Approximation Schemes for Clustering Problems in Finite Metrics and High Dimensional Spaces

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Abstract

We give polynomial time approximation schemes (PTASs) for the problem of partitioning an input set of n points into a fixed number k of clusters so as to minimize the sum over all clusters of the sum of pairwise distances in a cluster. Our algorithms work for arbitrary metric spaces as well as for points in $\mathbb{R}^d$ where the distance between two points x, y is measured by $\|x-y\|_2^2$ (notice that $(\mathbb{R}^d, \|\cdot\|_2^2)$ is not a metric space). Our algorithms can be modified to handle other objective functions, such as minimizing the sum over all clusters of the sum of distances to the best choice for a cluster center. The method of solution of this paper depends on some new techniques which could be also of independent interest.

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1 Introduction

Problem statement and motivation. The problem of partitioning a data set into a small number of *clusters*, each containing a set of seemingly related items, has a crucial role in many information retrieval and data analysis applications, such as web search and classification [5, 19], or interpretation of experimental data in molecular biology [24]. For example, when searching or mining massive unstructured data sets, data items are often processed and represented as points in a high dimensional space $\mathbb{R}^d$, where some standard distance function measures affinity (see, for example, [7, 25, 11, 5]).

This paper deals with the question of designing good algorithms for an attractive criterion for clustering quality in such a setting. More specifically, we consider a set V of n points endowed with a distance function $\delta : V \times V \to \mathbb{R}$. These points have to be partitioned into a fixed number k of subsets $C_1, C_2, \ldots, C_k$ so as to minimize the cost of the partition, which is defined to be the sum over all clusters of the sum of pairwise distances in a cluster. We call this problem k-Clustering. We also deal with the k-Median and the k-Center problems. In the k-Median problem the cost of a clustering is the sum over all clusters of the sum of distances between cluster points and the best choice for a cluster center. In the k-Center problem, the cost of a clustering is the maximum distance between a point and its cluster center. In the settings that we consider, these optimization problems are NP-hard (by similar arguments as in [9, 8]) to solve exactly even for $k = 2$.

Our results. Our algorithms deal with the case that δ is an arbitrary metric (including, in particular, points in $\mathbb{R}^d$ with distances induced by some norm). We also handle the non-metric case of points in $\mathbb{R}^d$ where the distance between two points x, y is measured by $\delta(x, y) = \|x - y\|_2^2$. We refer to instances of the latter form as ℓ_2^2 instances.

For the k-Clustering problem, we present algorithms for every fixed integer k and for every fixed $\epsilon > 0$ that compute a partition into k clusters $C_1, C_2, \ldots, C_k$ of cost at most $1 + \epsilon$ times the cost of an optimum partition. The algorithm is randomized and its running time is $O(n^{2k} + n^{k+1} 2^{\tilde{O}(1/\epsilon^{3k+1})})$. In the ℓ_2^2 case, the algorithms are deterministic, and their running time is $n^{O(k/\epsilon^2)}$. Our algorithms can be modified to output, for all $\zeta > 0$, a clustering that excludes at most ζn outliers and has cost at most $1 + \epsilon$ times the optimum cost. In the case of the square of Euclidean distance, we can do this in probabilistic time $O(n^3 \log n)$, where the hidden term in the $O()$ grows (rapidly) with k, $\frac{1}{\epsilon}$, and $\frac{1}{\zeta}$. We do not present the modification in this extended abstract.

The k-Median problem can be solved optimally in polynomial time for fixed k in finite metrics, because the number of choices for centers is polynomial. However, if the points are located in a larger space, such as $\mathbb{R}^d$, and the centers can be picked from this larger space, the problem may become hard. For ℓ_2^2 instances, we give k-Median algorithms that partition the input point-set into k clusters of cost at most $1 + \epsilon$ of the optimum cost in probabilistic time $O(g(k, \epsilon) \cdot n \cdot (\log n)^k)$, where g grows (rapidly) with k and $\frac{1}{\epsilon}$. Some of our algorithms can be modified trivially to derive polynomial time approximation schemes for other objective functions, such as the k-Center problem. We do not elaborate on these modifications in this extended abstract.

Related work. The k-Clustering problem was proposed by Sahni and Gonzalez [22] in the setting of arbitrary weighted graphs. Unfortunately, only poor approximation guarantees are possible [17, 12]. Guttman-Beck and Hassin [15] initiated the study of the problem in metrics. Schulman [23] gave probabilistic algorithms for clustering ℓ_2^2 instances. (Thus he also handled other interesting cases of metrics that embed isometrically into this distance space, such as Euclidean metrics or L^1 metrics.) His algorithms find a clustering such that either its cost is within a factor of $1+\epsilon$ of the optimum cost, or it can be converted into an optimum clustering by changing the assignment of at most an ϵ fraction of the points. The running time is linear if $d = o(\log n / \log\log n)$ and otherwise the running time is $n^{O(\log\log n)}$. Thus our results improve and extend Schulman's results, giving a true polynomial time approximation scheme for arbitrary dimension.

Earlier, Fernandez de la Vega and Kenyon [9] presented a polynomial time approximation scheme for Metric Max Cut, an objective function that is the complement of Metric 2-Clustering. Indyk [16] used the Max Cut algorithm as a black box ingredient to derive a polynomial time approximation scheme for the latter problem. Thus our results extend Indyk's result to the case of arbitrary fixed k.

As mentioned above, instances of k-Median in finite metrics with fixed k are trivially solvable in polynomial time. (For arbitrary k, the problem is APX-hard [14].) This is not the case in geometric settings, including the ℓ_2^2 case discussed in this paper. This case was considered by Drineas, Frieze, Kannan, Vempala, and Vinay [10], who gave a 2-approximation algorithm. Ostrovsky and Rabani [21] gave a polynomial time approximation scheme for this case and other geometric settings. Bădoiu, Har-Peled, and Indyk [4] gave a polynomial time approximation scheme for points in Euclidean space with much improved running time (as well as results on other clustering objectives). Our results, derived independently of [4], improve significantly the running time for the ℓ_2^2 case. Our k-Median algorithms and analysis are in many respects similar to the algorithms in [4] (though they handle a different distance function).

It is interesting to note that both Schulman's algorithm for k-Clustering and the algorithm of Fernandez de la Vega and Kenyon for Metric Max Cut use a similar idea of sampling data points at random from a biased distribution that depends on the pairwise distances. In recent research on clustering problems, sampling has been the core idea in the design of provably good algorithms for various objective functions.

Notations. Throughout the paper we use V to denote the input set of points and δ to denote the distance function over pairs of points in V. The function δ can be given explicitly or implicitly (for example, if $V \subset \mathbb{R}^d$ and δ is derived from a norm on $\mathbb{R}^d$). Our time bounds count arithmetic operations and assume that computing $\delta(x,y)$ is a single operation. The reader may assume that the input is rational to avoid having to deal with unrealistic computational models. We use k, a fixed constant, to denote the desired number of clusters. We omit the ceiling notation from expressions such as $\lceil 1/\epsilon \rceil$. Our claims and proofs can be modified trivially to account for taking the ceiling of non-integers wherever needed.

Let $X, Y \subset V$ and $x \in V$. With a slight abuse of notation, we use $\delta(x,Y)$ to denote $\sum_{y\in Y} \delta(x,y)$, and we use $\delta(X,Y)$ to denote $\sum_{x\in X} \delta(x,Y)$.[1] We use $\delta(X)$ to denote $\delta(X,X)$.

[1] Notice that $\delta(\cdot,\cdot)$ is a symmetric bilinear form but is not a distance in the power set of V.

Let $C_1, C_2, \ldots, C_k$ be a partition of V into k disjoint clusters. Then, for all $i = 1, 2, \ldots, k$, we use $\text{cost}(C_i)$ to denote the cost of C_i, and we use $c = \text{cost}(C_1, C_2, \ldots, C_k) = \sum_i \text{cost}(C_i)$ to denote the cost of the clustering. In the k-Clustering problem, $\text{cost}(C_i) = \frac{1}{2}\delta(C_i)$. In the k-Median problem, $\text{cost}(C_i) = \min_{x \in \mathbb{R}^d} \{\delta(x, C_i)\}$. In the k-Center problem, $\text{cost}(C_i) = \min_{x \in \mathbb{R}^d} \max_{y \in C_i} \{\delta(x, y)\}$, and $\text{cost}(C_1, C_2, \ldots, C_k) = \max i = 1^k \text{cost}(C_i)$. We use $C_1^*, C_2^*, \ldots, C_k^*$ to denote a clustering of V of minimum cost c^*.

