A Scalable Algorithm for Individually Fair K-means Clustering

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Abstract

We present a scalable algorithm for the individually fair (p, k)-clustering problem introduced by Jung et al. (2020) and Mahabadi and Vakilian (2020). Given n points P in a metric space, let $\delta(x)$ for $x \in P$ be the radius of the smallest ball around x containing at least n/kpoints. A clustering is then called *individually* fair if it has centers within distance $\delta(x)$ of x for each $x \in P$. While good approximation algorithms are known for this problem no efficient practical algorithms with good theoretical guarantees have been presented. We design the first fast local-search algorithm that runs in $\tilde{O}(nk^2)$ time and obtains a bicriteria (O(1), 6) approximation. Then we show empirically that not only is our algorithm much faster than prior work, but it also produces lower-cost solutions.

1 Introduction

The (p, k)-clustering problems (with k-means, k-median and k-center as special cases) are widely used in many unsupervised machine-learning tasks for exploratory data analysis, representative selection, data summarization, outlier detection, social-network community detection and signal processing, e.g., Lloyd (1982); MacQueen (1967); Chawla and Gionis (2013); Kleindessner et al. (2019); Zhang et al. (2007); Bóta et al. (2015).

With such ubiquity of applications, it is fundamental to design fair algorithms for such problems. In this paper we focus on the notion of individually fair clustering Jung et al. (2020), which *combines* the ℓ_p cost objective with a k-center-based concept of fairness: A Alessandro EpastoSilvio Lattanziaepasto@google.comsilviol@cohengoogle.comGoogle ResearchGoogle Research

minimum level of treatment should be guaranteed for every data point. To better understand this formulation consider the case in which centers were chosen randomly. In this case any subset of n/k points would be expected to include one center. So each point desires to be assigned to a center among its n/k closest points. This notion can be captured by considering a different radius $\delta(x)$ for each x in the dataset and by adding the constraint that there should be a center within distance $\delta(x)$ for each x. Satisfying such constraints amounts to (a special case of) the priority k-center problem Plesník (1987); Alamdari and Shmoys (2017); Bajpai et al. (2021).

Shortly after Jung et al. (2020) proposed this problem and presented a 2-approximation for it, Mahabadi and Vakilian (2020) generalized it to an optimization setting where an ℓ_p norm cost function (such as k-means or k-median) is optimized within the space of individually fair solutions. In fact, they devise a local-search algorithm with bicriteria (84,7) approximation (for p = 1, that is k-median).

In recent years, several attempts have been made to improve these results, theoretically and practically. Chakrabarty and Negahbani (2021) uses LP rounding to improve the guarantee to $(2^{p+2}, 8)$, i.e., cost guarantee of 16 for k-means and 8 for k-median. In simultaneous work, Humayun et al. (2021) presents an SDP-based algorithm (without performance or runtime analysis), and Vakilian and Yalçiner (2022) presents LP-based bicriteria guarantees $(16^p + \epsilon, 3)$ for any pand $(7.081 + \epsilon, 3)$ for p = 1.

Three of the above—with the exception of Vakilian and Yalçiner (2022)—present experimental studies. However, a major limitation of these algorithms is their running times, having an exponent of at least 4 for the number of points n, making them impractical for real-world datasets of interest. Therefore, all prior experiments were run on small samples of size at most 1000. As we will see in our empirical studies, our work is the first to report experimental evaluation on $600 \times$ larger datasets.

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Another related line of work is that of Chhaya et al. (2022) (see also Braverman et al. (2022) for stateof-the-art bounds) that introduced core-set based algorithms for regression and clustering with individual fairness. This work has a running time of $O(nkd + k^8d^4 + (k \log n)^4)$ for individually fair clustering. While this reduces the running dependency on *n* from prior work, it scales with a large polynomial of *k* and *d*. This makes the work impractical for large dimensional datasets and when many centers are required. As we will show in the paper, our work improves significantly the dependency on *k*, *d* and allows us to report experiments with datasets with $5 \times$ more points, $10 \times$ more dimensions and $3 \times$ more clusters than all prior work.

Our contributions.

As mentioned, the previous algorithms (and our new result above) have poor runtime guarantees, making them impractical for real-world datasets of interest. To address this shortcoming, we design a fast local-search algorithm using ideas from the algorithm above as well as from the fast k-means algorithm of Lattanzi and Sohler (2019). For simplicity, we focus on k-means, which is more commonly used in practice although we notice that our approach can be generalized to all p-norms.

Theorem 1.1. There is an $\tilde{O}(nd+nk^2)$ -time algorithm for individually fair k-means with a 6-approximation for radii and an O(1)-approximation on costs.

