cdot r_i\right).$$

Lemma 6.1. *Let (X,δ) be a $(1+\varepsilon)$-stable clustering instance with optimal k-clustering O. A multiplicative ε-coreset of X contains at least one point from each cluster of O.*

Proof: Let Q be a multiplicative ε-coreset of X. We start by defining a k-clustering S_Q of Q. For each point q in Q, assign q to its cluster in the optimal clustering O. This results in some clustering with at most k clusters. Insert additional empty clusters to create a valid k-clustering S_Q of Q.

Assume that Q does not contain any points from some optimal cluster X_i^* of O. Consider the center point c_i^* of X_i^*. By the fact that Q is a multiplicative ε-coreset, c_i^* must be contained in a ball resulting from the expansion of each cluster of S_Q by an ε-fraction of its radius. In notation, let the cluster of S_Q whose expansion covers c_i^* be X_j, with center c_j and radius r_j. Then one has $\delta(c_j, c_i^*) \leq (1+\varepsilon) \cdot r_j$.

Because S_Q is constructed by restricting the optimal clustering O on Q, cluster X_j is a subset of some optimal cluster in O: $X_j \subseteq X_j^*$. This implies $r_j \leq r_j^*$. Additionally, c_j and c_i^* lie in different optimal clusters, as c_j is in Q and therefore does not lie in X_i^*. So by $(1+\varepsilon)$-center proximity:

$$\delta(c_j, c_i^*) > (1+\varepsilon) \cdot \delta(c_j, c_j^*) = (1+\varepsilon) \cdot r_j^* \geq (1+\varepsilon) \cdot r_j,$$

contradicting to $\delta(c_j, c_i^*) \leq (1+\varepsilon) \cdot r_j$. Therefore, Q must contain at least one point from each optimal cluster. □

Algorithm. We first compute a constant approximation to the clustering problem instance (X,δ). We then recursively construct a multiplicative coreset of size $O(k!/\varepsilon^{dk})$ [4, 44]. By taking $\varepsilon = 1$, the coreset has size $O(k!)$ and for 2-stable instances, the multiplicative 2-coreset Q contains at least one point from every optimal cluster by Lemma 6.1. After obtaining this coreset, we then need to reconstruct the optimal clustering. By [24, Corollary 9],

when our instance satisfies strict separation ($\alpha \geq 2+\sqrt{3}$), taking any point from each optimal cluster induces the optimal partitioning of X. To find k such points, each from a different optimal cluster, we try all possible k subsets of Q as the candidate k centers. For each set of centers we compute its cost (under polygonal metric) using the cost computation scheme of Section 5, then take the clustering with minimum cost. Finally, recompute the optimal centers using any 1-clustering algorithm on each cluster of O.

It is known constant approximation to any of the k-means, k-median, or k-center instance can be computed in $O(nk)$ time [42] and even in $\tilde{O}(n)$ time [30, 44] in constant-dimensional Euclidean spaces. Thus computing the multiplicative 2-coreset takes $O(nk^2 + k!)$ time [43]. Using the cost computation scheme from Section 5, after $O(n \log^{2d} n)$ preprocessing time, the cost of each clustering can be computed in $\tilde{O}(k^{2d-1})$ time. There are at most $O((k!)^k)$ possible choices of center set of size k.

We conclude the section with the following theorem.

Theorem 6.2. *Let X be a set with n points lying in $\mathbb{R}^d$ and $k \geq 1$ an integer. If the k-means, k-median, or k-center instance for X under the Euclidean distance is α-stable for $\alpha \geq 2+\sqrt{3}$ then the optimal clustering can be computed in $\tilde{O}(nk^2 + k^{2d-1} \cdot (k!)^k)$ time.*

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A Appendix

A.1 Stability Properties

Properties of α-center proximity. Let (X,δ) be a clustering instance satisfying α-center proximity, where δ is a metric and $\alpha > 1$. Let X_1 be a cluster with center c_1 in an optimal clustering. Let $p, p', p'' \in X_1$ and $q \in X \setminus X_1$ with c_2 the center of q's cluster. Then,

(1) $(\alpha-1)\cdot\delta(p,c_1) < \delta(p,q)$;

(2) $(\alpha-1)\cdot\delta(p,c_1) < \delta(c_1,c_2)$;

(3) $(\alpha-1)\cdot\delta(c_1,c_1) < (\alpha+1)\cdot\delta(p,q)$;

(4) $(\alpha-1)\cdot\delta(p,p') < \frac{2\alpha}{\alpha-1}\cdot\delta(p,q)$; $\qquad\qquad \delta(p,p') < \delta(p,q)$ for $\alpha \geq 2+\sqrt{3}$

(5) $(\alpha-1)\cdot\delta(p',p'') < \frac{2(\alpha+1)}{\alpha-1}\cdot\delta(p,q)$. $\qquad\qquad \delta(p',p'') < \delta(p,q)$ for $\alpha \geq 2+\sqrt{5}$

Proof:
(1) $\delta(p,q) \leq (\alpha-1)\cdot\delta(p,c_1)$ yields the following contradiction.

$$\begin{aligned} \alpha\cdot\delta(q,c_2) < \delta(q,c_1) \leq \delta(p,c_1)+\delta(p,q) \leq \alpha\cdot\delta(p,c_1) \quad &\Rightarrow \quad \delta(q,c_2) < \delta(p,c_1) \\ \alpha\cdot\delta(p,c_1) < \delta(p,c_2) \leq \delta(q,c_2)+\delta(p,q) \leq \delta(q,c_2)+(\alpha-1)\cdot\delta(p,c_1) \quad &\Rightarrow \quad \delta(p,c_1) < \delta(q,c_2) \end{aligned}$$

(2) Follows from $\alpha\cdot\delta(p,c_1) < \delta(p,c_2) \leq \delta(p,c_1)+\delta(c_1,c_2)$.

