

Clustering Under Perturbation Stability in Near-Linear Time

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Abstract

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

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1 Introduction

Clustering is a fundamental problem in unsupervised learning and data summarization, with wide-ranging applications that span myriad areas. Typically, the data points are assumed to lie in a Euclidean space, and the goal in center-based clustering is to open a set of k centers to minimize the objective cost, usually a function over the distance from each data point



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to its closest center. The k -median objective minimizes the sum of distances; the k -means minimizes the sum of squares of distances; and the k -center minimizes the longest distance. In the worst case, all these objectives are NP-hard even in 2D [48, 50].

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

Because of NP-hardness results, we cannot hope to compute an optimal solution in polynomial time, but in the worst case an approximate clustering can be different from an optimal clustering. We focus on the case when the optimal clustering can be recovered under some reasonable assumptions on the input that hold in practice. Such methodology is termed “beyond worst-case analysis” and has been adopted by recent work [2, 8, 23]. In recent years, the notion of *stability* has emerged as a popular assumption under which polynomial-time optimal clustering algorithms have been developed. An instance of clustering is called *stable* if any “small perturbation” of input points does not change the optimal solution. This is natural in real datasets, where often, the optimal clustering is clearly demarcated, and the distances are obtained heuristically. Different notions of stability differ in how “small perturbation” is defined, though most of them are related. In this paper, we focus on the notions of stability introduced in Bilu and Linial [23] and Awasthi, Blum, and Sheffet [14]. A clustering instance is α -*perturbation resilient* or α -*stable* if the optimal clustering does not change when all distances are perturbed by a factor of at most α . Similarly, a clustering instance is α -*center proximal* if any point is at least a factor of α closer to its own optimal center than any other optimal center. Awasthi, Blum, and Sheffet showed that α -stability implies α -center proximity [14]. This line of work designs algorithms to recover the *exact* optimal clustering – the ground truth – in polynomial time for α -stable instances.

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

1.1 Our Results

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

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

In the above theorem, the \tilde{O} notation suppresses logarithmic terms in n and the spread of the point set. The function $f(k)$ depends on the choice of algorithm, and we present the exact dependence below. We also omit terms depending solely on the dimension, d . Furthermore, the above theorem is robust in the sense that the algorithm is not restricted to choosing the input points as centers (*discrete setting*), and can potentially choose arbitrary

points in the Euclidean plane as centers (*continuous setting*, sometimes referred to as the *Steiner point setting*) – indeed, we show that these notions are identical under a reasonable assumption on stability.

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

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

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

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

► **Remark 2.** While the current analysis of the dynamic programming based algorithm suggests that it is better than the local-search and coreset based approaches, the latter are of independent interest – our local-search analysis is considerably simpler than the previous analysis [38], and coresets have mostly been used to compute approximate, rather than exact, solutions. We also note that our analysis of the local-search algorithm is probably not tight. Furthermore, variants of all three approaches might work for smaller values of α .

Techniques. The key difficulty with developing fast algorithms for computing the optimal clustering is that some clusters could have a very small size compared to others. This issue persists even when the instances are stable. Imagine a scenario where there are multiple small clusters, and an algorithm must decide whether to merge these into one cluster while splitting some large cluster, or keep them intact. Now imagine this situation happening recursively, so that the algorithm has multiple choices about which clusters to recursively split. The difference in cost between these options and the size of the small clusters can be small enough that any $(1 + \epsilon)$ -approximation can be agnostic, while an exact solution cannot. As such, work on finding exact optima use techniques such as dynamic programming [10] or local search with large number of swaps [26, 38] in order to recover small clusters. Other work makes assumptions lower-bounding the size of the optimal clusters or the spread of their centers [34].