Our polynomial time approximation schemes handle the case where δ induces an arbitrary metric on V, as well as the non-metric case of $V \subset \mathbb{R}^d$ and $\delta(x, y) = \|x - y\|_2^2$. Instances of points in $\mathbb{R}^d$ are computationally hard if d is part of the input.[2]

2 A PTAS for Metric Instances

In this section we present our algorithm for clustering metric spaces. Before we describe the algorithm, we need some definitions.

2.1 Preliminaries

The main property of metric spaces that we use is the following proposition, which follows easily from the triangle inequality.

Proposition 1. Let $X, Y, Z \subseteq V$. Then,

$$|Z|\delta(X, Y) \leq |X|\delta(Y, Z) + |Y|\delta(Z, X).$$

It is straightforward to generalize this to more than 3 sets, and we will occasionnally do so. Here is a useful corollary.

Corollary 2. Let $C \subseteq V$. For every vertex $v \in C$ we have

$$\delta(v, C) \geq \frac{\delta(C)}{2|C|}.$$

Let $n_1 \geq n_2 \geq \cdots \geq n_k$ be given.

Definition 1. Define the sequence (ϵ_i) by:

$$\begin{cases} \epsilon_0 = 1 \\ \epsilon_1 = \epsilon \\ \forall i > 1, \quad \epsilon_i = \epsilon_{i-1}^2 \epsilon^2 \end{cases}$$

Let $I_j = (\epsilon_{j+1}, \epsilon_j]$. Let $j_0 \leq k$ be the minimum j such that for every i, the ratio n_i/n_1 is outside the interval I_j. Call a cluster index i *large* if $n_i \geq \epsilon_{j_0} n_1$ and *small* if $n_i < \epsilon_{j_0+1} n_1$.

[2] An exception to this rule is the case of Euclidean distance. The hardness of the problems considered here in the Euclidean case is an open problem.

In our proofs, the following quantities will come up frequently as upper or lower bounds to various cluster sizes, so we use some specific notations for them.

Notation 1.

$$\begin{aligned} M &= n_1 = \max\{n_i\} \\ m &= \min\{n_i \mid i \text{ large}\} \\ s &= \max\{n_i \mid i \text{ small}\} \end{aligned}$$

The advantage of the above definition is that there is a large gap between the sizes of large and of small clusters, much larger than between the sizes of any two large clusters. This will be useful in several places in the analysis and is expressed in the following fact.

Fact 3.

$$\frac{s}{m} \leq \frac{m}{M} \cdot \epsilon^2.$$

Consider two large clusters. They can be far apart, or they can be close together.

Notation 2. Let

$$\beta = \frac{M}{m\epsilon}.$$

Definition 2. Let A and B be two large clusters.We say that A and B are *close* if

$$\delta(A, B) < \beta(\delta(A) + \delta(B)),$$

and that they are *large* otherwise.

Now, the algorithm uses random sampling to have some rough estimate of the position of the clusters in the metric space. In fact, we will use just one sample point per cluster. For the algorithm to work, those sample points must be representative.

Definition 3. Let C be a set of points. An element c of C is *representative* of C if

$$\delta(c, C) \leq 2\frac{\delta(C)}{|C|}.$$

The following is an easy observation from elementary probability.

Lemma 4. Consider a partition $(C_1, \ldots, C_k)$ of V such that C_i has size n_i. For each large i, let c_i be a random uniform element of V. Then, with probability at least $(\epsilon_{j_0}/(2k))^k$, we have the following: for every large i, point c_i is a representative element of C_i.

The algorithm will only work when that event occurs. (As usual, we can always run the algorithm several times to boost up its success probability). When this occurs, the large cluster representatives have the following additional property, which will also come into play in the course of the analysis.

Lemma 5. Let C_i^* and C_j^* be two large clusters, and c_i, c_j their representatives. Assume that C_i^* and C_j^* are close to each other. Then:

$$\delta(c_i, c_j) \leq \frac{2M}{m\epsilon}\frac{OPT}{m^2}.$$

We also use the following propoerty of representatives, which follows easily from Proposition 1.

Lemma 6. Let c be a representative point of cluster C. Then, for any x in V, we have:

$$|\delta(x, C) - |C|\delta(x, c)| \leq 2\frac{\delta(C)}{|C|}.$$

Our algorithm uses, as a black box, an approximation scheme for Metric Max-k-Cut which is already known in the litterature. The Metric Max-k-Cut problem takes as input a set V of n points from an arbitrary metric space, and outputs a partition of V into k clusters $C_1, C_2, \ldots, C_k$ so as to maximize the total distance between pairs of points in different clusters, $\sum_i \sum_{j>i} \delta(C_i, C_j)$. For any partition into k clusters, the sum of the Max-k-Cut value and of the k-Clustering value is constant and equal to the sum of all distances, thus the same partition is optimal for both objective functions. Unfortunately, from the viewpoint of approximation, which involves controlling the relative error, the two problems are quite different, since in general the optimal k-clustering value could be much smaller than the optimal Max-k-Cut value. However, the Max-k-Cut approximation algorithm is still useful when the clusters are close together.

Theorem 7 ([9, 8]). Let k be a fixed integer. Then there is a polynomial time approximation scheme for Metric Max-k-Cut.[3] The running time is $O(n^2 + nk2^{O(1/\epsilon^3)})$.

2.2 The k-Clustering Algorithm

We are now ready to describe the k-clustering algorithm. Intuitively, this algorithm is natural: imagine that the space has a huge number of points. In a nutshell, here is the algorithm. Take a small sample of points. By exhaustive search, find their classification in the(unknown)optimal clustering. Use the information on the sample to classify the rest of the points. Temporarily merge clusters which are too close to one another. Remove outliers. Separate close clusters using the more sophiticated Max-h-Cut algorithm from the litterature, and recursively cluster the outliers into the appropriate number of (small) clusters.

Now, here is the formal description. Fix $\epsilon > 0$. Our algorithm consists of taking the best of all partitions that are generated as follows.

1. By exhaustive search, guess the optimal cluster sizes $n_1 \geq n_2 \geq \cdots \geq n_k$. Define large and small as in Definition 1.

[3]Theorem 7 is actually an easy extension of the Max Cut approximation scheme of [9]. The same reduction which is used for Max Cut also applies to Max-k-Cut, and the resulting weighted dense graph is only a variant of dense graphs in the usual sense, so that the Max-k-Cut approximation schemes for dense graphs (see [13, 3]) apply. An alternative algorithm can be found in [8].

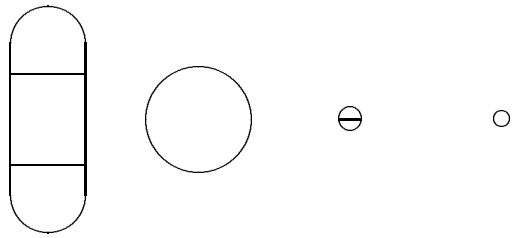

Figure 1: A typical situation for k-clustering. Here $k = 7$, there are 4 large clusters, of which three form a group and one is well-separated from the others, and 3 small clusters, for which the problem will be solved recursively.

2. Define far and close as in Definition 2. By exhaustive search, for each pair of large cluster indices i and j, guess whether C_i^* and C_j^* are close to each other.

3. Taking the equivalence relation which is the transitive closure of the relation "C_i^* and C_j^* are close to each other", define a partition of large cluster indices into groups.

4. For each large cluster C_i^*, let c_i be a random uniform element of V. Assign each point $x \in V$ to the group G which minimizes

$$\min_{i \in G}[n_i \delta(x, c_i)].$$

5. By exhaustive search, for each group G thus constructed, guess $|G \cap S|$, where $S = \cup_{i \text{ small}} C_i^*$ is the union of small clusters. For each x assigned to group G, let

$$f(x) = \min_{i \in G} \delta(x, c_i).$$

   Remove from G's assignment the $|G \cap S|$ elements with largest value $f(x)$.

6. Partition each group of large clusters into the appropriate number h of clusters using the PTAS for Max-h-Cut with error parameter $\epsilon' = \epsilon^2 \epsilon_{j_0}^3 / (3k^3)$.