(3) Follows by $\delta(c_1,c_2) \leq \delta(c_1,p)+\delta(p,q)+\delta(q,c_2) \overset{(1)}{<} \left(\frac{2}{\alpha-1}+1\right)\cdot\delta(p,q) = \frac{\alpha+1}{\alpha-1}\cdot\delta(p,q)$.

(4) Follows by

$$\begin{aligned} (\alpha-1)\cdot\delta(p,p') \quad &\leq \quad (\alpha-1)\cdot\delta(p,c_1)+(\alpha-1)\cdot\delta(p',c_1) \overset{(1),(2)}{<} \delta(p,q)+\delta(c_1,c_2) \\ &\overset{(3)}{<} \quad \delta(p,q)+\frac{\alpha+1}{\alpha-1}\cdot\delta(p,q) = \frac{2\alpha}{\alpha-1}\cdot\delta(p,q). \end{aligned}$$

(5) Follows by

$$(\alpha-1)\cdot\delta(p',p'') \leq (\alpha-1)\cdot\delta(p',c_1)+(\alpha-1)\cdot\delta(p'',c_1) \overset{(2)}{<} 2\cdot\delta(c_1,c_2) \overset{(3)}{<} \frac{2(\alpha+1)}{\alpha-1}\cdot\delta(p,q).$$

□

Proof (Proof of Lemma 2.3): Let c_1 and c_2 be the centers of cluster X_1 and q's cluster, respectively.
(i) First we show that $\delta(c_1,c_2) < \frac{\alpha+1}{\alpha-1}\cdot\delta(p'',q)$:

$$\begin{aligned} \delta(p'',q) &\geq \delta(q,c_1)-\delta(p'',c_1) \\ &\geq \delta(c_1,c_2)-\delta(q,c_2)-\delta(p'',c_1) \\ &> \delta(c_1,c_2)-\big(\delta(q,p'')+\delta(p'',q)\big)/(\alpha-1). \end{aligned}$$

Rearranging the inequality proves the claim.

Now $\alpha\cdot\delta(p,c_1) < \delta(p,c_2) \leq \delta(p,c_1)+\delta(c_1,c_2)$, which implies that $(\alpha-1)\cdot\delta(p,c_1) < \delta(c_1,c_2)$. It follows that

$$\begin{aligned} \delta(p,p') &\leq \delta(p,c_1)+\delta(p',c_1) \\ &< 2\cdot\delta(c_1,c_2)/(\alpha-1) \\ &< \frac{2(\alpha+1)}{(\alpha-1)^2}\cdot\delta(p'',q) \\ &\leq \delta(p'',q), \end{aligned}$$

where the last inequality holds when $\alpha \geq 2+\sqrt{5}$.

(ii) Let us assume $\delta(c_1, c_2) = 1$. We know that $\delta(p, c_2) > \alpha \cdot \delta(p, c_1)$ for all $p \in X_1$. The set of points p with $\delta(p, c_2) = \alpha \cdot \delta(p, c_1)$ is known as Apollonian Circle A_1 (with c_1 inside, but not centered at c_1!), see Fig. A.1. X_1 must be contained inside this circle A_1, or sphere in higher dimensions. Similarly, there is a sphere A_2 enclosing q's cluster (relative to X_1).

We take the classical fact that these are circles as given, but we want to understand the involved parameters. Of course, the circle A_1 has to be centered on the line ℓ through c_1 and c_2. Let a and b be the intersections of A_1 with ℓ, with b on the segment c_1c_2. $\delta(c_1, b) = \alpha\delta(c_2, b) = \alpha(1 - \delta(c_1, b))$, hence $\delta(c_1, b) = \frac{1}{\alpha+1}$. Similarly, $\delta(c_1, a) = \alpha\delta(c_2, a) = \alpha(1 + \delta(c_1, a))$, hence $\delta(c_1, a) = \frac{1}{\alpha-1}$. This sets the diameter of A_1 to $\frac{1}{\alpha+1} + \frac{1}{\alpha-1} = \frac{2\alpha}{\alpha^2-1}$, and the distance between A_1 and A_2 to $1 - 2 \cdot \frac{1}{\alpha+1} = \frac{\alpha-1}{\alpha+1}$. It follows that $\delta(p', p'')/\delta(p''', q) < \frac{2\alpha}{\alpha^2-1} / \frac{\alpha-1}{\alpha+1} = \frac{2\alpha}{(\alpha-1)^2}$. □

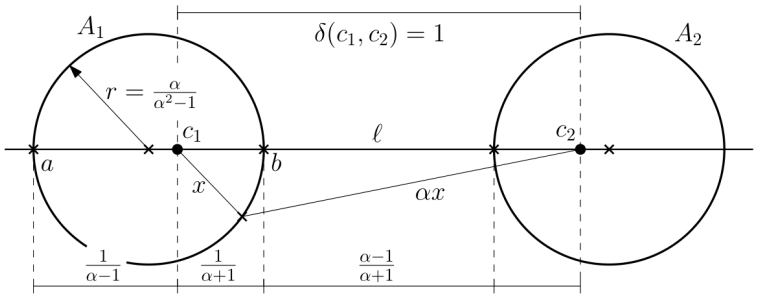

Figure A.1. The Apollonian Circles (with parameter α) for clusters centered at c_1 and c_2.