Non-Center-Based Clustering Under Bilu-Linial Stability

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***Abstract*—In this paper, we give the first analyses of the non-center-based clustering objectives of sum-of-diameters and sum-of-radii under Bilu-Linial stability. Specifically, for the sum-of-diameters problem, we give polynomial-time algorithms for instances that are 2-stable, accompanied by a matching hardness result for stability below 2. For sum-of-radii clustering, we give an analysis showing that 2-stable instances are polynomial-time solvable. THIS PAPER IS ELIGIBLE FOR THE STUDENT PAPER AWARD.**

I. Introduction

In this paper, we give the first results on **minimizing sum-of-diameters (MSD)** (and also, in the Appendix, **minimizing sum-of-radii (MSR)**) clustering under a stability assumption first introduced by Bilu and Linial [1] that is motivated by the observation that many real-world NP-hard problems can be solved efficiently in practice. Informally, **Bilu-Linial stability** assumes the optimal solution for a problem of interest does not change under small perturbation of the input.

In particular, we give structural properties that show that single-linkage and complete-linkage algorithms give exact solutions to 2-stable sum-of-diameters (MSD) instances, and we show that instances that are strictly less than 2-stable are NP-hard under randomized reductions. For the closely related problem of sum-of-radii clustering (MSR), we also present some structural properties that allow the single-linkage algorithm to solve 2-stable instances and the complete-linkage algorithm to solve 3-stable instances. We defer these results to the Appendix.

Many problems have been studied under Bilu-Linial stability, including max-cut [1], [2], max independent set [3], and center-based clustering such as k-means, k-median [4]–[6], k-center [7] and min-sum [8]. Other metric based problems include the traveling salesman problem [9] and the Steiner tree problem [10]. These works are also closely related to robust algorithms [2] and certified algorithms [11], as well as to an interesting connection between stability and independent systems/matroids [12]. Despite extensive research on center-based clustering, the MSD and MSR problems, which possess distinct, non-center-based structures, have yet to be analyzed under Bilu-Lineal stability.

The MSD and MSR problems are closely related and an exact solution to one is a 2-approximation to the other. Under a general metric, MSD and MSR are both known to be NP-hard [13], [14]. There are various approximation algorithms for these problems (see e.g. [15]), as well as exact algorithms studied under different metrics [16]–[19].

II. Preliminaries

Given a clustering instance (P, d) where P is a set of n points and $d(\cdot,\cdot)$ is a metric on P, we study the problem of dividing the points into k clusters $\{C_1, \ldots, C_k\}$ under a non-center-based objective, namely the MSD objective, where the goal is to minimize the sum of diameters of all the clusters. The diameter of a cluster C is

$$\rho(C) := \max_{(x,y)\in C} d(x, y).$$

A closely related objective that minimizes the sum of radii is known as MSR, and the radius is

$$r(C) := \min_{c\in C} \max_{p\in C} d(c, p).$$

Notice that a solution to MSR is a 2-approximation to MSD and vice versa, because for each cluster we have $r \leq \rho \leq 2r$, and

$$\sum_{i=1}^{i=k} r_i^* \leq \sum_{j=1}^{j=k} \rho_j, \;\; \sum_{i=1}^{i=k} \rho_i^* \leq \sum_{j=1}^{j=k} 2r_j$$

where r_i^*, ρ_i^* correspond to the radii and diameters of the optimal MSR or MSD solution, and r_j, ρ_j correspond to any feasible solution.

We use $\mathrm{dist}(C_1, C_2)$ to represent the distance between two clusters, which is the distance between the closest pair of points from each cluster, i.e.,

$$\mathrm{dist}(C_1, C_2) := \min_{a\in C_1, b\in C_2} d(a, b).$$

We denote the optimal clustering as $\mathrm{OPT} := \{C_1^*, \ldots, C_k^*\}$ and its value as $\mathrm{cost}(\mathrm{OPT})$.

