Applications of Weighted Voronoi Diagrams and Randomization to Variance-Based k-Clustering

(Extended Abstract)

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Abstract

In this paper we consider the k-clustering problem for a set S of n points $p_i = (x_i)$ in the d-dimensional space with variance-based errors as clustering criteria, motivated from the color quantization problem of computing a color lookup table for frame buffer display. As the inter-cluster criterion to minimize, the sum of intra-cluster errors over every cluster is used, and as the intra-cluster criterion of a cluster S_j,

$$|S_j|^{\alpha-1} \sum_{p_i \in S_j} \|x_i - \bar{x}(S_j)\|^2$$

is considered, where $\| \cdot \|$ is the L_2 norm and $\bar{x}(S_j)$ is the centroid of points in S_j, i.e., $(1/|S_j|) \sum_{p_i \in S_j} x_i$. The cases of $\alpha = 1, 2$ correspond to the sum of squared errors and the all-pairs sum of squared errors, respectively.

The k-clustering problem under the criterion with $\alpha = 1, 2$ are treated in a unified manner by characterizing the optimum solution to the k-clustering problem by the ordinary Euclidean Voronoi diagram and the weighted Voronoi diagram with both multiplicative and additive weights. With this framework, the problem is related to the generalized primary shutter function for the Voronoi diagrams. The primary shutter function is shown to be $O(n^{O(kd)})$, which implies that, for fixed k, this clustering problem can be solved in a polynomial time. For the problem with the most typical intra-cluster criterion of the sum of squared errors, we also present an efficient randomized algorithm which, roughly speaking, finds an ϵ-approximate 2-clustering

in $O(n(1/\epsilon)^d)$ time, which is quite practical and may be used to real large-scale problems such as the color quantization problem.

1 Introduction

Clustering is the grouping of similar objects and a clustering of a set is a partition of its elements that is chosen to minimize some measure of dissimilarity. It is very fundamental and used in various fields in computer science such as pattern recognition, learning theory, image processing and computer graphics. There are various kinds of measure of dissimilarity, called criteria, in compliance with the problem.

Definition of the k-clustering problem: The general k-clustering problem can be defined as follows. A k-clustering is a partition of the given set S of n points $p_i = (x_i)$ $(i = 1, \ldots, n)$ in the d-dimensional space into k disjoint nonempty subsets $S_1, \ldots, S_k$, called clusters. A k-clustering is measured by the following two criteria.
(**Intra-cluster criterion**) For each cluster S_j, the measure (or error) $\mathrm{Intra}(S_j)$ of S_j, representing how good the cluster S_j is, is defined appropriately by applications. Typical intra-cluster criteria are the diameter, radius, variance, variance multiplied by $|S_j|$ (sum of squared errors) and variance multiplied by $|S_j|^2$ (all-pairs sum of squared errors) of point set S_j.
(**Inter-cluster criterion**) The inter-cluster criterion defines the total cost of the k-clustering, which is a function of $\mathrm{Intra}(S_j)$ $(j = 1, \ldots, k)$ and is denoted by $\mathrm{Inter}(y_1, y_2, \ldots, y_k)$ where $y_j = \mathrm{Intra}(S_j)$. Typical function forms are $\max\{ y_j \mid j = 1, \ldots, k \}$ and $\sum_{i=1}^{k} y_k$.
Then, the k-clustering problem is to find a k-clustering which minimizes the inter-cluster criterion:

$$\min\{ \mathrm{Inter}(\mathrm{Intra}(S_1), \ldots, \mathrm{Intra}(S_k)) \mid$$
$$k\text{-clustering } (S_1, \ldots, S_k) \text{ of } S \}$$

Previous results concerning diameter and radius: In computational geometry, many results have

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been obtained for the clustering problem. The diameter and radius problems are rather well studied. They include an $O(n \log n)$-time algorithm for finding a 2-clustering of n points in the plane which minimizes the maximum diameter (Asano, Bhattacharya, Keil and Yao [1]), an $O(n^2 \log^2 n)$-time algorithm for finding a 3-clustering of planar point set which minimizes the maximum diameter (Hagauer and Rote [5]), and an $O(n \log^2 n / \log \log n)$-time algorithm for finding a 2-clustering which minimizes the sum of the two diameters (Hershberger [10]). When k is regarded as a variable, most k-clustering problems become NP-hard (e.g., see Megiddo and Supowit [14], Feder and Greene [4]). For fixed k, the k-clustering problem using the diameter and radius as the intra-cluster criterion and a monotone function, including taking the maximum and the summation, as the inter-cluster criterion can be solved in a polynomial time (Capoyleas, Rote and Woeginger [3]).

