On Clusters that are Separated but Large

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Abstract

Given a set $P$ of $n$ points in $\mathbb{R}^d$, consider the problem of computing $k$ subsets of $P$ that form clusters that are well-separated from each other, and each of them is large (cardinality wise). We provide tight upper and lower bounds, and corresponding algorithms, on the quality of separation, and the size of the clusters that can be computed, as a function of $n, d, k, s, \Phi$, where $s$ is the desired separation, and $\Phi$ is the spread of the point set $P$.

1. Introduction

Clustering is one of the fundamental problems in data and computer science. We consider a variant of clustering where we are interested in computing clusters that are tight and well-separated in relation to each other. Unlike the classical settings, we do not require the clusters to cover all the points, and instead we want the clusters to be as large as possible, while providing the desired separation properties. One can interpret our problem as a variant of clustering with noise (or outliers) – which is a notoriously hard problem [DHS01].

Figure 1.1: A point set, two well-separated subsets (i.e., clusters), and the two associated balls.

On different notions of separation. In our settings a cluster is simply a subset of the points. The size of a cluster is the number of points in it, and when computing a collection of clusters, the quality of clustering is the cardinality of the smallest cluster among the clusters computed. A desired property is that clusters are separated from each other. Specifically, the distance between any pair of clusters is some function of their diameters. For example, two sets $C_1, C_2 \subseteq \mathbb{R}^d$ are well $s$-separated if

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\[
d(C_1, C_2) \geq s \max(\text{diam}(C_1), \text{diam}(C_2)),
\]
where \(d(C_1, C_2)\) is the minimum distance between points in the two sets, and \(\text{diam}(C_i)\) is the diameter of \(C_i\). Here \(s > 0\) is the \textit{separation} parameter, and the larger it is, the more separated the clusters are. An alternative way to view such well-separated sets is to consider the two smallest enclosing balls of the two clusters and require that these two balls are far from each other, see Figure 1.1. If we demand that both clusters are of large size, than there is a trade-off between the separation of the clusters, and their quality (i.e., the minimum number of points in either cluster).

A somewhat weaker notion is \textit{semi-\(s\)-separation}, where we require that for the two clusters \(C_1, C_2\), we have
\[
d(C_1, C_2) \geq s \min(\text{diam}(C_1), \text{diam}(C_2)),
\]
see Figure 1.2 for an example.

If one considers more than two clusters, say \(C_1, \ldots, C_k\), then one can further strengthen the notion of separation, requiring that the distance between clusters is determined by the cluster with the largest diameter. Formally, these \(k\) clusters are \textit{strongly \(s\)-separated} if
\[
\forall i \neq j \quad d(C_i, C_j) \geq s \cdot \max_{\ell=1}^{k} \text{diam}(P_{i}).
\]

These three notions of separations, for more than two clusters, are illustrated in Figure 1.3.

\textbf{Previous work on separation in computational geometry.} Callahan and Kosaraju [CK95] showed that a set \(P\) of \(n\) points in \(\mathbb{R}^d\) can be decomposed into \(O(s^d n)\) pairs, such that all pairs of points are covered by some pair in the decomposition, and all pairs are \(s\)-separated. This decomposition is known as \textit{well-separated pairs decomposition} (WSPD). There is also work on semi-separated pair decomposition, where one can get a near linear bound on the total size of listing all the pairs explicitly [Var98, AH12]. Both notions are widely used in geometric approximation algorithms, as they provide compact representation of the metric structure of the point set.

\textbf{Separation in clustering.} The ratio \(\min_{i<j} d(C_i, C_j)/\max_i \text{diam}(C_i)\) is known as the \textit{Dunn index}, and dates back to the work of Dunn from 1973 [Dun73], and is used to measure the quality of clustering (this corresponds to the notion of strong \(s\)-separation defined above). There are a lot of other measures of quality of clustering, including the \textit{Davies–Bouldin} and \textit{Silhouette} indices, among others. Such indices are used in cluster analysis [ELLS11]. Assumptions that lead to stable clustering can be interpreted as constraints on the separation between the “true” clusters [Lux10].
The task at hand. Here, we investigate the trade-off between the quality of separation (under the different notions) and clusters quality/size, and provide bounds quantifying it and algorithms for computing such good clusterings.

Our results. In the following $P$ is a set of $n$ points in $\mathbb{R}^d$, $s$ is the desired separation, $k$ is the number of clusters, and $\Phi$ is the spread of $P$. We remind the reader that for $k$ clusters $C_1, \ldots, C_k \subseteq P$, the quality of clustering is the size of the smallest cluster, that is $\min_i |C_i|$. We start with two easy upper bounds on the quality of clustering computed.

(A) **Quality must depend on the spread (well/strong separation).** In Lemma 3.2, we show that the standard exponential point set, implies that even for two clusters $C_1, C_2 \subseteq P$ in one dimension, the quality of the clustering can be at most $O(n/\log \Phi)$.