We focus on the MSD problem under the notion of stability first introduced by Bilu and Linial [1], which is usually referred to as "perturbation resilience" in the context of clustering [4].

Definition II.1 (γ-Perturbation). *Given a clustering instance (P, d), we say a function $d' : P \times P \to [0, \infty)$ is a γ-perturbation of (P, d) if $\forall x, y \in P$, we have $d(x, y) \leq d'(x, y) \leq \gamma \cdot d(x, y)$. Note that d' may not be a metric.*

Definition II.2 (Perturbation Resilience). *For $\gamma > 1$, we say a clustering instance (P, d) is γ-perturbation-resilient if for any γ-perturbation d', the unique optimal clustering $\{C_1^*, \ldots, C_k^*\}$ of (P, d) stays the same under d', i.e., $\mathrm{OPT} = \mathrm{OPT}'$ where OPT' is the optimal solution of the perturbed instance.*

III. Algorithm for MSD Under Stability

In this section we first present some properties of MSD under stability assumptions, then we use these properties to show that the single-linkage and complete-linkage algorithms combined with dynamic programming finds the optimal clustering of 2-stable instances.

A. Properties Following Stability

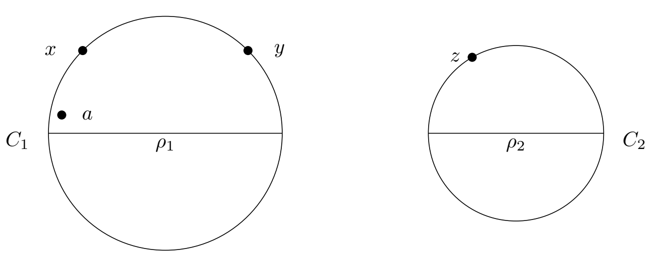

Fig. 1: Properties of stable MSD instances.

Lemma III.1 (MSD properties from stability). *Given a γ-stable MSD clustering instance, suppose C_1 and C_2 are clusters in* OPT *with diameters ρ_1 and ρ_2 respectively, then we have the following:*

1) *$\forall z \notin C_1, \exists a \in C_1$ s.t. $d(a, z) > \gamma \cdot \rho_1$.*
2) *$\forall x, y \in C_1, \forall z \notin C_1, (\gamma - 1) \cdot d(x, y) < d(y, z)$. In particular, if $\gamma \geq 2$, $d(x, y) < d(y, z)$.*
3) *$(\gamma - 1) \cdot \rho_1 < \mathrm{dist}(C_1, C_2)$. In particular, if $\gamma \geq 2$, $\rho_1 < \mathrm{dist}(C_1, C_2)$.*

Proof.

1) Suppose not, then under the perturbation where all pair-wise distances in C_1 are perturbed by γ, z can be moved to C_1 in OPT' without increasing the cost so that $\mathrm{OPT}' \neq \mathrm{OPT}$, contradicting the stability assumption.

2) Suppose $\exists x, y \in C_1$ and $z \in C_2$ s.t. $(\gamma - 1) \cdot d(x, y) \geq d(y, z)$, which means $d(y, z) \leq (\gamma - 1) \cdot \rho_1$. $\forall a \in C_1$, we have $d(a, y) \leq \rho_1$, therefore $d(a, z) \leq d(a, y) + d(y, z) \leq \gamma \cdot \rho_1$, contradicting property 1.

3) Suppose not, then $\exists y \in C_1$ and $z \in C_2$ s.t. $d(y, z) \leq (\gamma - 1) \cdot \rho_1$, by a same argument as above we have a contradiction.

□

B. Algorithms for 2-Stable MSD Instances

The single-linkage and complete-linkage algorithms are popular heuristics for clustering, and they both belong to the family of agglomerative hierarchical clustering algorithms [20]. In this section we show that for stable MSD instances with $\gamma \geq 2$, these simple heuristics produce a tree structure where the optimal clustering is a pruning of the tree, which can then be found using dynamic programming (Cf. [6] Section 4.2.)