7. Recursively partition the removed elements into the appropriate number of clusters.

A typical case is presented in figure 2.2.

Theorem 8. For any fixed positive integer k, the algorithm presented in Section 2.2 is a PTAS for the Metric k-Clustering problem. The running time of the algorithm is $O(n^{3k} f(k, \epsilon))$, where $f(k, \epsilon)$ has a leading factor of $exp((1/\epsilon)^{2^k})$.

The running time analysis can be proved by inspection of the algorithm. The rest of this section will be devoted to analyzing the cost of the clustering constructed by the algorithm. The proof is a rather long and technical, sometimes tricky, but not particularly interesting elementary calculation, involving a careful management of the various error terms. The interesting facts have already been spelled out in subsection 2.1. We only provide the proof sketches to enable the dedicated reader to verify correctness.

2.3 Analysis of step 4

We first analyze the mistakes made in step 4 of the algorithm. For any two large clusters i and j which belong to different groups, let $F(i,j)$ denote the set of points $x \in C_i^*$ such that $\min_\ell n_\ell \delta(x, c_\ell) = n_j \delta(x, c_j)$. These points, which really should be in i's group, are mistakenly placed by the algorithm in j's group.

Let

$$C_i = C_i^* + \cup_j F(j,i) - \cup_j F(i,j)$$

for i large, and $C_i = C_i^*$ for i small cluster.

Proposition 9.

$$\sum_i \delta(C_i) \leq \sum_i \delta(C_i^*)(1 + 80k^3\epsilon).$$

To prove this Proposition, we need the following Lemma.

Lemma 10.

$$\delta(F(j,i), C_i^*) - \delta(F(j,i), C_j^*) \leq \frac{2}{m}(\delta(C_i^*) + \delta(C_j^*))|F(j,i)|.$$

Proof: Let $x \in F(j,i)$. By Lemma 6, we have

$$\delta(x, C_i^*) \leq n_i \delta(x, c_i) + 2\frac{\delta(C_i^*)}{n_i}.$$

By the choice of the algorithm, $n_i \delta(x, c_i) \leq n_j \delta(x, c_j)$. By Lemma 6 again, we have

$$n_j \delta(x, c_j) \leq \delta(x, C_j^*) + 2\frac{\delta(C_j^*)}{n_j}.$$

Thus

$$\delta(x, C_i^*) \leq \delta(x, C_j^*) + \frac{2}{m}(\delta(C_i^*) + \delta(C_j^*)).$$

Summing over $x \in F(j,i)$ concludes the proof of the lemma. □

To be able to use Lemma 10, we need an upper bound on $|F(j,i)|$.

Lemma 11.

$$|F(j,i)| \leq \frac{8}{1 - 8\epsilon} m\epsilon.$$

Proof: Let $F = F(j,i)$ for shorthand. Since i and j are in different groups, C_i^* and C_j^* are far from each other, so

$$\delta(C_i^* \cup C_j^*) > \beta(\delta(C_i^*) + \delta(C_j^*)). \tag{1}$$

Consider $x \in F$. By Proposition 1, we have

$$\delta(C_i^* \cup C_j^*) \leq 2\delta(x, C_i^* \cup C_j^*)|C_i^* \cup C_j^*|.$$

Summing over $x \in F$, we get

$$|F|\delta(C_i^* \cup C_j^*) \leq 4M(\delta(F, C_i^*) + \delta(F, C_j^*)).$$

We now use the result of Lemma 10.

$$|F|\delta(C_i^* \cup C_j^*) \leq 4M(2\delta(F, C_j^*) + \frac{2}{m}(\delta(C_i^*) + \delta(C_j^*))|F|).$$

Since $F \subset C_j^*$, we have $\delta(F, C_j^*) \leq \delta(C_j^*)$. Combining with Equation 1 and factoring in $|F|$ gives

$$|F|(\delta(C_i^*) + \delta(C_j^*)(\beta - \frac{8M}{m}) \leq 8M\delta(C_j^*).$$

We conclude that $|F| \leq \frac{8M}{\beta - 8M/m}$, and it only remains to replace β by its value to get the statement of the Lemma. □

Plugging the result of Lemma 11 into Lemma 10 (for the first inequality), or using Proposition 1 followed by Lemma 11 (for the next two inequalities), yields the following Corollary.

Corollary 12.

- $$\delta(F(j,i), C_i^*) - \delta(F(j,i), C_j^*) \leq \epsilon \frac{16}{1-8\epsilon} OPT;$$
- $$\delta(F(j,i)) \leq \epsilon \frac{16}{1-8\epsilon} OPT;$$
- $$\delta(F(i,j), F(i,j')) \leq \epsilon \frac{16}{1-8\epsilon} OPT.$$

Lemma 13.

$$\delta(F(j,i), F(j',i)) \leq \epsilon \frac{16}{1-8\epsilon} OPT.$$

Proof: By Proposition 1, we have

$$\delta(F(j,i), F(j',i)) \leq \frac{|F(j',i)|\delta(F(j,i), C_i^*) + |F(j,i)|\delta(F(j',i), C_i^*)}{|C_i^*|}.$$

By Lemma 11, this yields

$$\delta(F(j,i), F(j',i)) \leq \frac{8}{1-8\epsilon}\epsilon(\delta(F(j,i), C_i^*) + \delta(F(j',i), C_i^*)).$$

By the first statement of Corollary 12, this can be replaced by

$$\delta(F(j,i), F(j',i)) \leq \frac{8}{1-8\epsilon}\epsilon(\delta(F(j,i), C_j^*) + \delta(F(j',i), C_{j'}^* + \epsilon \frac{32}{1-8\epsilon} OPT).$$

Since $F(j,i) \subset C_j^*$ and $F(j',i) \subset C_{j'}^*$, we have:

$$\delta(F(j,i), C_j^*) + \delta(F(j',i), C_{j'}^* \leq OPT,$$

hence the Lemma. □

We are now equipped to prove Proposition 9.

Proof: We write:

$$\begin{aligned}\sum_i \delta(C_i) &= \sum_i \delta(C_i^* + \cup_j F(j,i) - \cup_j F(i,j)) \\ &= \sum_i \delta(C_i^*) + [\sum_{i,j} \delta(C_i^*, F(j,i)) - \sum_{i,j} \delta(C_i^*, F(i,j))] + \sum_i \delta(\cup_j F(j,i) - \cup_j F(i,j)).\end{aligned}$$

We exchange the roles of i and j in the third sum to bound the brackedted quantity using the first statement of Corollary 12. We use bilinearity of $\delta(\cdot,\cdot)$ and appeal to the rest of the Corollary to bound the other terms. This gives the bound of the Proposition. □

2.4 Analysis of step 5

Before we can continue modifying the clustering, we need to prove that C_a is not too different from C_a^*. The following Lemma easily follows from Lemma 11.

Lemma 14.

$$||C_a| - |C_a^*|| \leq \frac{8k}{1-8\epsilon}\epsilon|C_a^*|.$$

Let (C_i') denote the clustering obtained from (C_i) as follows. Let G denote a group, and for each cluster C_i of G, let $\mathrm{Out}(i)$ denote the elements of C_i which are (mistakenly) removed from G by the algorithm. Let $\mathrm{In}(G)$ denote the elements of S which (mistakenly) get to stay in G. We have:

$$|\mathrm{In}(G)| = \sum_{i \text{ cluster of } G} |\mathrm{Out}(i)|.$$

Thus, we can pair up the vertices of $\cup_i \mathrm{Out}(i)$ in a one-to-one fashion with the vertices of $\mathrm{In}(G)$.

For i large, let C_i' denote the elements of C_i which get to stay in G, plus the elements of $\mathrm{In}(G)$ which are paired up with elements of $\mathrm{Out}(i)$.

For i small, let C_i' denote the elements of C_i which stay outside the groups, plus the elements paired up with elements of C_i which end up in large groups.

By convention, we will always use (v, v') for elements which are paired, with v denoting the element which goes out of the large cluster and v' the element which goes out of the small cluster.