(B) **Quality drops with the dimension.** In Lemma 3.1, we show that the natural grid in $\mathbb{R}^d$ implies that under any notion of $s$-separation, the quality can be at most $O(n/s^d)$.

In particular, in high dimension, one can not get anything useful in the worst case:
Figure 1.4: A summary of results.

(C) **Quality drops exponentially with dimension.** Using the Johnson-Lindenstrauss lemma, we show an almost uniform point-set in $O(\log n)$ dimensions, such that any 2-separated clusters are useless (i.e., the smaller cluster of the two contains a single point). See Lemma 3.9.

We next combine (A) and (B), to get a more nuanced upper bound:

(D) **A stronger upper bound using exponential grid.** In Section 3.4, we show that a carefully constructed exponential grid, implies that the quality of any two clusters that are well $\delta$-separated is bounded by $O(n/(\delta^d \log \Phi))$. Intuitively, this is to be expected from combining the above two examples, but the details are somewhat involved and require care.

This upper bound construction also leads to an improved bound for the case of $k$ clusters, showing that for such clusters to be well/strongly $\delta$-separated, in the worst case, the quality is bounded by $O(n/(k \delta^d \log \Phi))$. See Corollary 3.7.

Next, in Section 4 we study algorithms for computing such clusterings.

(E) **Algorithm for computing semi $\delta$-separated $k$ clusters.** In Lemma 4.1, we show how to compute $k$ clusters that are semi $\delta$-separated, and the quality of the computed clusters is $\Omega(n/(\delta^d \log \Phi))$. This matches the above upper bound of Lemma 3.1.

(F) **Algorithm for computing well/strong $\delta$-separated $k$ clusters.** In Section 4.2, we present an algorithm to compute $k$ clusters that are strongly (and thus also well) $\delta$-separated, and the quality of the clusters is $\Omega(n/(k \delta^d \log \Phi))$. This matches the upper bound of Corollary 3.7 mentioned above.

(G) **The colored version.** We also study the colored variant, where we are given $k$ sets $P_1, \ldots, P_k \subseteq \mathbb{R}^d$ (each with $n$ points), and the task at hand is to compute clusters $C_1, \ldots, C_k$ that are $\delta$-separated, and $C_i \subseteq P_i$, for all $i$. Fortunately, a variant of the uncolored algorithm works in the colored case, and yields the same bound for the colored semi $\delta$-separated case. See Lemma 4.2.

Unfortunately, for three or more colors no useful clustering is possible if one wants strong separation, see Section 3.3.

The only remaining case is the colored well-separate case, where one can compute $k$ clusters, each of size $\Omega(n/(k \delta^d \log \Phi))$, see Lemma 4.4. Thus, the three notions of separations have different behaviors.

The results are summarized in Figure 1.4.
Techniques used. For the algorithms, we use as basic building blocks two tools: (i) fast approximation algorithm for smallest enclosing ball, and (ii) quorum clustering.

Connection to Ramsey theory. We are addressing here a natural question of finding large subset(s) of the data that have a good structure that is better than the one that holds for the whole input. A classical example of such a question is finding the largest clique in the graph (i.e., Ramsey numbers). There is also work in finite metric spaces showing that there is always a subset that is a “better” metric space [BLMN05].

Paper organization. We start by formally defining the different notions of separation in Section 2.1. We then describe, in Section 2.2, the two main algorithmic building blocks – tighter ball extraction and quorum clustering. For quorum clustering we prove a key property about their density in Lemma 2.6. In Section 3 we present the various upper bounds on the quality of clustering under the various notions of separations. The algorithms are presented in Section 4. We conclude in Section 5.

2. Preliminaries

2.1. Definitions

Definition 2.1. A metric space \((X, d)\) is a set \(X\) equipped with a metric \(d\). For two sets \(X, Y \subseteq X\), their distance is \(d(X, Y) = \min_{x \in X, y \in Y} d(x, y)\). The closest pair distance of a set of points \(P \subseteq X\), is \(\text{cp}(P) = \min_{p, q \in P, p \neq q} d(p, q)\). The diameter of \(P\) is \(\text{diam}(P) = \max_{p, q \in P} d(p, q)\). The spread of \(P\) is \(\Phi(P) = \frac{\text{diam}(P)}{\text{cp}(P)}\), which is the ratio between the diameter and closest pair distance.

Definition 2.2. Let \(P\) be a set of points in a metric space \((X, d)\). Consider \(k\) sets \(P_1, \ldots, P_k \subseteq P\), and a parameter \(\delta > 0\). The sets \(P_1, \ldots, P_k\) are:

- **strongly \(\delta\)-separated** if for all distinct \(i, j\), we have \(d(P_i, P_j) \geq \delta \cdot \max_{t=1}^{k} \text{diam}(P_t)\).
- **well \(\delta\)-separated** if for all distinct \(i, j\), we have \(d(P_i, P_j) \geq \delta \cdot \max(\text{diam}(P_i), \text{diam}(P_j))\).
- **semi \(\delta\)-separated** if for all distinct \(i, j\), we have \(d(P_i, P_j) \geq \delta \cdot \min(\text{diam}(P_i), \text{diam}(P_j))\).