We complement our theoretical result with an experimental study. In our experiments we use local search with swaps of size one, building on the work of Lattanzi and Sohler (2019) to find good swaps quickly (see also Beretta Beretta et al. (2023)). Whereas our algorithm scale to large datasets with 600,000 points dataset in less than two hours, prior methods can process with at most 4000–25000 points in one hour;¹ see Figure 1a.

It is also interesting to note that despite the worse approximation guarantees, we observe in Section 4 that this algorithm outperforms prior algorithms on cost and fairness objectives.²

Additional Related work. The k-means and kmedian problems are NP-Hard, even in Euclidean space where they are hard to approximate within a factor 1.36 and 1.08 respectively (Cohen-Addad and Karthik C. S. (2019); Cohen-Addad et al. (2022b, 2021) while the state-of-the-art approximation algorithms achieve a 5.94 and 2.40 approximation respectively Cohen-Addad et al. (2022a). There is an extensive literature on group fairness, where the goal is (in essence) to curb under- and over-representation in certain slices of the data (say, sensitive groups based on gender or age group) Chierichetti et al. (2017); Rösner and Schmidt (2018); Bera et al. (2019); Ahmadian et al. (2019, 2020b,a); Hotegni et al. (2023); Gupta et al. (2023); Froese et al. (2022). Another line of work concerns two generalizations of k-clustering problems to ℓ_p norm and ordered median objectives Byrka et al. (2018); Chakrabarty and Swamy (2018, 2019); Kalhan et al. (2019): Create a (non-increasingly) sorted vector out of the distances of points to their closest centers, and aim to minimize either the ℓ_p norm of this vector or the inner product of the vector with some given weight vector w. Note that $p = 1, 2, \log n$ yields k-median, k-means and k-center through the first generalization, whereas w = (1, 1, ..., 1) and w = (1, 0, ..., 0) yield k-median and k-center objectives through the latter. Chlamtác et al. (2022) combines the two generalizations into the notion of (p, q)-Fair Clustering problem, which is also a generalization of Socially Fair k-Median and k-Means Ghadiri et al. (2021); Abbasi et al. (2021); Makarychev and Vakilian (2021). Some of the above results are also motivated from the standpoint of solution robustness—the main motivation stated in Humavun et al. (2021). The widely popular k-means clustering implicitly assumes certain uniform Gaussian distributions for the data Raykov et al. (2016), and is known to be sensitive to sampling biases and outliers Wang et al. (2020). Beyond enforcing individual fairness or cluster-level consistency constraints (the focus of this work), researchers have tackled the above problem from various angles such as resorting to kernel methods Dhillon et al. (2004), adding regularization terms Georgogiannis (2016), and using trimming functions Georgogiannis (2016); Deshpande et al. (2020); Dorabiala et al. (2021).

2 Preliminaries

Let (X, dist) be a metric space, where X is a finite set of points and dist a distance function between the points in X. We define the distance between a point p and a finite set of points C as $\operatorname{dist}(p, C) = \min_{c \in C} \operatorname{dist}(p, c)$; if the set C is empty we define the distance to be ∞ . Let $\Delta = \max_{p,q} \operatorname{dist}(p,q) / \min_{p \neq q} \operatorname{dist}(p,q)$ denote the *aspect ratio* of the instance. We also let $\mu(X)$ denote the mean of a finite point set X.

Problem definition. Given a metric space (X, dist), the input to our problem is a tuple (A, C, k, δ) , where

¹Notice that the LP- or SDP-based algorithms require $\Omega(n^2)$ space, so those algorithms cannot scale to 100s of thousand point datasets even with several hours of runtime, as they run out of memory.

²Note that our algorithm, and some of the prior work Mahabadi and Vakilian (2020); Chakrabarty and Negahbani (2021); Vakilian and Yalçiner (2022), work for any vector δ of radius bounds so the results presented in the paper are more general than the classic individual fair clustering setting.

 $A \subseteq X$ is a set of points of the metric space, $C \subseteq X$ is a set of points of the metric space, k is a positive integer and $\delta : A \mapsto \mathbb{R}_+$ is the desired serving cost or *radius* of points. The goal is to output a set $S \subseteq C$ that minimizes $\sum_{a \in A} \operatorname{dist}(a, S)$ under the constraints that $|S| \leq k$ and $\forall a \in A : \operatorname{dist}(a, S) \leq \delta(a)$.