There are also proposed approximate algorithms for the diameter and radius whose approximation ratio is theoretically guaranteed. Feder and Greene [4] gave optimal approximate algorithms whose running time is $O(n \log k)$ for n points in the d-dimensional space for fixed d, and whose worst-case ratio is 2.

Motivation for the variance-based clustering: In this paper, we consider the k-clustering problem with variance-based measures as an intra-cluster criterion. This is motivated from the color quantization problem of computing a color lookup table for frame buffer display. Typical color quantization problems cluster hundreds of thousands of points in the RGB three-dimensional space into $k = 256$ clusters. Since k is large, a top-down approach to recursively divide the point set into 2 clusters is mostly employed. In this problem, the diameter and radius are not suited as an intra-cluster criterion, and the variance-based (Wan, Wong and Prusinkiewicz [15]) and L_1-based (median cut; Heckbert [9]) criteria are often used. In [15], [9], the top-down approach is used and in solving the 2-clustering problem both only treat separating planes orthogonal to some coordinate axis. These algorithms are implemented in rlequant of Utah Raster Toolkit, and ppmquant of X11R5 or tiffmedian of Tiff Soft. Although these implementations run rather fast in practice, roughly speaking in $O(n \log n)$ time, there is no theoretical guarantee about how good their solution k-clusterings are.

Rigorous definition of the variance-based clustering: Therefore, it is required to develop a fast 2-clustering algorithm and to determine the complexity of the k-clustering problem for the variance-based case. Before describing the existing computational-geometric results concerning variance-based case, let us define the variance-based intra-cluster criterion in a rigorous way. The variance $\mathrm{Var}(S)$ of points $p_i = (x_i)$ in S is defined by

$$\mathrm{Var}(S) = \frac{1}{|S|} \sum_{p_i \in S} \|x_i - \bar{x}(S)\|^2$$

where $\bar{x}(S)$ is the centroid of S:

$$\bar{x}(S) = \frac{1}{|S|} \sum_{p_i \in S} x_i.$$

For a parameter α, define $\mathrm{Var}^{\alpha}(S)$ by

$$\mathrm{Var}^{\alpha}(S) = |S|^{\alpha} \mathrm{Var}(S).$$

Var^0 is exactly the variance itself. Var^1 is represented as

$$\mathrm{Var}^1(S) = \sum_{p_i \in S} \|x_i - \bar{x}(S)\|^2$$

and hence is the sum of squared errors with respect to the centroid of S. Var^2 is represented as

$$\mathrm{Var}^2(S) = |S| \sum_{p_i \in S} \|x_i - \bar{x}(S)\|^2$$
$$= \sum_{p_i, p_l \in S, \ i < l} \|x_i - x_l\|^2$$

and hence is the all-pairs sum of squared errors in S. Adopting Var^{α} as the intra-cluster metric, as α becomes larger, the sizes of clusters in an optimum k-clustering becomes more balanced.

Previous results on the variance-based clustering: For the variance-based criteria, unlike the diameter and radius, the k-clustering problem adopting the maximum function as the inter-cluster criterion becomes hard to solve. For this inter-cluster criterion with the all-pairs sum of squared errors, only a pseudo-polynomial approximation scheme is known (Hasegawa, Imai, Inaba, Katoh and Nakano [7]). Also, in applications such as the color quantization problem, the summation function is adopted as an inter-cluster criterion [15]. In this paper, we consider only the summation case, that is, the k-clustering problem to minimize the summation of variance-based intra-cluster costs over clusters.