Algorithm 1: Single-linkage for MSD

$\mathcal{C} = \{\{p\} \mid p \in P\}$ start with all singletons;
while $|\mathcal{C}| > k$ **do**
  Merge $\underset{C_i, C_j}{\mathrm{argmin}}\ \mathrm{dist}(C_i, C_j)$;
end while

Algorithm 2: Complete-linkage for MSD

$\mathcal{C} = \{\{p\} \mid p \in P\}$ start with all singletons;
while $|\mathcal{C}| > k$ **do**
  Merge $\underset{C_i, C_j}{\mathrm{argmin}}\ \rho(C_i \cup C_j)$;
end while

Theorem III.2 (Algorithms for MSD). *The single-linkage algorithm 1 and complete-linkage algorithm 2 give exact solutions to MSD instances assuming stability $\gamma \geq 2$.*

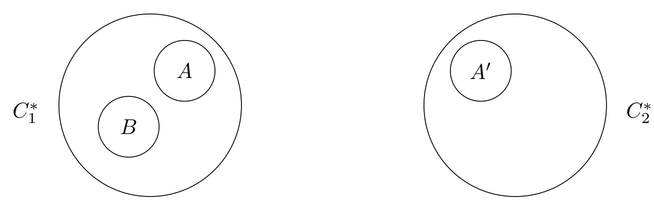

Fig. 2: Merge clusters during Algorithm 1 and 2.

Proof. We show by induction that in both algorithms the clusters after each merge are laminar to OPT, i.e., inside each remaining cluster, all points belong to the same cluster in OPT. This technique is inspired by the analysis in [5] for k-median clustering instances.

Base case: singleton clusters are laminar to OPT.

Induction step of merging: consider the clusters formed during the algorithm and a merge step (see Figure 2). Suppose $A \subset C_1^*$ where $\rho(C_1^*) = \rho_1^*$, we know that $\exists B \subset C_1^* \setminus A$ *s.t.* $\mathrm{dist}(A, B) \leq \rho(A \cup B) \leq \rho_1^*$. Let $A' \not\subset C_1^*$, by the induction hypothesis A' is fully contained in some cluster in OPT so without loss of generality we may assume $A' \subset C_2^*$, and $\rho(A \cup A') \geq \mathrm{dist}(A, A') \geq \mathrm{dist}(C_1^*, C_2^*) > \rho_1^*$ (by property 3). This means for single-linkage we have $\mathrm{dist}(A, B) < \mathrm{dist}(A, A')$, and for complete-linkage we have $\rho(A \cup B) < \rho(A \cup A')$, therefore the argmin pair of clusters chosen by the algorithms must belong to the same cluster in

OPT, and all the clusters remain laminar to OPT after the merge. □

In the Appendix, we prove the following related theorem for MSR clustering, showing that it also is polynomial-time solvable at 2-stability or higher.

Theorem III.3 (Algorithms for MSR)**.** *The single-linkage algorithm 1 gives exact solution to MSR if* $\gamma \geq 2$ *and the complete-linkage algorithm 2 gives exact solution if* $\gamma \geq 3$.

IV. A Matching Lower Bound for MSD

A. Non-Approximability of Sum-Of-Diameters Clustering

The following theorem from [13] states the non-approximability result for the MSD problem without any stability assumptions. We restate the theorem and the reduction setup here, and we will use the same reduction to show the NP-hardness result for MSD instances with $2-\epsilon$ stability.

Theorem IV.1 (Prop. 2 [13])**.** *Unless* $\mathrm{P} = \mathrm{NP}$*, for any* $\epsilon > 0$*, no polynomial time algorithm for the problem can provide a solution which satisfies the bound on the number of clusters and whose total diameter is within a factor* $2-\epsilon$ *of the optimal value.*

The result was shown using reduction from the clique problem. Given a clique problem to determine whether there exists a clique of size J in the graph $G = (V, E)$, we can reduce it to a MSD problem using the 2-1-metric: set $P = V$, and $d(u, v) = 1$ if $(u, v) \in E$, otherwise $d(u, v) = 2$. The number of clusters is set to $k = n + 1 - J$. If there exists a clique of size J, $\mathrm{cost}(\mathrm{OPT_{MSD}}) = 1$ consisting of 1 cluster of diameter 1 containing all the vertices in the clique, and $n - J$ singleton clusters with diameter 0 for each of the remaining vertex; otherwise $\mathrm{cost}(\mathrm{OPT_{MSD}}) \geq 2$.