Our main technical insight for the first two results is simple in hindsight, yet powerful: For a stable instance, if the Euclidean metric is replaced by another metric that is a good approximation, then the optimal clustering does not change under the new metric and in fact the instance remains stable albeit with a smaller stability parameter. In particular,

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

we replace the Euclidean metric with an appropriate *polyhedral metric* – that is, a convex distance function where each unit ball is a regular polyhedron – yielding efficient procedures for the following two primitives:

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

We next combine the insight of changing the metrics with additional techniques. For local search, we build on the approach in [26,31,38] that shows local search with t -swaps for large enough constant t finds an optimal solution for stable instances in polynomial time for any fixed-dimension Euclidean space. None of the prior analysis directly extends as is to 1-swap, which is critical in achieving near-linear running time – note that even when $t = 2$ there is a quadratic number of candidate swaps per step.

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

Due to length constraints of the paper, the coresets result, most of algorithmic details, and many proofs can be found in the full version of the paper.

1.2 Related Work

All of k -median, k -means, and k -center are widely studied from the perspective of approximation algorithms and are known to be hard to approximate [36]. Indeed, for general metric spaces, k -center is hard to approximate to within a factor of $2 - \epsilon$ [43]; k -median is hard to $(1 + 2/e)$ -approximate [44]; and k -means is hard to $(1 + 8/e)$ -approximate in general metrics [29], and is hard to approximate within a factor of 1.0013 in the Euclidean setting [47]. Even when the metric space is Euclidean, k -means is still NP-hard when $k = 2$ [7,32], and there is an $n^{\Omega(k)}$ lower bound on running time for k -median and k -means in 4-dimensional Euclidean space under the exponential-time hypothesis [27].

There is a long line of work in developing $(1 + \epsilon)$ -approximations for these problems in Euclidean spaces. The holy grail of this work has been the development of algorithms that are near-linear time in n , and several techniques are now known to achieve this. This includes randomly shifted quad-trees [11], coresets [4,15,37,40,41], sampling [46], and local search [26,28,30], among others.

There are many notions of clustering stability that have been considered in literature [1,6,13,17,18,22,35,45,52]. The exact definition of stability we study here was first introduced in Awasthi et al. [14]; their definition in particular resembles the one of Bilu and Linial [23] for max-cut problem, which later has been adapted to other optimization problems [9,10,19,49,51]. Building on a long line of work [14,16,20,21], which gradually reduced the stability parameter, Angelidakis et al. [10] present a dynamic programming based polynomial-time optimal algorithm for discrete 2-stable instances for all center-based objectives.

Chekuri and Gupta [25] show that a natural LP-relaxation is integral for the 2-stable k -center problem. Recent work by Cohen-Addad [31] provides a framework for analyzing local search algorithms for stable instances. This work shows that for an α -stable instance with $\alpha > 3$, any solution is optimal if it cannot be improved by swapping $\lceil 2/(\alpha - 3) \rceil$

centers. Focusing on Euclidean spaces of fixed dimensions, Friggstad et al. [38] show that a local-search algorithm with $O(1)$ -swaps runs in polynomial time under a $(1 + \delta)$ -stable assumption for any $\delta > 0$. However, none of the algorithms for stable instances of clustering so far have running time near-linear in n , even when the stability parameter α is large, points lie in \mathbb{R}^2 , and the underlying metric is Euclidean.

On the hardness side, solving $(3 - \delta)$ -center proximal k -median instances in general metric spaces is NP-hard for any $\delta > 0$ [14]. When restricted to Euclidean spaces in arbitrary dimensions, Ben-David and Reyzin [22] showed that for every $\delta > 0$, solving discrete $(2 - \delta)$ -center proximal k -median instances is NP-hard. Similarly, the clustering problem for discrete k -center remains hard for α -stable instances when $\alpha < 2$, assuming standard complexity assumption that $\text{NP} \neq \text{RP}$ [20]. Under the same complexity assumption, discrete α -stable k -means is also hard when $\alpha < 1 + \delta_0$ for some positive constant δ_0 [38]. Deshpande et al. [34] showed it is NP-hard to $(1 + \epsilon)$ -approximate $(2 - \delta)$ -center proximal k -means instances.