For the variance-based clustering problem with the summation function as an inter-cluster metric, the following are known. Concerning Var^1, the sum of squared errors, it is well known that an optimum 2-clustering is linearly separable and that an optimum k-clustering is induced by the Voronoi diagram generated by k points (e.g., see [2, 7, 15]). Using this characterization together

with standard computational-geometric techniques, the 2-clustering problem with Var^1 as the intra-cluster metric can be solved in $O(n^2)$ time and $O(n)$ space, and the k-clustering problem is solvable in a polynomial time when k is fixed [7]. Concerning Var^2, the all-pairs sum of squared errors, an optimum 2-clustering is circularly separable (Boros and Hammer [2]), and a finer characterization by using the higher-order Voronoi diagram is given in [7]. Using this characterization, the 2-clustering problem with Var^2 as the intra-cluster metric can be solved in $O(n^{d+1})$ time, and also it is seen that the k-clustering problem for this case can be solved in a polynomial time $O(n^{(d+1)k(k-1)/2})$ when k is fixed [6].

There is also proposed an approximate algorithm for the k-clustering problem with Var^1 as an intra-cluster metric. Hasegawa, Imai, Inaba, Katoh and Nakano [7] gave an $O(n^{k+1})$-time algorithm for fixed d whose worst-case ratio is 2. This algorithm solve the k-clustering problem with constraining the representative point of each cluster to be one of points in the cluster.

Our results: In this paper, the k-clustering problem under the intra-cluster criterion Var^α with $\alpha = 1, 2$ is treated in a unified way by characterizing the optimum solution to the k-clustering problem by the ordinary Voronoi diagram and the weighted Voronoi diagrams with both multiplicative and additive weights.

With this framework, the problem is related to the generalized primary shutter function for the Voronoi diagrams, which is roughly the number of partitions of n points in the d-dimensional space induced by the Voronoi diagram generated by k generator points. The primary shutter function of the Euclidean Voronoi diagram is shown to be $O(n^{dk})$, and that for the Voronoi diagram with additive and multiplicative weights $O(n^{(d+2)k})$. Based on these, the k-clustering problem for n points in the d-dimensional space with a variance-based criterion can be solved in $O(n^{(d+2)k+1})$ time. This greatly improves the previous bound $O(n^{O(dk^2)})$. We have thus given a polynomial-time algorithm for the case of fixed k, but its degree is large even for moderate values of d and k.

To develop a practically useful 2-clustering algorithm, for the problem with the most typical intra-cluster criterion of the sum of squared errors, we present an efficient randomized algorithm which, roughly speaking, finds an ϵ-approximate 2-clustering in $O(n(1/\epsilon)^d)$ time, which is quite practical and may be used to real large-scale problems such as the color quantization problem. In the analysis, a fact that this intra-cluster cost has its statistical meanings by definition is used. This randomized algorithm can be easily generalized to the k-clustering

problem.

2 A unified approach to the variance-based k-clustering by weighted Voronoi diagrams

The variance-based k-clustering problem is described as follows:

$$\min\{\sum_{j=1}^{k}\text{Var}^\alpha(S_j) \mid k\text{-clustering }(S_1,\ldots,S_k)\text{ of }S\}$$

In [7], a parametric characterization was given for the case of $\alpha = 2$ (all-pairs case) by using a general parametric technique for minizing quasiconcave functions developed by Katoh and Ibaraki [12], which enabled us to characterize an optimal 2-clustering for $\alpha = 2$ by means of higher-order Voronoi diagram, and to obtain a pseudo polynomial approximation scheme for the 2-clustering problem for Var^2 and the maximum function as the inter-cluster metric.

In this paper, we concentrate on the case where the summation function is adopted for the inter-cluster criterion, and give a more direct characterization for the problem with $\alpha = 1, 2$.

We may make use of partitions of n points induced by weighted Voronoi diagrams. Consider k points $q_j = (\mu_j)$ in the d-dimensional space with multiplicative weight ν_j and additive weight σ_j $(j = 1, \ldots, k)$. Define the Voronoi region $\text{Vor}(q_j)$ of q_j by

$$\text{Vor}(q_j) = \bigcap_{l=1}^{k}\{p = (x) \mid$$
$$\nu_j\|x - \mu_j\|^2 + \sigma_j \leq \nu_l\|x - \mu_l\|^2 + \sigma_l\}$$

For any point in $\text{Vor}(q_j)$, q_j is the closest point among q_l $(l = 1, \ldots, k)$ with respect to the weighted distance. $\text{Vor}(q_j)$ $(j = 1, \ldots, k)$ partitions the space, which is called the *weighted Voronoi diagram* generated by these k points q_j. When $\sigma_j = 0$ and $\nu_j = 1$ $(j = 1, \ldots, k)$, this weighted Voronoi diagram reduces to the ordinary Euclidean Voronoi diagram.