The quality of the collection is \(\min_i |P_i|\). Such a collection of sets is **useless** if \(|P_i| = 1\) for some \(i\) (i.e., the quality is one).

Observation. For \(k = 2\), strong separation and well separation are the same. If a pair of sets \(X, Y\) is \(c\)-separated, then it is \(c'\)-separated for all \(c' \leq c\).

2.2. Basic tools

2.2.1. Tight ball extraction

Theorem 2.3 ([HR15]). Given a set \(P\) of \(n\) points in \(\mathbb{R}^d\) and a parameter \(\alpha\), one can compute, in expected linear time and with high probability, a ball \(b\) of radius \(r\), such that \(r_{\text{opt}}(P, \alpha) \leq r \leq 2r_{\text{opt}}(P, \alpha)\), where \(r_{\text{opt}}(P, \alpha)\) is the minimum radius of a ball covering \(\alpha\) points of \(P\). Furthermore, we have that \(b\) contains at least \(\alpha\) points of \(P\).
2.2.2. Quorum clustering and some properties

Let $P$ be a set of $n$ points in $\mathbb{R}^d$. Consider the process that, in the $i$th iteration, does the following:

(I) Computes the ball $b_i$ that contains $\geq \gamma$ points of $P$, where $r_i = \text{radius}(b_i) \leq 2\rho_i$, where $\rho_i = r_{\text{opt}}(P, \gamma)$ is the radius of the smallest ball containing $\gamma$ points of $P$.

(II) Select exactly $\gamma$ points of $P \cap b_i$ into a new set $P_i$.

(III) $P \leftarrow P \setminus P_i$.

This process is repeated till $P$ is an empty set, and assume that $b_m$ and $P_m$ are the last ball and set computed. (The last set $P_m$ might contain less than $\gamma$ points.)

The resulting partition is known as quorum clustering, and it can be computed in $O(n \log n)$ time [CDH+05, HR15] (for a constant dimension $d$).

Definition 2.4. The era starting at location $i$, is the longest subsequence $r_i, r_{i+1}, \ldots, r_j$ such that

$$\max(r_i, r_{i+1}, \ldots, r_j) \leq 4r_i.$$ 

Let $\text{era}(i)$ denote the index ending the epoch starting at $i$ (e.g., above we have $\text{era}(i) = j$).

Starting at the first location $r_1$, this naturally partitions the quorum clustering into epochs. Setting $f(1) = \text{era}(1)$, and $f(i) = \text{era}(f(i-1)+1)$, for $i > 1$. The $i$th epoch is the subsequence $r_{f(i-1)+1}, \ldots, r_{f(i)}$. The sequence of sets in the $i$th epoch is $\mathcal{B}_i = \{P_{f(i-1)+1}, \ldots, P_{f(i)}\}$.

Observation 2.5. (A) Let $\rho_i$ be the radius of the smallest ball containing $\gamma$ (unclustered) points in the beginning of the $i$th epoch. We have that $\rho_1 \leq \rho_2 \leq \cdots \leq \rho_m$. Let $r$ be a radius of any ball in $\mathcal{B}_i$ containing $\gamma$ points. By the definition of $\rho_i$, we have

$$\rho_i \leq r \leq 4r_i \leq 8\rho_i.$$ 

Therefore, the radius of any such ball in $\mathcal{B}_i$ lies in $[r/8, 8r]$.

(B) For all $i$, we have $\rho_{i+1} \geq (4r_i/2) \geq 2\rho_i$.

The above implies that the quorum clustering has at most $O(\log \Phi)$ epochs, and the following lemma implies that balls that are in the same epoch are sparse – they can not cover a point too many times.

Lemma 2.6. Let $\mathcal{B}_i$ be the set of balls computed in the $i$th epoch. Any point $p \in \mathbb{R}^d$ is contained in at most $d^{O(d)}$ balls of $\mathcal{B}_i$.

Proof: Fix arbitrary $p \in P$ and let $r$ denote the radius of the last ball in $\mathcal{B}_i$. By definition, and by Observation 2.5, all the balls of $\mathcal{B}_i$ have radius in the range $[r/8, 8r]$.