Lemma 15.

$$\sum \delta(v, v') \leq (2 + 6k\epsilon^2 + 2k^2\epsilon)\frac{OPT}{m}.$$

Proof: Let a be a large cluster and $v \in \mathrm{Out}(a)$, and let v' be the element which is paired with v, and let G denote a's group. Why did v' end up in G rather than v ? Because there is some large cluster b also in group G, such that

$$\delta(v', c_b) = f(v') < f(v) \leq \delta(v, c_a).$$

This yields

$$\delta(v, v') \leq \delta(v, c_a) + \delta(c_a, c_b) + \delta(c_b, v') \leq 2\delta(v, c_a) + \delta(c_a, c_b).$$

Since a and b are in the same group, there is a chain of at most k clusters connecting them, such that consecutive clusters along the chain are close. By Lemma 5, this implies

$$\delta(c_a, c_b) \leq k\frac{2M}{m\epsilon}\frac{OPT}{m^2}.$$

By Proposition 1, we have:

$$\delta(v, c_a) \leq \frac{\delta(v, C_a) + \delta(C_a, c_a)}{|C_a|}.$$

By the choice of the algorithm, we have

$$\delta(c_a, C_a) \leq \delta(c_a, C_a^*)|C_a|/|C_a^*| \leq 2(1 + \frac{8k}{1-8\epsilon}\epsilon)\frac{\delta(C_a^*)}{|C_a^*|} \leq 3\frac{OPT}{m}.$$

Hence

$$\delta(v, v') \leq 2\frac{\delta(v, C_a)}{m} + 6\frac{OPT}{m^2} + k\frac{2M}{m\epsilon}\frac{OPT}{m^2}.$$

Summing and realizing that the number of terms is at most the sum of the cardinalities of the small clusters, which is at most ks, we get

$$\sum \delta(v, v') \leq (2 + 6k\frac{s}{m} + k^2\frac{2M}{m\epsilon}\frac{s}{m})\frac{OPT}{m}.$$

Now, remember Fact 3:

$$\sum \delta(v, v') \leq (2 + 6k\epsilon^2 + 2k^2\epsilon)\frac{OPT}{m}.$$

□

Equipped with this Lemma, we are now ready to attack the analysis of the clustering (C_i').

Lemma 16. For every small i,

$$\delta(C_i') \leq \delta(C_i) + 3k(2 + 6k\epsilon^2 + 2k^2\epsilon)\epsilon^2 OPT.$$

Proof: Let b be a small cluster. Let $C_b' = C_b + P(b) - M(b)$. By bilinearity, we can write

$$\delta(C_b') = \delta(C_b) + [\delta(C_b, P(b)) - \delta(C_b, M(b))] + [\delta(P(b)) - \delta(P(b), M(b))] + [\delta(M(b)) - \delta(M(b), P(b))].$$

Since $\delta(u,v) - \delta(u,v') \leq \delta(v,v')$, it is easy to see that

$$\delta(P(b)) - \delta(P(b), M(b)) \leq |P(b)| \sum \delta(v,v') \leq ks(2+6k\epsilon^2+2k^2\epsilon)\frac{OPT}{m} \leq k(2+6k\epsilon^2+2k^2\epsilon)\epsilon^2 OPT.$$

Similarly,

$$\delta(M(b)) - \delta(M(b), P(b)) \leq k(2+6k\epsilon^2+2k^2\epsilon)\epsilon^2 OPT.$$

Now, let $v \in P(b)$ and v' paired with v. We write with Proposition 1

$$\delta(v, C_b) \leq |C_b|\delta(v,v') + \delta(v', C_b).$$

Summing, we get

$$\delta(P(b), C_b) \leq ks \sum_v \delta(v,v') + \delta(M(b), C_b).$$

We apply Lemma 15 to yield

$$\delta(P(b), C_b) - \delta(M(b), C_b) \leq ks(2+6k\epsilon^2+2k^2\epsilon)\frac{OPT}{m} \leq k(2+6k\epsilon^2+2k^2\epsilon)\epsilon^2 OPT.$$

Summing our various inequalities gives the lemma. □

The only thing left to do is analyze the modifications to the large clusters.

Lemma 17. For every large a, $\delta(C'_a) \leq \delta(C_a) + (6k\epsilon^2 + 2k^2\epsilon)OPT$.

Proof: We use the same notations as in the proof of Lemma 15. Similarly to the pervious Lemma we can easily get

$$\delta(C'_a) \leq \delta(C_a) + [\delta(C_a, P(a)) - \delta(C_a, M(a))] + 2k(3+2k^2\epsilon)\epsilon^2 OPT.$$

Now, recall that $\delta(c_a, C_a) \leq 3OPT/m$. By Proposition 1,

$$\delta(v', C_a) \leq \delta(v', c_a)|C_a| + 3\frac{OPT}{m}.$$

$$\delta(v', c_a) \leq \delta(v', c_b) + \delta(c_b, c_a) \leq \delta(v, c_a) + k\frac{2M}{m\epsilon}\frac{OPT}{m^2}.$$

Hence

$$\delta(v', C_a) \leq |C_a|\delta(v, c_a) + k\frac{2M}{m\epsilon}\frac{OPT}{m} + 3\frac{OPT}{m}.$$

Now,

$$|C_a|\delta(v, c_a) \leq \delta(v, C_a) + \delta(C_a, c_a) \leq \delta(v, C_a) + 3\frac{OPT}{m}.$$

Replacing and summing over $v' \in P(a)$, and remembering that $|P(a) = |M(a)| \leq ks$, we obtain

$$\begin{aligned}
\delta(P(a), C_a) &\leq \delta(M(a), C_a) + (6 + k\frac{2M}{m\epsilon})\frac{OPT}{m}ks \\
&\leq \delta(M(a), C_a) + (6k\frac{s}{m} + 2\frac{k^2}{\epsilon}\frac{M}{m}\frac{s}{m})OPT \\
&\leq \delta(M(a), C_a) + (6k\epsilon^2 + 2k^2\epsilon)OPT.
\end{aligned}$$

□

2.5 Analysis of step 6

Finally, we need to analyze the use of Max-h-Cut in step 6 of the algorithm; we will present the analysis as if the group was perfect, i.e. consisted of the clusters C_i^*. (It is easy to see that the proof also goes through when replacing the C_i^* by C_i', at the cost of some bookkeeping of the small errors introduced at every step of the calculation.) In the groups of large clusters, we can prove that c^* is $\Omega(\sum_{V\times V}\delta(x,y))$ as follows.

Consider a group $C_1^*\cup C_2^*\cup\cdots\cup C_h^*$. Let $c=\delta(C_1^*)+\cdots+\delta(C_h^*)$ and $W=\delta(C_1^*\cup\cdots\cup C_h^*)=\sum_{i,j}\delta(C_i^*,C_j^*)$. We have:

$$\begin{aligned}\delta(C_i^*,C_j^*) &\le n_j\delta(C_i^*,c_i)+n_in_j\delta(c_i,c_j)+n_i\delta(c_j,C_j^*)\\ &\le M2\frac{\delta(C_i^*)}{m}+M^2k\frac{2M}{m\epsilon}\frac{c}{m^2}+M2\frac{\delta(C_j^*)}{m}.\end{aligned}$$

Summing over the k^2 terms gives

$$W\le 4\frac{M}{m}kc+\frac{2k^3}{\epsilon}(\frac{M}{m})^3c\le 3\frac{k^3}{\epsilon}(1/\epsilon_{j_0})^3c.$$

Run the PTAS for Max-h-Cut with error parameter

$$\epsilon'=\frac{\epsilon\epsilon_{j_0}^3}{3k^3}\epsilon.$$

The error is then at most $\epsilon' W\le\epsilon c$.

Overall, the algorithm produces a cut of value at most $(1+O(k^4\epsilon+k^2\epsilon^2))OPT$. Assuming that $\epsilon<1/k$, this is $OPT(1+O(k^2\epsilon^2))$.

3 Properties of the Square of Euclidean distance

Throughout this section we put $\delta(x,y)=\|x-y\|_2^2$. For a finite set $X\subset\mathbb{R}^d$ we denote by $\mathrm{conv}(X)$ the *convex hull* of X. Let $X=\{x^1,x^2,\ldots,x^n\}$. Let $y=\sum_{i=1}^n\alpha_ix^i$ be a point in $\mathrm{conv}(X)$, and suppose that there are integers $r,q_1,q_2,\ldots,q_n$ such that $\alpha_i=q_i/r$ for all $i=1,2,\ldots,n$. We associate with y a multi-subset Y of X of size r, obtained by taking q_i copies of x^i, for all $i=1,2,\ldots,n$. We denote by $\overline{Y}$ the center of mass of Y. I.e., $\overline{Y}=\cdot\sum_{i=1}^n q_ix^i/r$. Notice that $y=\overline{Y}$.