By the Voronoi diagram generated by these k weighted points, n points in the given set S are naturally partitioned into k clusters (we here ignore the case in this definition where a point in S is equidistant from two points among these k weighted points). We call this partition a *Voronoi partition* of n points in S by k weighted generators. Apparently, not all k-clusterings are Voronoi partitions. In fact, we can characterize optimal k-clusterings by the Voronoi partition. The case of $\alpha = 1$ is well known, and we here state only the

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theorem.

Theorem 1 ([2, 7, 15]) *Suppose that $(S_1^*, \ldots, S_k^*)$ is an optimum k-clustering for the k-clustering problem with Var^1 ($\alpha = 1$) as the intra-cluster metric. Then, an optimum k-clustering is a Voronoi partition by the ordinary Euclidean Voronoi diagram for k points $q_j = (\mu_j^*)$ ($\mu_j^* = \bar{x}(S_j^*)$).* $\square$

Now, we prove the following theorem for the case of Var^2, i.e., all-pairs sum of squared errors.

Theorem 2 *Suppose that $(S_1^*, \ldots, S_k^*)$ is an optimum k-clustering for the k-clustering problem with Var^2 ($\alpha = 2$) as the intra-cluster metric. Then, an optimum k-clustering is a Voronoi partition by the weighted Voronoi diagram for k points $q_j = (\mu_j^*)$ ($\mu_j^* = \bar{x}(S_j^*)$) with multiplicative weight $\nu_j^* = |S_j^*|$ and additive weight σ_j defined by $\sigma_j = \sum_{p_i \in S_j^*} \|x_i - \bar{x}(S_j^*)\|^2$.*

Proof: First, observe the following relation.

$$\sum_{p_i \in S_j} \|x_i - x\|^2$$
$$= \sum_{p_i \in S_j} \|(x_i - \bar{x}(S_j)) + (\bar{x}(S_j) - x)\|^2$$
$$= |S_j| \cdot \|x - \bar{x}(S_j)\|^2 + \sum_{p_i \in S_j} \|x_i - \bar{x}(S_j)\|^2$$

where it should be noted that $\sum_{p_i \in S_j}(x_i - \bar{x}(S_j)) = 0$.

Now, suppose that, in the weighted Voronoi diagram above, a point $p_i \in S_j^*$ is not contained in $\mathrm{Vor}(q_j)$ for $q_j = (\bar{x}(S_j^*))$, and is in $\mathrm{Vor}(q_{j'})$. Then, moving p_i from S_j^* to $S_{j'}^*$, the total cost is strictly reduced from the above formula (note that Var^2 is the all-pairs sum of squared errors), which contradicts the optimality of $(S_1^*, \ldots, S_k^*)$. Hence, each $p_j \in S_j^*$ is contained in $\mathrm{Vor}(q_j)$ for $j = 1, \ldots, k$, and the theorem follows. $\square$

By Theorem 1 and Theorem 2, the variance-based k-clustering problem with $\alpha = 1, 2$ can be solved by enumerating all the Voronoi partitions of n points generated by k weighted points, and finding a partition with minimum one.

The number of distinct Voronoi partitions has strong connection with the generalized primary shutter function for k-label space introduced by Hasegawa [6, 8] which has applications in computational learning theory. We here analyze this number by showing that Voronoi partitions are duals of arrangements of algebraic surfaces in the $O(dk)$-dimensional space.

Theorem 3 *The number of Voronoi partitions of n points by the Euclidean Voronoi diagram generated by k points in the d-dimensional space is $O(n^{dk})$, and all*

the Voronoi partitions can be enumerated in $O(n^{dk+1})$ time.