B. Hardness Under Stability Assumptions

In this section, we provide a matching lower-bound of $2-\epsilon$ on the stability parameter. The result is formally stated in Theorem IV.2.

Theorem IV.2. *Unless* $\mathrm{P} = \mathrm{NP} = \mathrm{RP}$*, no polynomial time algorithm can solve a* $(2-\epsilon)$*-stable instance of the sum-of-diameters clustering problem for any* $\epsilon > 0$.

Notice that the reduction used in Theorem IV.1 produces a $(2-\epsilon)$-stable clustering instance if there exists a unique clique of size J in the clique problem. In other words, solving $(2-\epsilon)$-stable MSD instances is at least as hard as the Clique Promise Problem, which is a variation on the Clique problem where it is promised that there exists a unique optimal solution. We show the hardness of the Clique Promise Problem in Theorem IV.3, and then Theorem IV.2 follows.

Theorem IV.3 (Clique Promise Problem)**.** *The Clique Promise Problem (CPP), where the instance is promised to have a unique largest clique, is NP-hard under randomized reduction.*

Theorem IV.3 follows by combining two existing results. Lemma IV.5 states that SAT is parsimoniously reducible to the Clique problem, so we can apply Lemma IV.4 and choose A to be the Clique problem, which proves Theorem IV.3.

Lemma IV.4 (USAT Corollary 3.4 [21])**.** *Let A be any NP-complete problem to which satisfiability is parsimoniously reducible. The following "promise problem" is NP-hard under randomized reduction:*
Input: an instance x of A; Output: a solution to x; Promise: $\#A(x) = 1$.

Lemma IV.5 (#Clique is #P-complete [22])**.** *There is a parsimonious reduction from SAT to Clique.*

Here we include a modified version of the proof from [22] for completeness.

Proof. Step 1: #SAT $\leq_{\mathrm{p}}$ #3SAT.
Consider a SAT instance f, we will reduce it to a 3SAT formula f' where there is a one-to-one correspondence between any satisfiable assignment to f and f'. First introduce new variables a, b, c and new clauses

$$\overline{(a \vee b \vee c)} \iff (\overline{a} \vee b \vee c) \wedge (a \vee \overline{b} \vee c) \wedge (a \vee b \vee \overline{c}) \wedge (\overline{a} \vee \overline{b} \vee c) \wedge (\overline{a} \vee b \vee \overline{c}) \wedge (a \vee \overline{b} \vee \overline{c}) \wedge (\overline{a} \vee \overline{b} \vee \overline{c}) \ ,$$

so that f' is satisfiable if and only if a, b, c are all set to 0.

1) For clauses with 1 literal x_1, replace it with $(x_1 \vee a \vee b) \iff x_1$;
2) For clauses with 2 literals x_1, x_2, replace it with $(x_1 \vee x_2 \vee a) \iff (x_1 \vee x_2)$;
3) For clauses with 3 literals, do nothing;
4) For clauses with ≥ 4 literals $(x_1 \vee x_2 \vee y)$, where y is a disjunction of ≥ 2 literals, repeatedly reduce the number of literals by one by replacing the clause with

$$C = (x_1 \vee x_2 \vee w) \wedge (\overline{x_1} \vee x_2 \vee \overline{w}) \wedge (x_1 \vee \overline{x_2} \vee \overline{w}) \wedge (\overline{x_1} \vee \overline{x_2} \vee \overline{w}) \wedge (\overline{w} \vee y) \ .$$

Consider any satisfiable assignment to f,
- if $\overline{x_1 \vee x_2}$, i.e. $x_1 = 0,\ x_2 = 0,\ y = 1$, and $C \iff w \wedge (\overline{w} \vee y)$, so $w = 1$ in any satisfiable assignment to f' ;
- if $x_1 \vee x_2$, $C \iff \overline{w} \wedge (\overline{w} \vee y)$, so $w = 0$ in any satisfiable assignment to f' .