The following proposition characterizes the edge-cost of a cluster in terms of the center of mass.

Proposition 18. For every finite $X\subset\mathbb{R}^d$, $\delta(X)=|X|\delta(\overline{X},X)$.

Proof: On the one hand,

$$\begin{aligned}\delta(\overline{X},X) &= \sum_{x\in X}\|x-\frac{1}{|X|}\sum_{y\in X}y\|_2^2\\ &= \sum_{x\in X}\left(\|x\|_2^2+\frac{1}{|X|^2}\sum_{y\in X}\sum_{z\in X}y\cdot z-\frac{2}{|X|}\sum_{y\in X}x\cdot y\right)\\ &= \sum_{x\in X}\|x\|_2^2-\frac{1}{|X|}\sum_{x\in X}\sum_{y\in X}x\cdot y.\end{aligned}$$

On the other hand,

$$\begin{aligned}\delta(X) &= \frac{1}{2}\sum_{x\in X}\sum_{y\in X}\|x-y\|_2^2 \\ &= \frac{1}{2}\sum_{x\in X}\sum_{y\in X}\left(\|x\|_2^2+\|y\|_2^2-2x\cdot y\right) \\ &= |X|\sum_{x\in X}\|x\|_2^2-\sum_{x\in X}\sum_{y\in X}x\cdot y. \qquad \square\end{aligned}$$

The following simple propositions will come in handy.

Proposition 19. Let Y be a multi-subset of $\mathbb{R}^d$. Then $\overline{Y}$ minimizes $\delta(Y,z)$ over z. In other words, $\overline{Y} = \arg\min_{z\in\mathbb{R}^d}\{\delta(Y,z)\}$.

Proof: As $\delta(Y,z) = \sum_{i=1}^d\sum_{y\in Y}(y_i-z_i)^2$, we can minimize each coordinate separately. The derivative of $\delta(Y,z)$ with respect to z_i is $-2\sum_{y\in Y}(y_i-z_i)$, which is 0 exactly when $z_i = \frac{1}{|Y|}\sum_{y\in Y}y_i$. As the second derivative with respect to z_i is $2|Y|$ which is positive, this is the unique global minimum. $\square$

Proposition 20. For every $x,y,z\in\mathbb{R}^d$, $\delta(x,z)\le\delta(x,y)+\delta(y,z)+2\sqrt{\delta(x,y)\cdot\delta(y,z)}$.

Proof: By the triangle inequality for Euclidean distance, $\sqrt{\delta(x,z)}\le\sqrt{\delta(x,y)}+\sqrt{\delta(y,z)}$. Squaring this inequality gives the desired result. $\square$

Proposition 21. For every $x\in\mathbb{R}^d$, for every multi-subset Y of $\mathbb{R}^d$, we have:

$$\delta(x,Y)\ge|Y|\delta(x,\overline{Y}).$$

Proof: It is easy to see that

$$\delta(x,\overline{Y}) = \sum_{i=1}^d\left(\frac{1}{|Y|}\sum_{y\in Y}(x_i-y_i)\right)^2.$$

On the other hand, it is also easy to see that

$$\frac{1}{|Y|}\delta(x,Y) = \sum_{i=1}^d\frac{1}{|Y|}\sum_{y\in Y}(x_i-y_i)^2.$$

Now, apply the Cauchy-Schwartz inequality to each of the d terms. $\square$

The first part of the following lemma is attributed to Maurey [6]. We provide a proof for completeness. We denote the diameter of Y by $\mathrm{diam}(Y) = \max_{x,y\in Y}\delta(x,y)$.

Lemma 22. Let $Y\subset\mathbb{R}^d$ and $\epsilon>0$.

1. **(Maurey)** For every $x \in \mathrm{conv}(Y)$, there exists a multi-subset Z of Y containing $\frac{1}{\epsilon}$ points and whose center of mass is close to x:

$$\delta(x, \overline{Z}) \leq \epsilon \cdot \mathrm{diam}(Y).$$

2. There exists a multi-subset Z of Y containing $\frac{1}{\epsilon}$ points and whose center of mass is close to the center of mass of Y:

$$\delta(\overline{Y}, \overline{Z}) \leq \epsilon \frac{\delta(Y, \overline{Y})}{|Y|}.$$

Proof: We start with the first assertion. Let $t = 1/\epsilon$ and $x = \sum_{y \in Y} \alpha_y y$, where the α_y's are non-negative and sum up to 1. We use the probabilistic method. Pick a multiset $Z = \{z^1, z^2, \ldots, z^t\}$ at random, where the z^i-s are i.i.d. random variables with $\Pr[z^i = y] = \alpha_y$. Now, it is easy to see that

$$\begin{aligned} E\left[\delta(x, \overline{Z})\right] &= E\left[\frac{1}{t^2} \sum_{i=1}^{t} \sum_{j=1}^{t} \left(x - z^i\right) \cdot \left(x - z^j\right)\right] \\ &= \frac{1}{t^2} \sum_{i=1}^{t} \left(E\left[\|x - z^i\|_2^2\right] + \sum_{j \neq i} E\left[\left(x - z^i\right) \cdot \left(x - z^j\right)\right] \right). \end{aligned}$$

Since z^i and z^j are independent, we have $E\left[(x - z^i) \cdot (x - z^j)\right] = \sum_{l=1}^{d} E\left[(x_l - z_l^i)\right] E\left[\left(x_l - z_l^j\right)\right]$ which is 0 by our choice of distribution. Thus,

$$E(\delta(x, \overline{Z})) = \frac{1}{t^2} \sum_{i=1}^{t} E\left[\|x - z^i\|_2^2\right] \leq \frac{1}{t} \mathrm{diam}(Y).$$

Therefore there exists a choice of Z such that $\delta(x, \overline{Z}) \leq \frac{1}{t} \mathrm{diam}(Y)$.

For the second assertion, we start the proof in the same way, with $x = \overline{Y}$, and replace the last part of the calculation by the following slightly finer estimate:

$$\frac{1}{t^2} \sum_i E(\delta(\overline{Y}, z^i)) = \frac{1}{t^2} \sum_i \sum_{y \in Y} \frac{1}{|Y|} \delta(\overline{Y}, y) = \frac{\delta(\overline{Y}, Y)}{t|Y|}. \qquad \square$$

Lemma 22 can be used to derive a high-probability result as follows.

Lemma 23. There exists a constant κ such that the following holds. Let $Y \subset \mathbb{R}^d$ and $\epsilon, \rho > 0$. Let Z be a random multi-subset of Y generated by taking $\kappa \cdot \frac{1}{\epsilon^2} \cdot \log \frac{1}{\rho}$ i.i.d. points distributed uniformly in Y. Then, with probability at least $1 - \rho$, we have:

$$\delta(\overline{Y}, \overline{Z}) \leq \epsilon \frac{\delta(Y, \overline{Y})}{|Y|}.$$

Proof: Let $s = \frac{\kappa}{2} \cdot \frac{1}{\epsilon} \cdot \log(1/\rho)$ and $t = \frac{2}{\epsilon}$. Consider Z as s samples $Z_1, Z_2, \ldots, Z_s$ of size t each. By Proposition 21, $\delta(\overline{Y}, \overline{Z}) \leq \frac{1}{s} \cdot \sum_{i=1}^{s} \delta(\overline{Y}, \overline{Z_i})$. Therefore, $\Pr\left[\delta(\overline{Y}, \overline{Z}) > \epsilon \cdot \delta(Y, \overline{Y})/|Y|\right] \leq \Pr\left[\sum_{i=1}^{s} \delta(\overline{Y}, \overline{Z_i}) > \epsilon s \cdot \delta(Y, \overline{Y})/|Y|\right]$. Put $\chi_i = |Y| \delta(\overline{Y}, \overline{Z_i}) / \delta(Y, \overline{Y})$ for all $i = 1, 2, \ldots s$. The χ_i are i.i.d. random variables taking values in the range $[0, 1]$. By Lemma 22, $E\left[\chi_i\right] \leq \frac{1}{2}\epsilon$ for all i. Using standard Chernoff bounds we get that $\Pr\left[\sum_{i=1}^{s} \chi_i > \epsilon s\right] < \left(\frac{e}{4}\right)^{\epsilon s/2}$. Defining $\kappa = 4/\log(4/e)$, the right hand side is equal to ρ. $\square$

4 A PTAS for ℓ_2^2 Instances

In this section we consider $V \subset \mathbb{R}^d$ and the distance function $\delta(x,y) = \|x-y\|_2^2$. The main idea behind this algorithm is similar to that of the metric algorithm. The center of mass of a cluster acts as its representative element. It is also the point that minimizes the sum of distances to cluster points. This latter property allows us to ignore the difference between well-separated and not well-separated clusters. The main difficulty is that there is an exponential number of potential centers of mass.