Proof: In the ordinary Voronoi diagram, all multiplicative weights are one and all additive weights are zero, i.e., $\nu_j = 1$, $\sigma_j = 0$ ($j = 1, \ldots, k$). Parameters are μ_j ($j = 1, \ldots, k$). Consider the (dk)-dimensional vector space consisting of μ with $\mu = (\mu_1, \mu_2, \ldots, \mu_k)$. In this (dk)-dimensional space, we can define an equivalence relation among points such that two points are in the equivalence relation if their corresponding Voronoi partitions are identical. The equivalence relation produces a subdivision of this space into equivalence classes.

For each pair of distinct μ_{j_1} and μ_{j_2} among μ_j ($j = 1, \ldots, k$) and each point $p_i = (x_i)$ among p_i ($i = 1, \ldots, n$), consider an algebraic surface in this dk-dimensional space defined by

$$\|x_i - \mu_{j_1}\|^2 - \|x_i - \mu_{j_2}\|^2 = 0$$

where x_i is regarded as a constant vector. The number of such surfaces is $nk(k-1)/2$. The arrangement of these $nk(k-1)/2$ algebraic surfaces coincides with the subdivision defined by the equivalence relation from Voronoi partitions. The number of Voronoi partitions is bounded by the combinatorial complexity of the arrangement of $nk(k-1)/2$ constant-degree algebraic surfaces, and the theorem follows. $\square$

A further detailed analysis about the primary shutter function of the k-Voronoi space is done by Ishiguro [11]. In that paper, the linearization technique is applied in the analysis, and an algorithm using hyperplane arrangements is given based on it. Also, an application of the primary shutter function to learning an unknown k-Voronoi space from examples is shown.

Theorem 4 *The number of Voronoi partitions of n points by the weighted Voronoi diagram generated by k weighted points with a multiplicative weight and an additive weight in the d-dimensional space is $O(n^{(d+2)k})$, and all the Voronoi partitions can be enumerated in $O(n^{(d+2)k+1})$ time.* $\square$

The proof is similar, and is omitted in this version. Combining these results, we have the following.

Theorem 5 *(1) The k-clustering problem for Var^1 can be solved in $O(n^{dk+1})$ time.*

(2) The k-clustering problem for Var^2 can be solved in $O(n^{(d+2)k+1})$ time.

It should be noted that, from the linear separability or circular separability, of an optimum 2-clustering for

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Var^1 and Var^2, respectively, as shown by [2, 7], the k-clustering problem for Var^1 and Var^2 is readily seen to be solvable in $O(n^{dk(k-1)/2})$ and $O(n^{(d+1)k(k-1)/2})$ time, respectively, using similar arguments in [3] for the diameter and radius. Only with the linear/circular separability for the 2-clustering, an algorithm of order $n^{O(dk^2)}$ may be best possible for the k-clustering problem. Our algorithms run in $O(n^{O(dk)})$ time, and improve the $O(n^{O(dk^2)})$ bound greatly. This becomes possible by the fine characterization of optimum k-clusterings by the weighted Voronoi diagram, and by evaluating the primary shatter function of the weighted Voronoi partitions in a tighter manner.

3 Randomized algorithms for the case of the sum of squared errors

The results in the previous section are interesting from the theoretical viewpoint, and the time complexity is polynomial when k is considered as a constant. However, even for $k = 3, 4, 5$, its polynomial degree is quite high, which makes it less interesting to implement the algorithms for practical problems such as the color quantization problem. The k-clustering problem is NP-complete in general when k is regarded as a variable, and in this respect the results are best possible we may expect to have.

To develop a practically useful algorithm, utilizing randomization may be a good candidate, since the intra-cluster metric we are using has its intrinsic statistical meanings. In this section, we develop randomized algorithms for the k-clustering problem with Var^1, the sum of squared error, as the intra-cluster metric.