Step 2: #3SAT $\leq_{\mathrm{p}}$ #Clique.
Consider #3 SAT instance $f = C_1 \wedge \ldots \wedge C_k$. Construct a graph G:
- Vertices: for each clause C_i introduce 7 vertices corresponding to the 7 assignments that satisfy C ;
- Edges: an edge exists between 2 vertices if and only if the assignments represented by the vertices do not contradict each other. In particular, there are no edges among vertices from the same clause.

There is a one-to-one correspondence between a satisfiable assignment to f and a clique of size k in G. □

It remains an open question to prove a similar lower bound for the MSR objective.

Appendix

In this appendix, we give an analysis of Algorithms 1 and 2 for the MSR objective. Given the similarity to the analysis for MSD, we have relegated these results to this appendix.

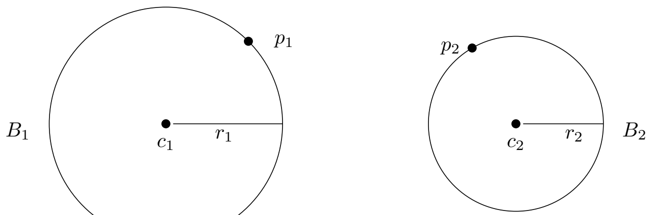

Fig. 3: Properties of stable MSR instances.

Lemma A.1 (MSR properties from stability)**.** *Given a γ-stable MSR clustering instance, suppose B_1 and B_2 are clusters in* OPT *centered at c_1, c_2 with radii r_1 and r_2 respectively, then we have the following:*

1) $\forall p_2 \notin B_1,\ d(c_1, p_2) > \gamma \cdot r_1$.
2) $d(c_1, c_2) > \frac{\gamma}{2}(r_1 + r_2)$.
In particular, if $\gamma > 2$, $d(c_1, c_2) > r_1 + r_2$, i.e., clusters are separated.
3) *If $\gamma \geq 2$, each point belongs to its closest center, i.e., $\forall p_1 \in B_1,\ d(p_1, c_1) < d(p_1, c_2)$ $\forall c_2$ that is a center of another cluster.*
4) $(\gamma - 1) \cdot r_1 < \mathrm{dist}(B_1, B_2)$.
$(\gamma - 1) \cdot d(p_1, c_1) < d(p_1, p_2)$ $\forall p_1 \in B_1,\ p_2 \in B_2$.
In particular, if $\gamma \geq 2$, $r_1 < \mathrm{dist}(B_1, B_2)$ and $d(p_1, c_1) < d(p_1, p_2)$.
If $\gamma \geq 3$, $\rho(B_1) \leq 2r_1 < \mathrm{dist}(B_1, B_2) \leq \rho(B_1 \cup B_2)$.
5) *Notably we don't have "center proximity", a property implied by perturbation resilience used in [4] instead of perturbation resilience, i.e., it's possible that $\gamma \cdot d(p_1, c_1) > d(p_1, c_2)$.*

Proof.

1) Suppose not, and consider the perturbation where $\forall p_1 \in B_1, d(c_1, p_1)$ is perturbed by γ, then we can move p_2 to B_1 in OPT' without increasing the cost so that $\mathrm{OPT}' \neq \mathrm{OPT}$, contradicting the stability assumption.

2) Following property 1, $d(c_1, c_2) > \gamma \cdot r_1$ and $d(c_1, c_2) > \gamma \cdot r_2$, combined we have $d(c_1, c_2) > \frac{\gamma}{2}(r_1 + r_2)$.