4.1 The ℓ_2^2 Algorithm

1. By exhaustive search, guess the optimal cluster sizes $|C_i| = n_i$, $n_1 + n_2 + \cdots + n_k = n$. By exhaustive search, consider all possible sequences $A_1, A_2, \ldots, A_k$, where the A_i-s are mutually disjoint multisets, each containing $16/\epsilon^2$ (not necessarily distinct) points from V.

2. Compute a minimum cost assignment of points to clusters $C_1, C_2, \ldots, C_k$, subject to the conditions that exactly n_i points are assigned to C_i, and the cost of assigning a point x to C_i is $\hat{\delta}(x, C_i) = n_i \cdot \delta(x, \overline{A_i})$, for all $i = 1, 2, \ldots, k$.

3. Output the best such clustering over all choices of $\mathcal{A} = (A_1, \ldots, A_k)$ and $N = (n_1, \ldots, n_k)$.

4.2 Analysis of the ℓ_2^2 Algorithm

Our algorithm is motivated by the following bound.

Lemma 24. Let Y be a multi-subset of V and $1 \geq \epsilon > 0$. Then there exists a multi-subset Z of Y of size $|Z| = 16/\epsilon^2$ such that $\delta(Y, \overline{Z}) \leq (1+\epsilon)\delta(Y, \overline{Y})$.

Proof: By Proposition 20, for every $y \in Y$, $\delta(y, \overline{Z}) \leq \delta(y, \overline{Y}) + \delta(\overline{Y}, \overline{Z}) + 2\sqrt{\delta(y, \overline{Y})\delta(\overline{Y}, \overline{Z})}$. By the Cauchy-Schwarz inequality, $\sum_{y \in Y} \sqrt{\delta(y, \overline{Y})} \leq \sqrt{|Y| \sum_{y \in Y} \delta(y, \overline{Y})}$. Therefore, summing the previous expression over $y \in Y$, we get that $\delta(Y, \overline{Z}) \leq \delta(Y, \overline{Y}) + |Y|\delta(\overline{Y}, \overline{Z}) + 2\sqrt{|Y|\delta(Y, \overline{Y})\delta(\overline{Y}, \overline{Z})}$. Plugging in the bound for $\delta(\overline{Y}, \overline{Z})$ from Lemma 22, we get that $\delta(Y, \overline{Z}) \leq (1 + \frac{\epsilon}{2} + \frac{\epsilon^2}{16})\delta(Y, \overline{Y}) \leq (1+\epsilon)\delta(Y, \overline{Y})$. $\square$

We are now ready for the analysis of our algorithm.

Theorem 25. The algorithm presented in Section 4.1 is a PTAS for the ℓ_2^2 k-Clustering problem. Its running time is $n^{O(k/\epsilon^2)}$.

Proof: By Lemma 24 applied to $Y = C_i^*$, for every $i = 1, 2, \ldots, k$, there exists a multi-subset Z_i of C_i^* of size $|Z_i| = 16/\epsilon^2$, such that $\delta(C_i^*, \overline{Z_i}) \leq (1+\epsilon)\delta(C_i^*, \overline{C_i^*})$. Consider the iteration of the algorithm where $A_i = Z_i$ and $n_i = |C_i^*|$ for every $i = 1, 2, \ldots, k$. Let $C_1, C_2, \ldots, C_k$ be

the clustering computed by the algorithm in this iteration. Then,

$$\begin{aligned}
\text{cost}(C_1, C_2, \ldots, C_k) &= \sum_{i=1}^{k} |C_i| \cdot \sum_{x \in C_i} \delta(x, \overline{C_i}) \\
&\leq \sum_{i=1}^{k} n_i \cdot \sum_{x \in C_i} \delta(x, \overline{A_i}) \text{ by Proposition 19 for } C_i \\
&\leq \sum_{i=1}^{k} n_i \cdot \sum_{x \in C_i^*} \delta(x, \overline{A_i}) \text{ as we compute the minimum cost assignment} \\
&\leq (1+\epsilon) \cdot \sum_{i=1}^{k} |C_i^*| \cdot \delta(C_i^*, \overline{C_i^*}) \\
&= (1+\epsilon) \cdot \text{cost}\left(C_1^*, C_2^*, \ldots, C_k^*\right).
\end{aligned}$$

The performance guarantee follows because the algorithm finds a partition whose cost is at least as good as $\text{cost}(C_1, C_2, \ldots, C_k)$.

As for the running time of the algorithm, there are less than n^k possible representations of n as a sum $n_1 + n_2 + \cdots + n_k$. There are less than n^{16k/ϵ^2} possible choices for $\mathcal{A}$. Computing a minimum cost assignment to clusters can be done using a minimum cost perfect matching algorithm in time $O(n^3 \log n)$. □

5 A PTAS for ℓ_2^2 Instances of k-Median

A simple variant of the algorithm presented in Section 4.1 solves the k-Median case and has similar running time. Here we give a faster randomized polynomial time approximation scheme for ℓ_2^2 instances of k-Median. The running time of our algorithm, for fixed k, ϵ, and failure probability ρ, is just $O(n(\log n)^{O(1)})$.

5.1 The k-Median algorithm

The approximation scheme works as follows.

1. By exhaustive search, guess an approximation $n_1 \geq n_2 \geq \cdots \geq n_k$ on the sizes of the k clusters, where n_i is the power of $(1+\epsilon)$ larger than and closest to $|C_i^*|$.

2. Partition the k clusters into groups in a greedy fashion: 1 goes into the first group, and for i going from 2 to k, i goes into the current group if $n_i \geq (\epsilon/16k)^2 n_{i-1}$, and into a new group otherwise. Let T be the number of groups and let m_t denote the size of the largest cluster in the tth group. Put $m_{T+1} = 0$.

3. For t going from 1 to T, do the following:

   (a) Let U_t denote the points not yet clustered (initially $U_1 = V$).

(b) Let Z denote a random uniform sample of U_t, with replacement, of constant size (size $k^{2k}/(16\epsilon)^{2k} \cdot (\ln k)\gamma/\epsilon^6$, where $\gamma > 0$ is a constant).

(c) By exhaustive search, guess $A_i = Z \cap C_i^*$ for all i in the tth group. Define, for each such cluster C_i, the representative point as $c_i = \overline{A_i}$. (If $A_i = \emptyset$, take an arbitrary point as the representative of C_i.)

(d) Assign $|U_t| - m_{t+1}16k^2/\epsilon$ points from U_t to the clusters in groups 1 through t, where point x is assigned to a cluster C_i that minimizes $\delta(x, c_i)$.

4. Output the best clustering of all the ones constructed above.

This completes the specification of the algorithm. We now proceed with its analysis.

5.2 Analysis of the k-Median algorithm

Consider the iteration of the algorithm where all the guesses are correct. For all $t = 1, 2, \ldots, T$, let a_t denote the index of the first and largest cluster in the tth group (so that $m_t = n_{a_t}$), and let b_t denote the index of the last and smallest cluster in that group.

Lemma 26. For all $t \in \{1, 2, \ldots, T\}$, the number of points in the smallest and in the largest clusters of group t are not very different:

$$\left(\frac{\epsilon}{16k}\right)^{2(k-1)} n_{a_t} \leq n_{b_t} \leq n_{a_t}.$$

Proof: Use the definition of group t and the fact that a group contains at most k clusters. □

Consider the situation when the algorithm starts iteration t. For each j in group t, let $U_{jt} = C_j^* \cap U_t$ denote the points which have not yet been classified and which we hope the algorithm will place in cluster j during iteration t.