Consider the (hyper)cube $\Box$ of side length $32r$ centered at $p$. Any ball of $\mathcal{B}_i$ that covers $p$ is contained inside $\Box$. Consider the partition of $\Box$ into a grid of cells with sidelength $r/\lceil 32\sqrt{d} \rceil$. Formally we partition $\Box$ into a grid of $c^d$ equal sizes cubes, where $c \leq 2 + 16r/(r/32\sqrt{d}) = O(\sqrt{d})$. Every cell in this grid has diameter at most $r/32$, and is contained as such in a ball of radius $r/16$. If the number of balls in $\mathcal{B}_i$ that covers $p$ exceeds $c^d$, then the $\Box$ contains at least $(c^d+1)\gamma$ points in the beginning of the epoch. Namely, one of the grid cell contains at least $\gamma$ points at this point in time. Namely, $r_{\text{opt}}(P; \gamma) \leq r/16$, which implies that the first ball in this epoch must have radius $< r/8$. But this is impossible. □
3. Upper bounds on quality of clustering

3.1. Upper bound for the uniform case

Lemma 3.1. Let \( n > 0 \) be an integer number, such that \( N = n^{1/d} \) is an integer. Consider the grid point set \( P = [N]^d \subseteq \mathbb{R}^d \), and parameters \( k \) and \( \delta > 0 \), where \( [N] = \{1, \ldots, N\} \). Any strong, well or semi \( \delta \)-separated \( k \) clusters \( C_1, \ldots, C_k \subseteq P \) have the property that \( \min_i |C_i| = \Theta(n/(k\delta^d)) \).

Proof: Let \( C_1, \ldots, C_k \) be such a clustering. Let \( t = \lceil cn/(k\delta^d) \rceil \) for a sufficiently large constant \( c \), and assume, for the sake of contradiction, that \( |C_i| \geq t \), for all \( i \). A grid set \( S \) with diameter \( \ell \) is contained inside a hypercube of sidelength \( \ell + 1 \), and thus \( |S| \leq (\ell + 1)^d \leq 2^{d+1} \) points. We conclude that \( \text{diam}(S) \geq |S|^{1/d}/2 \). This implies that \( \text{diam}(C_i) \geq \beta^{1/d}/2 \geq \beta \cdot n^{1/d}/(k^{1/d}\delta) \) points (if \( c \) is sufficiently large), for all \( i \), where \( \beta \) is a constant to be specified shortly. Now, we have that

\[
\text{d}(C_i, C_j) \geq \delta \min(\text{diam}(C_i), \text{diam}(C_j)) \geq \delta \cdot \frac{\beta^{1/d}/(k^{1/d}\delta)}{2^{1/d}} \geq \frac{\beta n^{1/d}/(k^{1/d}\delta)}{2^{1/d}} \geq \beta n^{1/d}/2^{1/d}. 
\]

Let \( \ell = (\beta/(2\sqrt{d})) n^{1/d}/2^{1/d} \). Assign each point of the grid \( [N]^d \) to the cluster closest to it (resolve equality in an arbitrary fashion). It is easy to verify that each cluster gets assigned at least \( (\ell/2)^d \) points. This would imply that \( (\ell/2)^d k \leq n \), which fails if \( \beta \) is sufficiently large, as

\[
(\ell/2)^d k = \left( \frac{\beta/(2\sqrt{d}) n^{1/d}}{2^{1/d}} \right)^d \geq \frac{\beta}{4^d d^d}. 
\]

3.2. Upper bound with inverse logarithmic dependency on the spread

We start by constructing an exponentially spaced point set admitting only useless clustering. Thus, any bound on the quality of clustering must have (inverse) logarithmic dependency on the spread of the point set.

Lemma 3.2. There exists a point set \( P \) of \( n \) points in the real line, with spread \( 2^{n+1} \), such that all strongly (or well) \( 1 \)-separated pairs are useless. Namely, for any two clusters \( C_1, C_2 \subseteq P \) that are strongly \( 1 \)-separated we have that \( \min(|C_1|, |C_2|) = 1 \).

Proof: For \( i = 1, \ldots, n \), let \( p_i = \sum_{j=0}^{i} 2^j = 2^{i+1} - 1 \), and let \( P = \{p_1, \ldots, p_n\} \). The distance \( |p_i - p_{i+1}| = |p_0 - p_i| - 1 \). Consider two sets \( B_1, B_2 \subseteq P \) that are \( 1 \)-separated, where, without loss of generality, all the points of \( B_2 \) are bigger than all the points of \( B_1 \). By the \( 1 \)-separation, we have that \( \text{diam}(B_2) \leq \text{d}(B_1, B_2) = \text{max} B_1 - \text{min} B_2 \). As such, if \( p_i, p_{i+\Delta} \in B_2 \), for some \( \Delta > 0 \), then we have

\[
\text{max} B_1 \leq \text{min} B_2 - \text{diam}(B_2) \leq p_i - (p_{i+\Delta} - p_i) = 2 \cdot 2^{i+1} - 2 - 2^{i+\Delta+1} + 1 \leq -1, 
\]

which is impossible. It follows that the set \( B_2 \) can contain only a single point. Namely, this pair is useless. \( \Box \)

In light of this disappointing example, we restrict ourselves to bounds that depends on the spread of \( P \), when looking for well-separation.
3.3. Strong separation is hopeless for three colors

**Lemma 3.3.** There are three sets $P_1, P_2, P_3$ of $n$ points each on the real line, such that $P = \bigcup_i P_i$ has spread $O(n^2)$. Furthermore, for any strong 3-separated clustering $C_1, C_2, C_3$, with $C_i \subseteq P_i$, for $i = 1, 2, 3$, we have that $\min_i |C_i| = 1$.