2 Definitions and Preliminaries

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

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

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

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

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

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

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► **Lemma 3.** *Let (X, δ) be an α -stable clustering instance with $\alpha > 1$. Then the optimal clustering O of (X, δ) is unique.*

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

► **Lemma 4.** *Given point set X , let δ and δ' be two metrics satisfying $\delta(p, q) \leq \delta'(p, q) \leq \beta \cdot \delta(p, q)$ for all p and q in X for some β . Let (X, δ) be an α -stable clustering instance with $\alpha > \beta$. Then the optimal clustering of (X, δ) is also the optimal clustering of (X, δ') , and vice versa. Furthermore, (X, δ') is an (α/β) -stable clustering instance.*

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

Since N is centrally symmetric, δ_N is symmetric and thus a metric. The unit ball under δ_N is a convex polyhedron, thus the name polyhedral metric. By construction, an easy calculation shows that for any p and q in \mathbb{R}^d , $\|p - q\| \geq \delta_N(p, q) \geq (1 - \epsilon) \cdot \|p - q\|$. By scaling each vector in N by a $1 + \epsilon$ factor, we can ensure that $(1 + \epsilon) \cdot \|p - q\| \geq \delta_N(p, q) \geq \|p - q\|$. By taking ϵ to be small enough, the optimal clustering for α -stable clustering instance $(X, \|\cdot\|, \$)$ is the same as that for $(X, \delta_N, \$)$ by Lemma 4, and the new instance $(X, \delta_N, \$)$ is $(1 - \epsilon)\alpha$ -stable if the original instance $(X, \|\cdot\|, \$)$ is α -stable.

Center proximity. A clustering instance (X, δ) satisfies α -center proximity property [14] if for any distinct optimal clusters X_i and X_j with centers c_i and c_j and any point $p \in X_i$, one has $\alpha \cdot \delta(p, c_i) < \delta(p, c_j)$. Awasthi, Blum, and Sheffet showed that any α -stable instance satisfies α -center proximity [14, Fact 2.2] (also [10, Theorem 3.1] under metric perturbation). Optimal solutions of α -stable instances satisfy the following separation properties.²

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

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

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

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

² We give an additional list of known separation properties in the full version of the paper.

³ They are known as *weak center proximity* [20] and *strict separation property* [18, 22] respectively.

► **Lemma 6.** *For any α -stable instance $(X, \delta, \$_\delta)$ with $\alpha \geq 2 + \sqrt{3}$, any continuous optimal k -clustering is a discrete optimal k -clustering and vice versa.*

3 Efficient Dynamic Programming

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

► **Theorem 7.** *Let X be a set with n points lying in \mathbb{R}^d and $k \geq 1$ an integer. If the k -means, k -median, or k -center instance for X under the Euclidean metric is α -stable for $\alpha \geq 2 + \sqrt{3} + \varepsilon$ for any constant $\varepsilon > 0$, then the optimal clustering can be computed in $O(nk^2 + n \text{ polylog } n)$ time. For $d = 2$ the assumption can be relaxed to $\alpha \geq 2 + \sqrt{3}$.*

3.1 Fast Dynamic Programming

The following lemma is the key observation for our algorithm.

► **Lemma 8.** *Let $(X, \delta, \$)$ be an α -stable k -clustering instance with $\alpha \geq 2 + \sqrt{3}$ and $k \geq 2$, and let T be the minimum spanning tree of X under metric δ . Then (1) The two endpoints u and v of the longest edge e in T do not belong to the same cluster; (2) each cluster lies in the same connected component of $T \setminus \{e\}$.*

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

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

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

⁴ Tree \mathbf{R} is nothing but the minimum spanning tree constructed by Kruskal's algorithm.

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

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

3.2 Efficient Implementation

In this section, we show how to obtain the minimum spanning tree and compute $\mu(X_v; 1)$ efficiently for 1-mean, 1-center, and 1-median when $X \subseteq \mathbb{R}^d$. We can compute the Euclidean minimum spanning tree T in $O(n \log n)$ time in \mathbb{R}^2 [54]. We can then compute $\mu(X_v; 1)$ efficiently either under Euclidean metric (for 1-mean), or switch to the L_1 -metric and compute $\mu(X_v; 1)$ efficiently using Lemma 4 (for 1-center and 1-median).