Definition 4. For $j \in [a_t, b_t]$, we say that C_j^* is a *well-represented* cluster if $|U_{jt}| \geq \epsilon^3/16^3 \cdot n_j$. Otherwise C_j^* is called *poorly represented.*

Lemma 27. Fix a cluster index j and let t be j's group. For every $\rho > 0$ and for every sufficiently large $\lambda > 0$, there exists $\gamma > 0$ (the γ used to define the size of Z) such that with probability at least $1 - \frac{\rho}{k}$, if j is a surviving index then we have:

$$|A_j| \geq \frac{\lambda}{\epsilon^4} \ln k.$$

Proof: Use Lemma 26 and survivability so as to bound $|U_{jt}|/|U_t|$ from below, then use standard Chernov bounds for A_j. □

The following Lemma motivates the terminology of well-represented clusters.

Lemma 28. For every $\rho > 0$ there exist $\lambda > 0$ and $\gamma > 0$ such that with probability at least $1 - \rho$, we have:

$$\forall t, \forall j \text{ surviving index}, \quad \left|\delta(U_{jt}, c_j) - \delta(U_{jt}, \overline{U_{jt}})\right| \leq \frac{\epsilon}{8} \cdot \delta(U_{jt}, \overline{U_{jt}}). \tag{2}$$

Proof: (Suggested sketch): Combines Lemma 23, Lemma 27, Cauchy-Schwartz, and the union bound. □

Proof: Apply Lemma 23 to the sample A_j in U_{jt}, so that for j surviving and $|A_j|$ large enough, with probability at least $1 - \rho/(3k)$ we have

$$\delta(c_j, \overline{U_{jt}}) \leq \frac{\epsilon^2}{2^{10}} \cdot \delta(U_{jt}, \overline{U_{jt}})/|U_{jt}|. \tag{3}$$

(this defines λ). Set γ according to Lemma 27 so that if j is surviving, then A_j is large enough with probability at least $1 - \rho/(3k)$. By the proof of Lemma 24, Equation 3 then implies $\left|\delta(U_{jt}, c_j) - \delta(U_{jt}, \overline{U_{jt}})\right| \leq (\epsilon/8) \cdot \delta(U_{jt}, \overline{U_{jt}})$. Summing failure probabilities then concludes the proof. □

¿From now on, in the rest of the analysis we will assume that Equation 2 holds.

For $x \in X$, denote by j_x the index of the cluster that x gets assigned to by the algorithm, and denote by j_x^* the index of the cluster that x gets assigned to by the optimal clustering.

Let D_t denote the set of points which are assigned during iteration t of the loop in step 3 of the algorithm. Such points can be classified into three categories:

- *regular* points: $x \in D_t$ is regular if its optimal cluster j_x^* has $j_x^* \leq b_t$ and is well-represented.
- *premature* points: $x \in D_t$ is premature if $j_x^* > b_t$, i.e. the optimal cluster of x is too small to bet taken into consideration yet. Let P_t denote the premature points in D_t.
- *leftover* points: $x \in D_t$ is leftover if $j_x^* \leq b_t$ and cluster j_x^* is poorly represented. Let L_t denote the premature points of D_t.

We start the analysis with the easiest category, that of regular points.

Lemma 29.

$$\sum_{x \text{ regular}} \delta(x, c_{j_x}) \leq \left(1 + \frac{\epsilon}{8}\right) \cdot \sum_{j \text{ well-represented}} \delta(C_j^*, \overline{C_j^*}).$$

Proof: (Suggested sketch): When x is assigned, its cluster representative $c_{j_x^*}$ is already in existence, so $\delta(x, c_{j_x}) \leq \delta(x, c_{j_x^*})$. We then use Lemma 28 and Proposition 19. □

Proof: Take x a regular point and let t be the group containing j_x^*. Then $x \in U_{j_x^* t}$. Thus the left hand side of the sum ranges over U_{jt}, where j is well-represented. The assignment of x by the algorithm has value $\delta(x, c_{j_x}) \leq \delta(x, c_{j_x^*})$ by definition of the algorithm. Thus:

$$\begin{aligned}
\sum_{x \text{ regular}} \delta(x, c_{j_x}) &\leq \sum_{x \text{ regular}} \delta(x, c_{j_x^*}) \\
&\leq \sum_{j \text{ well-represented}} \delta(U_{jt}, c_j) \\
&\leq (1 + \frac{\epsilon}{8}) \sum_{j \text{ well-represented}} \delta(U_{jt}, \overline{U_{jt}}) \text{ by Lemma 28}
\end{aligned}$$

$$\leq (1+\frac{\epsilon}{8}) \sum_{j \text{ well-represented}} \delta(U_{jt}, \overline{C_j^*}) \text{ by Proposition 19}$$

$$\leq (1+\frac{\epsilon}{8}) \sum_{j \text{ well-represented}} \delta(C_j^*, \overline{C_j^*}).$$

□

We now deal with the next easiest category, that of premature points. The proof of this lemma crucially uses the specific feature of the algorithm according to which one keeps assigning unsufficiently many points to the clusters under consideration. Thus this is one of the key points in the analysis.

Lemma 30.

$$\sum_{x \text{ premature}} \delta(x, c_{j_x}) \leq \frac{\epsilon}{8} \cdot \sum_{x \text{ not premature}} \delta(x, c_{j_x}).$$

Proof: First note that by definition of premature points, P_t has size at most $|\cup_{j>b_t} C_j^*| \leq km_{t+1}$.

By definition of the algorithm, the number of points in U_{t+1} is exactly $16k^2 m_{t+1}/\epsilon$. Since $|\cup_{j>b_t} C_j^*|$ has size at most km_{t+1}, in U_{t+1} there must be at least $m_{t+1}(16k^2/\epsilon - k) > m_{t+1} 8k^2/\epsilon$ points which belong to $C_1^* \cup \cdots \cup C_{b_t}^*$ (hence which are not premature). Among those, let S_t denote the $|P_t|$ points such that $\delta(x, c_{j_c^*})$ is smallest.

Since the algorithm chooses a minimum cost assignment and prefers P_t over S_t in doing so during iteration t, we have:

$$\begin{aligned}
\sum_{P_t} \delta(x, c_{j_x}) &\leq \sum_{S_t} \delta(x, c_{j_x^*}) \\
&\leq \frac{|S_t|}{|U_{t+1} \cap (C_1^* \cup \cdots \cup C_{b_t}^*)|} \sum_{x \in U_{t+1}, x \text{ not premature}} \delta(x, c_{j_x}) \\
&\leq \frac{\epsilon}{8k} \sum_{x \text{ not premature}} \delta(x, c_{j_x}).
\end{aligned}$$

Summing over t yields the Lemma. □

Finally, we deal with the leftover points.

Lemma 31.

$$\sum_{x \text{ leftover}} \delta(x, c_{j_x}) \leq \sum_{j \text{ poorly represented}} \delta(C_j, \overline{C_j^*}) + O(\epsilon^3) \sum_{y \text{ premature}} \delta(y, c_{j_y}) +$$

$$2\sqrt{\sum_{j \text{ poorly represented}} \delta(C_j, \overline{C_j^*}) O(\epsilon^3) \sum_{y \text{ premature}} \delta(y, c_{j_y})}.$$

Proof: Suggested sketch: Let C_j^* be a poorly represented cluster and t be its group. By definition of poor representation, most of the points of C_j^* were assigned before their turn, i.e., they got assigned to some cluster of index $< a_t$; thus most of the points of C_j^* were premature. Take $x \in C_j^*$, x leftover, and $y \in C_j^*$, y premature. We have:

$$\delta(x, c_{j_x}) \leq \delta(x, c_{j_y}) \leq \delta(x, y) + \delta(y, c_{j_y}) + 2\sqrt{\delta(x, y)\delta(y, c_{j_y})}.$$

We sum over $x \in C_j^* \cap L$ (leftover) and $y \in C_j^* \cap P$ (premature), and appealing to Cauchy-Schwartx twice and to Proposition 18. □

Proof: Let C_j^* be a poorly represented cluster and t be its group. By definition of poor representation, most of the points of C_j^* were assigned before their turn, i.e., they got assigned to some cluster of index $< a_t$; thus most of the points of C_j^* were premature. Take $x \in C_j^*$, x leftover, and $y \in C_j^*$, y premature. We have:

$$\delta(x, c_{j_x}) \leq \delta(x, c_{j_y}) \leq \delta(x, y) + \delta(y, c_{j_y}) + 2\sqrt{\delta(x, y)\delta(y, c_{j_y})}.$$