In this extended abstract, we mainly consider the 2-clustering problem with Var^1, but most of the following discussions carry over to the k-clustering problem. First, let us consider how to estimate $\text{Var}^1(S)$ for the set S of n points $p_i = (x_i)$ $(i = 1, \ldots, n)$ by random sampling. Let T be a set of m points obtained by m independent draws at random from S. If the original point set S are uniformly located, $(n/(m-1))\text{Var}^1(T)$ may be a good estimate for $\text{Var}^1(S)$. However, this is not necessarily the case. For example, suppose that a point p_i in S is far from the other $n-1$ points in S, and the other $n-1$ points are very close to one another. Then, $\text{Var}^1(S)$ is nearly equal to the squared distance between p_i and a point in $S - \{p_i\}$, while with high probability $\text{Var}^1(T)$ is almost zero. This indicates that $\text{Var}^1(T)$ cannot necessarily provide a good estimate for $\text{Var}^1(S)$.

On the other hand, the centroid $\bar{x}(T)$ of T is close to the centroid $\bar{x}(S)$ of S with high probability by the law of large numbers, and we obtain the following lemma.

Lemma 1 *With probability $1 - \delta$,*

$$\|\bar{x}(T) - \bar{x}(S)\|^2 < \frac{1}{\delta m}\text{Var}^0(S).$$

Proof: First, observe that

$$\text{E}(\bar{x}(T)) = \bar{x}(S), \qquad \text{E}(\|\bar{x}(T) - \bar{x}(S)\|^2) = \frac{1}{m}\text{Var}^0(S)$$

and then apply the Markov inequality to obtain the following.

$$\Pr\left(\|\bar{x}(T) - \bar{x}(S)\|^2 > \frac{1}{\delta m}\text{Var}^0(S)\right) < \delta. \quad \square$$

Lemma 2 *With probability $1 - \delta$,*

$$\sum_{p_i \in S} \|x_i - \bar{x}(T)\|^2 < (1 + \frac{1}{\delta m})\text{Var}^1(S).$$

Proof: Immediate from Lemma 1 and the following.

$$\sum_{p_i \in S} \|x_i - \bar{x}(T)\|^2 = \text{Var}^1(S) + |S| \cdot \|\bar{x}(T) - \bar{x}(S)\|^2. \quad \square$$

Thus, we can estimate $\text{Var}^1(S)$ by random sampling. For the 2-clustering problem, we have to estimate $\text{Var}^1(S_1)$ and $\text{Var}^1(S_2)$ for a 2-clustering (S_1, S_2) by estimating the centroids of S_1 and S_2. Now, consider the following algorithm.

A randomized algorithm for the 2-clustering:

1. Sample a subset T of m points from S by m independent draws at random;

2. For every linearly separable 2-clustering (T_1, T_2) of T, execute the following:

   Compute the centroids t_1 and t_2 of T_1 and T_2, respectively;

   Find a 2-clustering (S_1, S_2) of S by dividing S by the perpendicular bisector of line segment connecting t_1 and t_2;

   Compute the value of $\text{Var}^1(S_1) + \text{Var}^1(S_2)$ and maintain the minimum among these values;

3. Output the 2-clustering of S with minimum value above.

The idea of this randomized algorithm is to use all pairs of centroids of linearly separable 2-clusterings for the sampled point set T. Let (S_1^*, S_2^*) be an optimum 2-clustering of S for Var^1, and let s_1^* and s_2^* be the centroids of S_1^* and S_2^*, respectively. By considering all linearly separable 2-clusterings for T, the algorithm handles the 2-clustering (T_1', T_2') obtained by dividing T by the perpendicular bisector of line segment connecting s_1^* and s_2^*. Then, from the centroids of T_1' and T_2', we obtain a 2-clustering (S_1', S_2') in the algorithm.

Since T is obtained from m independent draws,

$$\mathrm{E}(|T_j'|) = \frac{m}{n}|S_j^*| \quad (j = 1, 2).$$

From Lemma 2, $\text{Var}^1(S_j^*)$ can be estimated by using $|T_j'|$. The sizes $|T_j'|$ $(j = 1, 2)$ are determined by independent Bernoulli trials, and is dependent on the ratio of $|S_1^*|$ and $|S_2^*|$. For the sampling number m, we say that S is $f(m)$-balanced if there exists an optimum 2-clustering (S_1^*, S_2^*) with

$$\frac{m}{n}\min\{|S_1^*|, |S_2^*|\} \geq f(m),$$

and the optimum 2-clustering is called an $f(m)$-balanced optimum 2-clustering. We then have the following.