**Proof:** Let $P_1 = \mathbb{N} = \{1, \ldots, n\}$, $P_2 = n + \mathbb{N} = \{n + x \mid x \in \mathbb{N}\}$, and $P_3 = \{1 + (1 + i)n \mid i \in \mathbb{N}\}$.

The spread of $\bigcup_i P_i$ is $O(n^2)$, See Figure 3.1. Consider any colorful strong 3-separated sets $C_1, C_2, C_3$, with $C_i \subseteq P_i$, for $i \in [3]$. If $|C_3| \geq 2$, then $\text{diam}(C_3) \geq n$. But this implies that $C_1$ and $C_2$ can not be strongly 3-separated, since

$$3n \leq 3\text{diam}(C_3) \leq d(C_1, C_2) \leq \text{diam}(P_1 \cup P_2) \leq 2n,$$

which is a contradiction. ■

3.4. Upper bound on quality by an exponential grid

**Construction.** For a point $p = (p_1, \ldots, p_d) \in \mathbb{R}^d$, and a number $c > 0$, let

$$p/c = (p_1/c, p_2/c, \ldots, p_d/c).$$

Similarly, for a set $X \subseteq \mathbb{R}^d$, let $X/c = \{p/c \mid p \in X\}$.

Let $n, \delta, \Phi$ be parameters. Let $h = \log_2 \Phi$ – for the sake of simplicity of exposition assume that $h$ is an integer. In the following, we assume that $n$ is sufficiently large compared to $\delta$ and $h$, and $\Phi \geq n$.

Let $R_1 = [-3,3]^d \setminus (-2,2)^d$ be a “ring”, and pick a maximum number $\ell$, such that the uniform grid $G_1$ with sidelength $\ell$ contains at least $n$ points in $R_1$. Let $P_1$ be a set of arbitrary $n$ points of $Q_1 = G_1 \cap R_1$. In the following, we assume that $n$ is sufficiently large, such that $|G_1 \cap [-3,3]^d| \leq 6n$.

For $i = 2, \ldots, h$, let $P_i = P_1/3^{i-1}$, $Q_i = Q_1/3^{i-1}$, and $R_i = R_1/3^{i-1}$. Let $P = \bigcup_{i=1}^h P_i$. See Figure 3.2.
Analysis. We have that the spread of \( P \) is bounded by \( O(n3^h) = \Phi^{O(1)} \). Also, \( |P| = \Theta(n \log \Phi) \).

Lemma 3.4. The rank of a cluster \( C \subseteq P \), denoted by \( r(C) \), is the smallest index \( j \), such that \( C \) contains points of \( P_j \). If the rank of \( C \) is \( t \), and \( C \) contains at least \( cn/\delta^d \) points of \( P \), then \( \text{diam}(C) \geq 2\text{diam}(R_t)/\delta \), for \( c \) a sufficient large constant that depends only on \( d \).

Proof: If \( C \) contains points of \( \cup_{r > t} P_r \), then by the ring property we have that
\[
\text{diam}(C) \geq \frac{\text{diam}(R_t)}{6\sqrt{d}} \geq \frac{2\text{diam}(R_t)}{\delta}
\]
(see purple segment in Figure 3.2), which establishes the claim.

Otherwise, \( C \subseteq P_t \). By scaling, we can assume that \( t = 1 \). Let \( Q = G_1 \cap [-3,3]^d \), we have by construction (and the assumption that \( n \) is sufficiently large), that \( |Q| \leq 6|P_t| \leq 6n \). A point set \( S \subseteq Q \) that contains at least \( \gamma|Q| \geq 1 \) points of \( Q \), for some \( \gamma \in (0,1] \), must have diameter \( \rho \geq \gamma^{1/d}\text{diam}(Q)/(4d) \) (this follows from the same argument used in Lemma 3.1). In particular, for \( c \) sufficiently large, if \( C \) contains at least \( cn/\delta^d \) points of \( Q \), then
\[
\text{diam}(C) \geq \left( \frac{c}{63^d} \right)^{1/d} \cdot \frac{1}{4d} \cdot \text{diam}(Q) \geq \frac{2}{\delta} \text{diam}(R_t),
\]
for \( c \) sufficiently large. \( \blacksquare \)

Lemma 3.5. For any two clusters \( C_1, C_2 \subseteq P \), such that \( \text{d}(C_1, C_2) \geq \delta \cdot \max(\text{diam}(C_1), \text{diam}(C_2)) \), we have that \( \min(|C_1|, |C_2|) = O(n/\delta^d) \).