Summing over $x \in C_j^* \cap L$ (leftover) and $y \in C_j^* \cap P$ (premature), and using Cauchy-Schwartz, we get:

$$|C_j^* \cap P| \sum_{C_j^* \cap L} \delta(x, c_{j_x}) \leq \delta(C_j^*) + |C_j^* \cap L| \sum_{C_j^* \cap P} \delta(y, c_{j_y}) + 2\sqrt{\delta(C_j^*)|C_j^* \cap L| \sum_{C_j^* \cap P} \delta(y, c_{j_y})}.$$

Now, by definition of leftover points, we have

$$|C_j^* \cap L| \leq \frac{\epsilon^3}{16^3} n_j \text{ and } |C_j^* \cap P| \geq n_j(1 - \frac{\epsilon^3}{16^3}).$$

Thus, replacing, we have:

$$\sum_{C_j^* \cap L} \delta(x, c_{j_x}) \leq (1 + O(\epsilon^3))\frac{\delta(C_j^*)}{|C_j^*|} + O(\epsilon^3) \sum_{C_j^* \cap P} \delta(y, c_{j_y}) + 2\sqrt{\frac{\delta(C_j^*)}{|C_j^*|} O(\epsilon^3) \sum_{C_j^* \cap P} \delta(y, c_{j_y})}.$$

It only remains to apply Proposition 18, sum over j, use Cauchy-Schwartz again to deduce the statement of the Lemma. □

We are now ready to prove the main theorem of this section.

Theorem 32. With constant probability the algorithm in section 5.1 computes a solution whose cost is within a factor of $1+\epsilon$ of the optimum cost. The running time of the algorithm is $O(g(k, \epsilon) \cdot n \cdot (\log n)^k)$, where $g(k, \epsilon) = \exp\left(\frac{1}{\epsilon^8} \cdot k^3 \ln k \cdot \left(\ln \frac{1}{\epsilon} + \ln k\right)\right)$.

Proof: Suggested sketch: The clustering output by the algorithm has value less than $\sum_{x \in X} \delta(x, c_{j_x})$. We separate the sums into three parts R, P, L corresponding to regular, premature and leftover points, apply the three lemmas above to each parts, and a short algebraic manipulation then yields that the cost is $OPT(1 + O(\epsilon))$.

The running time result follows by inspection of the algorithm. □

Proof: The clustering output by the algorithm has value

$$\begin{aligned}\mathrm{cost}(C_1, C_2, \ldots, C_k) &= \sum_{j=1}^{k} \sum_{x \in C_j} \delta(x, \overline{C_j}) \\ &\leq \sum_{j=1}^{k} \sum_{x \in C_j} \delta(x, c_j) \\ &= \sum_{x \in X} \delta(x, c_{j_x}).\end{aligned}$$

We separate the sums into three parts R, P, L corresponding to regular, premature and left-over points, apply the three lemmas above to each parts, and a short algebraic manipulation then yields that the cost is $OPT(1 + O(\epsilon))$.

As for the running time of the algorithm, the number of sequences $n_1, n_2, \ldots, n_k$ that the algorithms has to enumerate over is $O\left(\left(\log_{1+\epsilon} n\right)^k\right)$. The size of T is at most

$$2^{\left(\frac{1}{\epsilon^4} \cdot k^3 \ln k \cdot \left(\ln \frac{1}{\epsilon} + \ln k\right)\right)}.$$

Computing the augmentation at each node of T requires $O(n)$ distance computations, where the hidden constant depends mildly on k and ϵ. □

References

[1] N. Alon, S. Dar, M. Parnas, and D. Ron. Testing of clustering. In *Proc. of the 41th Ann. IEEE Symp. on Foundations of Computer Science(FOCS)* 2000, 240-250.

[2] N. Alon and B. Sudakov. On two segmentation problems. *Journal of Algorithms*, 33:173–184, 1999.

[3] S. Arora, D. Karger, and M. Karpinski. Polynomial time approximation schemes for dense instances of NP-hard problems. *J. Comp. System. Sci.*, 58:193–210, 1999.

[4] M. Bădoiu, S. Har-Peled, and P. Indyk. Approximate clustering via Core-Sets. *Proc. 34th ACM STOC (2002)*, pages 250-257.

[5] A. Broder, S. Glassman, M. Manasse, and G. Zweig. Syntactic clustering of the Web. In *Proc. of the 6th Int'l World Wide Web Conf.*(WWW), 1997, pages 391–404.

[6] B. Carl and I. Stephani. *Entropy, Compactness and the Approximation of Operators.* Cambridge University Press, 1990.

[7] S. Deerwester, S.T. Dumais, T.K. Landauer, G.W. Furnas, and R.A. Harshman. Indexing by latent semantic analysis. *Journal of the Society for Information Science*, 41(6):391–407, 1990.

[8] W. Fernandez de la Vega, M. Karpinski, and C. Kenyon. A polynomial time approximation scheme for metric MIN-BISECTION. *ECCC TR02-041*, 2002.

[9] W. Fernandez de la Vega and C. Kenyon. A randomized approximation scheme for metric MAX CUT. In *Proc. of the 39th Ann. IEEE Symp. on Foundations of Computer Science (FOCS)*, 1998, pages 468-471, also in JCSS 63 (2001). pages 531-541.

[10] P. Drineas, A. Frieze, R. Kannan, S. Vempala, and V. Vinay. Clustering in large graphs and matrices. In *Proc. of the 10th Ann. ACM-SIAM Symp. on Discrete Algorithms (SODA)*, 1999, pages 291–299.

[11] C. Faloutsos, R. Barber, M. Flickner, J. Hafner, W. Niblack, D. Petkovic, and W. Equitz. Efficient and effective querying by image content. *Journal of Intelligent Information Systems*, 3(3):231–262, 1994.

[12] N. Garg, V. Vazirani, and M. Yannakakis. Approximate max-flow min-(multi)cut theorems and their applications. *SIAM Journal on Computing*, 25(2):235–251, 1996.

[13] O. Goldreich, S. Goldwasser, and D. Ron. Property testing and its connection to learning and approximation. *J. of the ACM*, 45:653–750, 1998.

[14] S. Guha and S. Khuller. Greedy strikes back: Improved facility location algorithms. In *Proc. of the 9th Ann. ACM-SIAM Symp. on Discrete Algorithms (SODA)*, January 1998, 649-657.

[15] N. Guttmann-Beck and R. Hassin. Approximation algorithms for min-sum p-clustering. *Disc. Applied Math.*, 89:125–142, 1998.

[16] P. Indyk. A sublinear time approximation scheme for clustering in metric spaces. In *Proc. of the 40th Ann. IEEE Symp. on Foundations of Computer Science (FOCS)*, 1999, 154-159.

[17] V. Kann, S. Khanna, J. Lagergren, and A. Panconesi. On the hardness of approximating Max k-Cut and its dual. In *Proc. of the 4th Israeli Symp. on Theory of Computing and Systems (ISTCS)*, 1996. Also in *Chicago Journal of Theoretical Computer Science*, 1997.

[18] J. Kleinberg, C. Papadimitriou, and P. Raghavan. Segmentation problems. In *Proc. of the 30th Ann. ACM Symp. on Theory of Computing (STOC)*, 1998, pages 473–482.

[19] Manjara. `http://cluster.cs.yale.edu/`

[20] N. Mishra, D. Oblinger, and L. Pitt. Sublinear time approximate clustering. In *Proc. of the 12th Ann. ACM-SIAM Symp. on Discrete Algorithms (SODA)*, January 2001, pages 439–447.

[21] R. Ostrovsky and Y. Rabani. Polynomial time approximation schemes for geometric clustering problems. *J. of the ACM*, 49(2):139–156, March 2002.

[22] S. Sahni and T. Gonzalez. P-complete approximation problems. *Journal of the ACM*, 23(3):555–565, 1976.

[23] L.J. Schulman. Clustering for edge-cost minimization. In *Proc. of the 32nd Ann. ACM Symp. on Theory of Computing (STOC)*, 2000, pages 547–555.

[24] R. Shamir and R. Sharan. Algorithmic approaches to clustering gene expression data. In T. Jiang, T. Smith, Y. Xu, M.Q. Zhang eds., *Current Topics in Computational Biology*, MIT Press, to appear.

[25] M.J. Swain and D.H. Ballard. Color indexing. *International Journal of Computer Vision*, 7:11–32, 1991.