There are two difficulties in extending the 2D data structures to higher dimensions. No near-linear time algorithm is known for computing the Euclidean minimum spanning tree for $d \geq 3$, and we can work with the L_1 -metric only if $\alpha \geq \sqrt{d}$ (Lemma 4). We address both of these difficulties by working with a polyhedral metric δ_N . Let $\alpha \geq 2 + \sqrt{3} + \Omega(1)$ be the stability parameter. By taking the number of vectors in N (defined by the polyhedral metric) to be large enough, we can ensure that $(1 - \epsilon)\|p - q\| \leq \delta_N(p, q) \leq \|p - q\|$ for all $p, q \in \mathbb{R}^d$. By Lemma 4, X is an α -stable instance under δ_N for $\alpha \geq 2 + \sqrt{3}$. We first compute the minimum spanning tree of X in $O(n \text{ polylog } n)$ time under δ_N using the result of Callahan and Kosaraju [24], and then compute $\mu(X_v, 1)$.

Data structure. We compute $\mu(X_v; 1)$ in a bottom-up manner. When processing a node v of \mathbb{R} , we maintain a dynamic data structure Ψ_v on X_v from which $\mu(X_v; 1)$ can be computed quickly. The exact form of Ψ_v depends on the cost function to be described below. Before that, we analyze the running time $\tau(n)$ spent on computing every $\mu(X_v; 1)$. Let w and z be the two children of v . Suppose we have Ψ_w and Ψ_z at our disposal and suppose $|X_w| \leq |X_z|$. We insert the points of X_w into Ψ_z one by one and obtain Ψ_v from which we compute $\mu(X_v; 1)$. Suppose $Q(n)$ is the update time of Ψ_v as well as the time taken to compute $\mu(X_v; 1)$ from Ψ_v . The total number of insert operations performed over all nodes of \mathbb{R} is $O(n \log n)$ because we insert the points of the smaller set into the larger set at each node of \mathbb{R} [42, 53]. Hence $\tau(n) = O(Q(n) \cdot n \log n)$. We now describe the data structure for each specific clustering problem.

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

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

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

We maintain the following four terms $\max_{p \in X_v} \langle p, e^+ \rangle$, $\min_{p \in X_v} \langle p, e^+ \rangle$, $\max_{p \in X_v} \langle p, e^- \rangle$, and $\min_{p \in X_v} \langle p, e^- \rangle$ at v . A point can be inserted in $O(1)$ time and ρ_v can be computed from these four terms in $O(1)$ time. Therefore, $Q(n) = O(1)$. For $d > 2$, we work with a polyhedral metric and compute the smallest ball $B(X_v)$ that contains X_v . For full details, see the full version of the paper.

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

4 k -Median: Single-Swap Local Search

We customize the standard local-search framework for the k -clustering problem [30, 31, 39]. In order to recover the optimal solution, we must define near-optimality more carefully. Let (X, δ) be an instance of α -stable k -median in \mathbb{R}^2 for $\alpha > 5$. By Lemma 6, it suffices to consider the *discrete* k -median problem. In Section 4, we describe a simple local-search algorithm for finding the optimal clustering of (X, δ) . In Section 4 we show that the algorithm terminates within $O(k \log(n\Delta))$ iterations. We obtain the following.

► **Theorem 9.** *Let (X, δ) be an α -stable instance of the k -median problem for some $\alpha > 5$ where X is a set of n points in \mathbb{R}^2 equipped with L_p -metric δ . The 1-swap local search algorithm terminates with the optimal clustering in $O(k \log(n\Delta))$ iterations.*

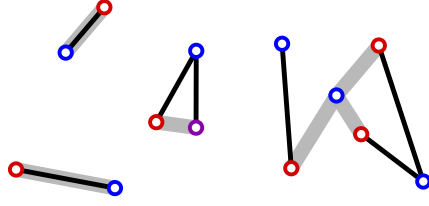
Local-search algorithm. The local-search algorithm maintains a k -clustering induced by a set S of k cluster centers. At each step, it finds a pair of points $x \in X$ and $y \in S$ such that $\$(X, S + x - y)$ is minimized. If $\$(X, S + x - y) \geq \(X, S) , it stops and returns the k -clustering induced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