Proof: Assume for contradiction that \( |C_i| \geq cn/\delta^d \), for \( i = 1,2 \), where \( c \) is the constant specified in Lemma 3.4. If \( r = r(C_1) \leq r(C_2) \) then \( C_1, C_2 \subseteq H_r = [-3.3]^d/3^{r-1} \). By Lemma 3.4, we have that \( \text{diam}(C) \geq 2\text{diam}(R_t)/\delta = 2\text{diam}(H_r)/\delta \). But this implies that
\[
\text{d}(C_1, C_2) \geq \delta \cdot \max(\text{diam}(C_1), \text{diam}(C_2)) \geq 2\text{diam}(H_r),
\]
which is a contradiction, as the two sets are contained in the hypercube \( H_r \).

The case that \( r(C_1) \geq r(C_2) \) is handled in a similar fashion. \( \blacksquare \)

This implies the following result.

Theorem 3.6. Given parameter \( \delta > 12d \), an integer \( n \) sufficiently large, and a parameter \( \Phi \geq n \), one can construct a point set \( P \) in \( \mathbb{R}^d \) of size \( N = O(n \log \Phi) \), such that \( \Phi(P) = \Phi^{O(1)} \). Furthermore, for any two clusters \( C_1, C_2 \subseteq P \) we have that if they are (strongly or well) \( \delta \)-separated then they are “small”. Formally, we have
\[
\text{d}(C_1, C_2) \geq \delta \cdot \max(\text{diam}(C_1), \text{diam}(C_2)) \implies \min(|C_1|, |C_2|) = O\left( \frac{N}{\delta^d \log \Phi} \right).
\]

The above extends to \( k \) clusters.

Corollary 3.7. Given parameter \( \delta > 12d \), an integer \( n \) sufficiently large, a parameter \( \Phi \geq n \), and an integer \( k > 2 \), one can construct a point set \( P \) in \( \mathbb{R}^d \) of size \( N = O(nk \log \Phi) \), such that \( \Phi(P) = \Phi^{O(1)} \). Furthermore, for any \( k \) clusters \( C_1, \ldots, C_k \subseteq P \), if they are strongly or well \( \delta \)-separated, see Definition 2.2, then \( \min_i |C_i| = O\left( \frac{N}{k \delta^d \log \Phi} \right) \).

Proof: Let \( P \) be the point set of Theorem 3.6, and let \( \Delta = \text{diam}(P) \). We take \( \lfloor k/2 \rfloor \) copies of \( P \), spacing them \( \Delta \) distance from each other along a line. If there \( k \) clusters, then at least two of them must belong to the same copy of the point set (if a cluster spans more than a single copy of the point set, then it is the only cluster involved in its point set because of the separation property). But then the bound of Theorem 3.6 applies the claim immediately. \( \blacksquare \)
3.5. Upper bound in high dimensions

Theorem 3.8 (Johnson-Lindenstrauss lemma, [JL84]). For any \( \varepsilon \in (0, 1) \), and a set of \( n \) points \( P \subseteq \mathbb{R}^n \), there exists a linear function \( f : \mathbb{R}^n \rightarrow \mathbb{R}^d \), for \( d = 8 \lceil \varepsilon^{-2} \ln n \rceil \), such that
\[
\forall p, q \in P \quad (1 - \varepsilon) \|p - q\| \leq \|f(p) - f(q)\| \leq (1 + \varepsilon) \|p - q\|.
\]

Lemma 3.9. For any \( d \) sufficiently large, there exists a point set \( P \subseteq \mathbb{R}^d \), of size \( \exp(\Omega(d)) \), such that all 2-separated pairs are useless.

In particular, there is a set of \( n \) points in \( \mathbb{R}^{O(\log n)} \), such that any two clusters that are 2-separated are useless.

Proof: Let \( e_1, \ldots, e_n \) be the standard orthonormal basis for \( \mathbb{R}^n \), and let \( P = \{e_i/\sqrt{2} \mid i = 1, \ldots, n\} \). By the Johnson-Lindenstrauss lemma, for all \( 0 < \varepsilon \), there exists an \((1 \pm \varepsilon)\)-embedding \( P \) into \( \mathbb{R}^d \), where \( d = 8 \lceil \varepsilon^{-2} \ln n \rceil \). Let \( P' \subseteq \mathbb{R}^d \) be this embedding of \( P \). Any subset \( Q' \subseteq P' \), with two or more points, has diameter in the range \( I = [1 - \varepsilon, 1 + \varepsilon] \). In particular, we have that for two such subsets \( Q'_1, Q'_2 \subseteq P' \), we have that \( d(Q'_1, Q'_2), \text{diam}(Q'_1), \text{diam}(Q'_2) \in I \). Since \( (1 - \varepsilon)(1 + 2\varepsilon) > 1 + \varepsilon \), we conclude that for \( P' \), for any \((1 + 2\varepsilon)\)-separated sets \( Q'_1, Q'_2 \), it must be that \( \min(|Q'_1|, |Q'_2|) = 1 \). Namely, all 2-separated pairs are useless.