Lemma 3 *Suppose there exists a $(\log_e m)$-balanced optimum 2-clustering (S_1^*, S_2^*). Then, with probability $1 - \dfrac{2}{m^{\beta^2/2}}$ for a constant β $(0 < \beta < 1)$, the following holds.*

$$\min\{|T_1^*|, |T_2^*|\} > (1-\beta)\frac{m}{n}\min\{|S_1^*|, |S_2^*|\}$$
$$\geq (1-\beta)\log m.$$

Proof: Set $\mu' = \dfrac{m}{n}\min\{|S_1^*|, |S_2^*|\}$. For m independent Bernoulli trials $X_1, X_2, \ldots, X_m$ with $\Pr(X_i = 1) = \mu'/m \leq \Pr(X_i = 0) = 1 - \mu'/m$, the Chernoff bound implies, for $X = X_1 + \cdots + X_m$,

$$\Pr(X < (1-\beta)\mu') < \exp(-\mu'\beta^2/2).$$

From the assumption,

$$\exp(-\mu'\beta^2/2) \leq \exp(-(\log m)\beta^2/2) = \frac{1}{m^{\beta^2/2}}. \quad \square$$

Theorem 6 *Suppose that the point set S is $f(m)$-balanced with $f(m) \geq \log m$. Then, the randomized algorithm finds a 2-clustering whose total value is within a factor of $1 + \dfrac{1}{\delta(1-\beta)f(m)}$ to the optimum value with probability $1 - \delta - \dfrac{2}{m^{\beta^2/2}}$ in $O(nm^d)$ time.*

Proof: From Lemmas 2 and 3, with probability $1 - \delta - \dfrac{2}{m^{\beta^2/2}}$,

$$\sum_{j=1}^{2} \sum_{p_i \in S_j'} \|x_i - \bar{x}(T_j')\|^2$$
$$\leq (1 + \frac{1}{\delta(1-\beta)f(m)})\sum_{j=1}^{2}\text{Var}^1(S_j^*)$$

holds. Furthermore, the left hand side is bounded from below by $\sum_{j=1}^{2}\text{Var}^1(S_j')$, whose value is computed in the algorithm. Hence, the minimum value found in the algorithm is within the factor.

Concerning the time complexity, all linearly separable 2-clusterings for T can be enumerated in $O(m^d)$ time. For each 2-clustering (T_1, T_2) of T, finding a pair of centroids and a 2-clustering of S generated by the pair together with its objective function value can be done in $O(n)$ time. Thus the theorem follows. $\square$

We have developed a randomized algorithm only for the 2-clustering problem so far, but this can be directly generalized to the k-clustering problem. If there exists a balanced optimum k-clustering, similar bounds can be obtained. It may be noted that the technique employed here has some connection with the technique used to obtain a deterministic approximate algorithm with worst-case ratio bounded by 2 for the k-clustering problem in [7].

The above theorem assumes some balancing condition. In some applications, a very small cluster is useless even if its intra-cluster is small. For example, when we apply a 2-clustering algorithm recursively in a top-down fashion to solve the k-clustering problem, a balancing condition on 2-clusterings may be imposed to 2-clustering subproblems so that the sizes of subproblems may become small quickly and the total clustering may have nicer properties. In such a case, the randomized algorithm naturally ignores such small-size cluster. Also, for the case of finding a good and balanced 2-clustering, we have only to apply a slightly modified version of the randomized algorithm directly. This is typical for the clustering problem in VLSI layout design. See, for example, Kernighan and Lin [13]. Generalizing Theorem 6 for such cases, we have the following.

Theorem 7 *For the problem of finding an optimum 2-clustering among (γm)-balanced 2-clusterings for a constant γ, the randomized algorithm finds a 2-clustering which is almost at least (γm)-balanced and whose value is within a factor of $1 + O(1/(\delta m))$ to the optimum value of this problem with probability $1 - \delta$ for small δ. $\square$*

In the proof of this theorem, we use results concerning the ϵ-net and ϵ-approximations. The details will be

given in the full version. We here restate the theorem in a rough way so that its essence can be understood direclty.