Local-search analysis. The high-level structure of our analysis follows Friggstad et al. [39], however new ideas are needed for 1-swap. In this subsection, we denote a k -clustering by the set of its cluster centers. Let S be a fixed k -clustering, and let O be the optimal clustering. For a subset $Y \subseteq X$, we use $\$(Y)$ and $\$(Y)$ to denote $\$(Y, S)$ and $\$(Y, O)$, respectively. Similarly, for a point $p \in X$, we use $\text{nn}(p)$ and $\text{nn}^*(p)$ to denote the nearest neighbor of p in S and in O , respectively; define $\delta(p)$ to be $\delta(p, S)$ and $\delta^*(p)$ to be $\delta(p, O)$. We partition X into four subsets as follows:

- $X_{00} := \{p \in X \mid \text{nn}(p) \in S \setminus O, \text{nn}^*(p) \in O \setminus S\}$;
- $X_{01} := \{p \in X \mid \text{nn}(p) \in S \setminus O, \text{nn}^*(p) \in S \cap O\}$;
- $X_{10} := \{p \in X \mid \text{nn}(p) \in S \cap O, \text{nn}^*(p) \in O \setminus S\}$;
- $X_{11} := \{p \in X \mid \text{nn}(p) \in S \cap O, \text{nn}^*(p) \in S \cap O\}$.

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

► **Lemma 10.** *Any C -good clustering S for an α -stable clustering instance $(X, \delta, \$)$ must be optimal for $\alpha \geq C + 1$.*



■ **Figure 1** Illustration of candidate swaps \mathcal{S} in \mathbb{R}^2 . The blue dots belong to set S , the red dots belong to set O ; the only purple dot is in $S \cap O$. The thick gray segments indicate pairs inside the stars; each star has exact one blue dot as its center. The black pairs are the candidate swaps. Notice that the partitions of S and O form connected components.

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

$$\tilde{\delta}(p', p) := \begin{cases} \alpha \cdot \delta(p', p) & \text{if } p \neq \text{nn}(p'), \\ \delta(p', p) & \text{otherwise.} \end{cases}$$

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

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

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

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

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

Next, we prove a lower bound on the improvement in the cost of a clustering that is not C -good after performing a 1-swap. Following Arya et al. [12], define the set of *candidate swaps* \mathcal{S} as follows: For each center i in S , consider the *star* Σ_i centered at i defined as the collection of pairs $\Sigma_i := \{(i, j) \in S \times O \mid \text{nn}(j) = i\}$. Denote $\text{center}(j)$ to be the center of the star where j belongs; in other words, $\text{center}(j) = i$ if j belongs to Σ_i .

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

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

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

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

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

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

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

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

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

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

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

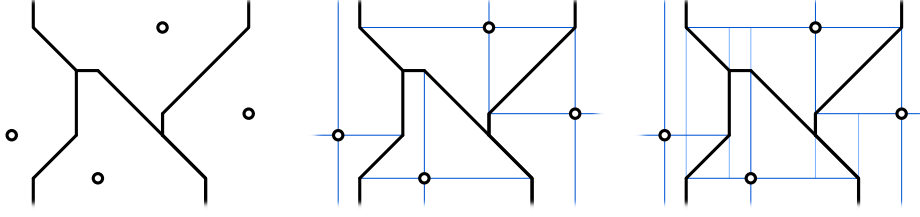
Using Lemma 11, we can prove the following.

► **Lemma 12.** *Let S be a k -clustering of (X, δ) that is not C -good for some fixed constant $C > 4 + \epsilon$ with arbitrarily small $\epsilon > 0$. There is always a 1-swap S' such that $\$(X) - \$^*(X) \leq (1 - \epsilon/(1 + \epsilon)k) \cdot (\$(X) - \$^*(X))$, where $\$'$ is the cost function defined with respect to S' .*

Proof. By Lemma 11 one has $\$(X) - \$'(X) \geq (\$(X) - \$^*(X) - \Psi(X_{00}))/k$ for some 1-swap S' and its corresponding cost function $\$'(\cdot)$. Since S is not C -good, $\$(X) - \$^*(X) > C \cdot \$^*(X_{00})$. Rearranging and plugging the definition of $\Psi(\cdot)$, we have

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

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



■ **Figure 2** L_1 Voronoi diagram V , quadrant decomposition \tilde{V} , and trapezoid decomposition V^\parallel .