Setting \( \varepsilon = 1/2 \), and stating \( n \) in terms of \( d \), we have
\[
\exp(d) = \exp(8 \lceil \varepsilon^{-2} \ln n \rceil) \leq e^8 n^{8/\varepsilon^2} \implies \exp(d/32 - 4) = \exp(8 \lceil \varepsilon^{-2} \ln n \rceil) \leq n.
\]

Remark. Lemma 3.2 and Lemma 3.9 imply that any useful bound on the quality of well-separated pairs requires the bound to depend exponentially on the dimension, and logarithmically on the spread of the point set.

4. Algorithms for computing heavy and separated \( k \) clusters

4.1. Semi-separated clusters

Lemma 4.1. Given a set \( P \) of \( n \) points in \( \mathbb{R}^d \), and parameters \( k \) and \( \delta \), one can compute, in \( O(nk) \) expected time, a semi \( \delta \)-separated collection of \( k \) sets \( C_1, \ldots, C_k \subseteq P \), such that \( \min_i |C_i| = \Omega(n/(k\delta^d)) \).

Proof: Let \( \alpha = \lceil cn/(k\delta^d) \rceil \), where \( c \) is some appropriate constant. Let \( P_0 = P \). In the \( i \)-th iteration, 2-approximate the smallest ball containing \( \alpha \) points of \( P_{i-1} \), and let \( b_i \) be this ball. Let \( C_i \) be \( \alpha \) points of \( P_{i-1} \) contained in \( b_i \). Set \( P_i = P_{i-1} \setminus b'_i \), where \( b'_i = (2\delta + 2)b_i \) is the scaling of \( b_i \) around its center by a factor of \( 2\delta + 2 \). The algorithm repeats this extraction step \( k \) times.

Observe, that \( b'_i \) can be covered by \( O(\delta^d) \) balls of radius \( \text{radius}(b_i)/2 \), and as each such ball contains at most \( \alpha \) points, it follow that \( |P_i| \geq |P_{i-1}| - O(\delta^d) \). As such, if \( c \) is chosen to be sufficiently large, we have that \( |P_{k-1}| \geq \alpha \), which ensures the algorithm succeeds in extracting the \( k \) clusters.

By construction, for any \( i \neq j \), we have that \( d(C_i, C_j) \geq 2\delta \text{radius}(b_i) \geq \delta \text{diam}(C_i) \), which implies that the two sets are semi \( \delta \)-separated.

We readily get the same result for the colored version.

Lemma 4.2. Given \( P_1, \ldots, P_k \subseteq \mathbb{R}^d \) be \( k \) sets of \( n \) points each, and a parameter \( \delta \), one can compute, in \( O(nk^2) \) expected time, a semi \( \delta \)-separated \( k \) sets \( C_1, \ldots, C_k \), such that \( \min_i |C_i| = \Omega(n/(k\delta^d)) \) and \( C_i \subseteq P_i \), for all \( i \).
Proof: Initially, all the \( k \) point sets \( P_1, \ldots, P_k \) are active.

Similar to the algorithm of Lemma 4.1, in the \( i \)th iteration, the algorithm 2-approximates for each active set \( P_i \) the smallest ball containing \( \alpha = [cn/(k\Delta d)] \) of this set, where \( c \) is some appropriate constant. The algorithm picks the smallest such ball to be \( b_i \). For simplicity of exposition, assume \( b_i \) was computed for \( P_i \). Set \( C_i \) to be \( \alpha \) points of \( P_i \) that lie inside \( b_i \), and mark \( P_i \) as inactive. The algorithm now removes all the points in the active sets that are inside the ball \((2 + 2\Delta)b_i\), and continues to the next iteration.

The correctness of this algorithm follows the same argument as in Lemma 4.1. 

4.2. Strongly separated pairs using quorum clustering

Theorem 4.3. Given a set \( P \) of \( n \) points in \( \mathbb{R}^d \) with spread \( \Phi \), and parameters \( k \) and \( \Delta \), one can compute \( k \) disjoint subsets, \( C_1, \ldots, C_k \subseteq P \), in \( O(n \log n) \) time, each of size at least

\[
\Omega_d \left( \frac{n}{(k\Delta d) \log \Phi} \right),
\]

such that these sets are strongly/well \( \Delta \)-separated.