Corollary 1 *When there is an optimum 2-clustering (S_1^*, S_2^*) of S such that*

$$|S_1^*|, \; |S_2^*| \geq \gamma |S| = n$$

for some constant γ $(0 < \gamma \leq 1/2)$, the randomized algorithm, which samples m points from S, finds a 2-clustering whose expected value is $1 + O(1/m)$ with high probability. $\square$

Corollary 2 *For the problem of finding an optimum 2-clustering among 2-clusterings (S_1, S_2) of S such that*

$$|S_1|, \; |S_2| \geq \gamma |S| = n$$

for some constant γ $(0 < \gamma \leq 1/2)$, the randomized algorithm, which samples m points from S, can be easily modified to find an approximate balanced 2-clustering whose expected value is $1 + O(1/m)$ with high probability. $\square$

On the other hand, if very small clusters with small intra-cluster metric should be found, we may enumerate such small clusters deterministically or in a randomized manner, since the number of such small clusters is relatively small. For the 2-clustering problem in the two-dimensional case, the number of linearly separable 2-clustering such that one cluster consists of at most k' points is $O(k'n)$ and can be enumerated efficiently. By enumerating k'-sets for an appropriate value of k', we obtain the following theorem.

Theorem 8 *The 2-clustering problem for n points in the plane with Var^1 as the intra-cluster metric can be solved in $O(n^{5/3}(\log n)^3)$ time with the approximation ratio within a factor of $1 + O(1/\log n)$ with probability $1 - O(1/\log n)$.*

Proof: Set $m = n^{1/3} \log n$. For this m, by the randomized algorithm, we find a good $(\log m)^2$-balanced 2-clustering. Also, by the deterministic algorithm enumerating $(\leq n^{2/3} \log n)$-sets, we find a best unbalanced 2-clustering. Setting $\delta = 1/\log m$ and β to a constant, the time complexity of the randomized algorithm is $O(n(n^{1/3} \log n)^2) = O(n^{5/3}(\log n)^2)$ and the approximation ratio is bounded by $1 + O(1/\log m)$ with probability $1 - O(1/\log m)$. The deterministic algorithm runs in $O(n(n^{2/3} \log n)(\log n)^2) = O(n^{5/3}(\log n)^3)$ time. $\square$

It should be noted that the time complexity in this theorem is subquadratic, compared with the deterministic quadratic exact algorithm.

4 Concluding remarks

We have demonstrated that optimum solutions to the variance-based k-clustering can be characterized by the (weighted) Voronoi diagram generated by k points, and have evaluated the primary shutter function of the k-Voronoi space. This primary shutter function can be used in computational learning theory in learning k-Voronoi spaces.

We have then presented a simple randomized algorithm for the k-clustering problem with Var^1 as an intra-cluster metric. This algorithm is practically useful when k is small and balanced k-clusterings are preferable. For example, for the problem of finding an optimum 2-clustering for n planar points among almost completely balanced 2-clusterings, an approximate 2-clustering which is approximately balanced and whose cost is within a factor of $1 + 1/3 = 4/3$ on the average to the optimum cost can be found by sampling 10 points from n points and spending $O(10^2 n) = O(n)$ time with probability $\sum_{i=3}^{7} \binom{10}{i}/2^{10} \approx 0.89$, or by sampling 20 points and spending $O(20^2 n) = O(n)$ time with probability $\sum_{i=3}^{17} \binom{20}{i}/2^{20} \approx 0.9996$.

The randomized algorithm, however, is not so suitable to find a good unbalanced 2-clustering. Also, although the randomized algorithm itself is valid for large k, the running time becomes inherently large since the primary shutter function for m sampled points is $O(m^{O(dk)})$. This implies that the variance-based k-clustering problem is harder in such a situation compared with the diameter- or radius-based k-clustering to which a good and fast approximate algorithm with worst-case ratio 2 is known [4].

Therefore, to solve the variance-based k-clustering for large k practically, say for $k = 256$ of the typical color quantization problem, we may apply the randomized 2-clustering algorithm proposed in this paper recursively in a top-down manner with sampling only a small number of points at each stage as mentioned above. We plan to implement this approach and experimentally evaluate its efficiency.

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