5 Efficient Implementation of Local Search

We describe an efficient implementation of each step of the local-search algorithm in this section. By Lemma 4, it suffices to implement the algorithm using a polyhedral metric δ_N . We show that each step of 1-swap can be implemented in $O(nk^{2d-1} \text{polylog } n)$ time under the assumption that $\alpha > 5$. We obtain the following:

► **Theorem 13.** *Let (X, δ) be an α -stable instance of the k -median problem where $X \subset \mathbb{R}^d$ and δ is the Euclidean metric. For $\alpha > 5$, the 1-swap local search algorithm computes the optimal k -clustering of (X, δ) in $O(nk^{2d-1} \text{polylog } n)$ time.*

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

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

Next, decompose each Voronoi cell $\text{Vor}(c)$ into four *quadrants* centered at c . Denote the resulting subdivision of V as \tilde{V} . We compute a *trapezoidal decomposition* V^\parallel of the diagram \tilde{V} by drawing a vertical segment from each vertex of \tilde{V} in both directions until it meets an edge of V ; V^\parallel has $O(k)$ trapezoids, see Figure 2. For each trapezoid $\tau \in V^\parallel$, let $X_\tau := X \cap \tau$. The cost of the new clustering S' can be computed as $\$(X, S') = \sum_{\tau \in V^\parallel} \(X_τ, S') .

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

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

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

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

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

■ **Figure 3** Efficient implementation of 1-swap under 1-norm.

The above query can be viewed as a 3-oriented polygonal range query [33]. We construct a 3-level range tree Ψ on X . Omitting the details (which can be found in [33]), Ψ can be constructed in $O(n \log^2 n)$ time and uses $O(n \log^2 n)$ space. Each node ξ at the third level of Ψ is associated with a subset $X_\xi \subseteq X$. We store $w(\xi, u) := \sum_{x \in X_\xi} \langle x, u \rangle$ for each $u \in \{\pm 1\}^2$ and $|X_\xi|$ at ξ . For a trapezoid τ , the query procedure identifies in $O(\log^3 n)$ time a set Ξ_τ of $O(\log^3 n)$ third-level nodes such that $X \cap \tau = \cup_{\xi \in \Xi_\tau} X_\xi$ and each point of $X \cap \tau$ appears as exactly one node of Ξ_τ . Then $\sum_{x \in X_\tau} \langle x, u \rangle = \sum_{\xi \in \Xi_\tau} w(\xi, u)$ and $|X_\tau| = \sum_{\xi \in \Xi_\tau} |X_\xi|$.

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

We summarize the implementation of 1-swap algorithm in Figure 3. The 1-swap procedure considers at most nk different k -clustering. Therefore we obtain the following.

► **Lemma 14.** *Let $(X, \delta, \$)$ be a given clustering instance where δ is the L_1 metric, and let S be a given k -clustering. After $O(n \log n)$ time preprocessing, we find a k -clustering $S' := S + x - y$ minimizing $\$(X, S')$ among all choices of (x, y) in $O(nk^2 \log^3 n)$ time.*

6 Conclusion

We presented near-linear time algorithms for finding optimal solutions of stable clustering instances for the k -means, k -medians, and k -center problem. We note that variants of all three approaches might work for smaller values of α . The value of α assumed in our results is larger than what is known for polynomial-time algorithm (e.g. $\alpha \geq 2$ in Angelidakis et al. [10]) and that in some applications the input may not satisfy our assumption, but our results are a big first step toward developing near-linear time algorithms for stable instances. We are not aware of any previous near-linear time algorithms for computing optimal clustering even for larger values of α . We leave the problem of reducing the assumption on α as an important open question.

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