Proof: Let \( \alpha = [cn/(k\Delta d \log \Phi)] \), for an appropriate constant \( c \). We compute the quorum clustering of \( P \) for the parameter \( \alpha \), in \( O(n \log n) \) time [HR15]. By the definition of \( \alpha \), there are \( N = \lceil n/\alpha \rceil = \Theta(ck\Delta d \log \Phi) \) balls computed by the quorum clustering. Let \( r_i \) be the radius of the first ball in the \( i \)th epoch. The radiiuses of the balls in the \( i \)th epoch is between \([r_i/8, 8r_i]\).

Observe that \( r_{i+1} > 4r_i \) by construction, which readily implies that the number of epochs is at most \( \log_2 \Phi \). As such, there must be an epoch that contains at least \( M = \Theta(ck\Delta d) \) balls. Consider a ball \( b \) in this epoch, and let \( p \) be its center and \( r \) be its radius. All the balls in distance \( \leq \Delta \cdot 4r \) from it are contained in a ball \( B \) of radius \((8 + 2\Delta)r \) centered at \( p \). By Lemma 2.6, the number of balls of this epoch covering any point in \( B \) is bounded by \( d^{O(d)} \). As such, the total number of balls that are not \( \Delta \)-separated from \( b \) is at most \((8 + 2\Delta)^d d^{O(d)} \). As such, we add \( b \) to \( C \), and remove all the balls contained in \( B \). Clearly, we can repeat this process \( M/(8 + 2\Delta)^d d^{O(d)} \) times. This quantity is at least \( k \), for \( c \) sufficient large, as desired.

As such, the algorithm compute the epoch with the most balls, and repeatedly pick a ball, add it to the clustering, and remove all the balls (in this epoch) that are not \( \Delta \)-separated from the set of balls picked so far. After \( k \) iterations, the resulting set of \( k \) balls are all pairwise strongly \( \Delta \)-separated, as desired. This later part of the algorithm can be computed in linear time using a grid, and we omit the straightforward details.

The quorum clustering can be computed in \( O(n \log n) \) time [HK14], the algorithm as described above is no more than computing an appropriate net of the centers of the balls in the large epoch, and this can be done in linear time [HR15]. Using the same techniques as [HR15], it is straightforward to compute, in the linear time, the points \( P \) that are contained in the selected balls.

4.3. Colored well-separated clustering

Lemma 4.4. Let \( P_1, \ldots, P_k \subseteq \mathbb{R}^d \) be \( k \) sets of \( n \) points each, such that the spread of \( P = \cup_i P_i \) is \( \Phi \). For any parameter \( \Delta > 0 \), one can compute, in \( O(nk \log \Phi) \) time, \( k \) clusters \( C_i \subseteq P_i \), for \( i = 1, \ldots, k \), such that these clusters are well \( \Delta \)-separated, and \( \min_i |C_i| = \Omega(\frac{n}{(k\Delta d \log \Phi)}) \).

Proof: We compute quorum clustering of each point set \( P_i \), with sets being of size \( \alpha = cn/(k\Delta d \log \Phi) \), where \( c \) is some constant to be specified shortly. Let \( B_i \) be the set of balls computed for the quorum
clustering of $P_i$, for $i = 1, \ldots, k$. Let $\mathcal{B} = \bigcup_i \mathcal{B}_i$. In the $i$th iteration, the algorithm repeatedly pick the smallest ball $b_i$ in $\mathcal{B}$, and assume it is a cluster of $P_i$. The algorithm add the points of $P_i$ covered by $b_i$ to the output, and remove all the balls of $\mathcal{B}_i$ from $\mathcal{B}$. In addition, all the balls that are not well $\delta$-separated from $b_i$ in $\mathcal{B}$ are removed from the set. The algorithm repeats till $k$ iterations are complete.

Observe, that in an epoch of $\mathcal{B}_j$ that involves balls that are of the roughly the same radius or larger than $b_i$, for $j \geq i$, there could be at most $O(\delta^d)$ balls that are not well $\delta$-separated from $b_i$, by the packing property of Lemma 2.6. As such, at most $O(\delta^d \log \Phi)$ balls are being thrown out of $\mathcal{B}_j$, for $j > i$, in the $i$th iteration. As such, for a sufficiently small $c$, the final set $\mathcal{B}_k$ is not empty, and the algorithm indeed computes $k$ clusters each of size at least $\alpha$.

The resulting clusters are well $\delta$-separated by construction.

\section{Conclusions}

We studied the problem of computing large separated clusters for a give point set, and provided upper bounds and algorithms for computing such “high” quality clusterings.

The clustering computed can be used to seed other clustering algorithms, such as the $k$-means method. We leave this as an open problem for further research.

Another interesting open problem is to compute the best such clustering for a given input. It is easy to show that this problem, in general, is as hard as computing the largest clique in a graph. As such, approximation algorithms approximating the optimal clustering that run in polynomial time in $d, k$ and $\delta$ are potentially interesting.

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