3) Suppose there exists another cluster's center c_2 s.t. $d(p_1, c_2) \leq d(p_1, c_1)$, then $d(c_1, c_2) \leq d(p_1, c_1) + d(p_1, c_2) \leq 2r_1 \leq \gamma \cdot r_1$, contradicting property 1.

4) Suppose $\exists p_1 \in B_1, p_2 \in B_2$ s.t. $d(p_1, p_2) \leq (\gamma - 1) \cdot r_1$, therefore $d(c_1, p_2) \leq d(c_1, p_1) + d(p_1, p_2) \leq \gamma \cdot r_1$, contradicting property 1.
Suppose $\exists p_1 \in B_1, p_2 \in B_2$ s.t. $d(p_1, p_2) \leq (\gamma - 1) \cdot d(p_1, c_1) \leq (\gamma - 1) \cdot r_1$, therefore $d(c_1, p_2) \leq d(c_1, p_1) + d(p_1, p_2) \leq \gamma \cdot r_1$, contradicting property 1.

5) Figure 4 shows a counter example where $\gamma \cdot d(p_1, c_1) > d(p_1, c_2)$ with $\gamma = 3$ and the number of clusters $k = 2$:

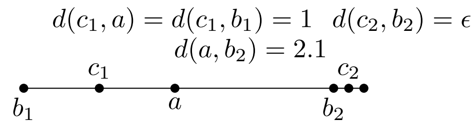

Fig. 4: A 3-stable MSR instance without the center proximity property.

In the figure above, $\mathrm{OPT} = d(a, c_1) + d(b_2, c_2) = 1 + \epsilon$.
Perturb $d(a, c_1) \to 3$, then $\mathrm{OPT} \to 3 + \epsilon$.
Consider an alternative solution OPT': move a to c_2, $\mathrm{OPT}' = d(b_1, c_1) + d(a, c_2) = 1 + 2.1 + \epsilon$, so the example is 3 stable, but $3 = 3d(a, c_1) > d(a, c_2) = 2.1 + \epsilon$, violating center proximity.

□

Now we are ready to prove Theorem III.3.

Proof. We show that in both algorithms the clusters after each merge are laminar to OPT by induction.

Single-linkage: Assume $\gamma \geq 2$ and we have $r_1^* < \mathrm{dist}(C_1^*, C_2^*)$ by property 4.
Base case: correct.
Induction step of merging: suppose $A \subset C_1^*$, we know $\exists B \subset C_1^* \setminus A$ *s.t.* $\mathrm{dist}(A, B) \leq r_1^*$ (let either A or B contain the center c_i). Let $A' \not\subset C_1^*$, by induction A' is fully contained in some cluster in OPT so w.o.l.g. we may assume $A' \subset C_2^*$ and $\mathrm{dist}(A, A') \geq \mathrm{dist}(C_1^*, C_2^*) > r_1^*$. This means $\mathrm{dist}(A, B) < \mathrm{dist}(A, A')$, and by the same argument as in the proof of Theorem III.2, the merge step is correct.

Complete-linkage: Assume $\gamma \geq 3$ and we have $\rho(C_1^*) < \mathrm{dist}(C_1^*, C_2^*)$ by property 4.
Base case: correct.
Induction step of merging: suppose $A \subset C_1^*$, we know $\exists B \subset C_1^* \setminus A$ *s.t.* $\rho(A \cup B) \leq \rho(C_1^*)$. Let $A' \not\subset C_1^*$, by induction A' is fully contained in some cluster in OPT so w.o.l.g. we may assume $A' \subset C_2^*$ and $\rho(A \cup A') \geq \mathrm{dist}(A, A') \geq \mathrm{dist}(C_1^*, C_2^*) > \rho(C_1^*)$. This means $\rho(A \cup B) < \rho(A \cup A')$, and by the same argument as in the proof of Theorem III.2, the merge step is correct. □

Acknowledgments

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