The elements of a solution $S \subseteq C$ are called *centers* or *facilities*. Given a set S of k centers, let $cost(S)_1$ denote the k-median cost of the set C for the centers S, i.e., $cost(S)_1 = \sum_{c \in A} dist(c, S)$. Similarly, we define the cost of the set C for the centers S for the k-means problem as $cost(S)_2 = \sum_{c \in A} dist(c, S)^2$. In both setting we denote with Opt_k the cost of an optimum solution S^* . When it is clear from the context we will drop the index 1 or 2 from the notation for the cost.

A solution is an (α, β) bicriteria approximation if the *k*-median (or *k*-means) cost of the solution *S* is at most α times that of the optimum, while the constraint that each *a* should be at distance at most $\delta(a)$ from a center of the solution *S* is violated by a factor at most β , i.e.: $\forall a, \operatorname{dist}(a, S) \leq \beta \delta(a).$

3 Fast algorithm

In this section we focus on the k-means problem and we show how to modify the local-search algorithm presented in Lattanzi and Sohler (2019) to obtain a bicriteria approximation for our problem, Theorem 1.1. The key intuition is to use the concept of anchor zones introduced below to allow only the swaps that preserve our fairness guarantees. To fit the page limit, the proof of the lemmas of this section have been postponed to Appendix C.

Algorithm 1: Scalable algorithm for individually fair k-means

- **Require:** an input point set X, a desired number of cluster k, a target number of iterations Z, an approximation parameter γ
- 1: $C \leftarrow \emptyset, S_0 \leftarrow \emptyset$
- 2: $S_0 \leftarrow \text{SEEDING}(X, \delta(\cdot), \gamma)$
- 3: Define each point $p \in S_0$ as an *anchor point*, and the ball B(p) of radius $\gamma \delta(p)$ around p as an *anchor zone*.
- 4: Let $T \subseteq X \setminus S_0$ be a set of $k |S_0|$ randomly selected points
- 5: $S \leftarrow S_0 \cup T$
- 6: for $i \leftarrow 2, 3, \ldots, Z$ do
- 7: $S \leftarrow$

CONSTRAINEDLOCALSEARCH++ $(X, S, B(\cdot))$ 8: return S

For simplicity of exposition in this section we consider the classic setting where A = C = X, we refer the

Algorithm 2: CONSTRAINEDLOCALSEARCH++
Require: $X, S, S_0, B(\cdot)$
1: Sample $p \in X$ with probability $\frac{\cot(\{p\},S)}{\sum_{q \in X} \cot(\{q\},S)}$
2: $Q \leftarrow \{q \in S \forall x \in S_0 : (S \setminus \{q\} \cup \{p\}) \cap B(x) \neq \emptyset\}$
3: $q^* \leftarrow \arg\min_{q \in Q} \operatorname{cost}(X, S \setminus \{q\} \cup \{p\})$
4: if $cost(X, S \setminus \{q^*\} \cup \{p\}) < cost(X, S)$ then
5: $S \leftarrow S \setminus \{q^*\} \cup \{p\}$
6: return S

Algorithm	3:	SEEDING
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Require: $A, \delta(\cdot), \gamma$
1: $S = \emptyset$
2: while $\exists p \in A : \operatorname{dist}(p, S) > \gamma \delta(p) \operatorname{do}$
3: $p^* \leftarrow \arg\min_{p' \in \{p \in A \operatorname{dist}(p,S) > \gamma \delta(p)\}} \delta(p')$
$4: S \leftarrow S \cup \{p^*\}$
5: Output S

interested reader to Appendix D for how the result can be extended to the more general case where $A, C \subseteq X$.

Toward this end, we need to change both the initialization and the swapping procedure of the local-search algorithm to take into account the radius constraints. As for initialization we first add a new center as long as there exists a point p at distance greater than $\gamma\delta(p)$ from the current set of centers, namely we use Algorithm 3 (whose correctness is proven in Appendix B). We refer to the obtained set of centers as S_0 . If $|S_0|$ is larger than k, then we know that the input is infeasible; otherwise we add additional points as centers until we obtain a set of k centers S. We say that a point is an anchor point if it is in S_0 . Furthermore we define the ball B(p) of radius $\gamma\delta(p)$ centered at p as the anchor zone for p.

As for the swaps, we choose a random point q using D^2 -sampling as in Lattanzi and Sohler (2019). If there is a subset S' obtained by swapping an element of S with q, such that (i) |S'| = k, (ii) every anchor zone contains at least one point in S', and (iii) $\sum_{p \in X} \operatorname{dist}(p, S)^2 > \sum_{p \in X} \operatorname{dist}(p, S')^2$, then we change our current solution from S to S'. Interestingly we show that after $O(k \log n\Delta)$ iterations, the solution will have constant-factor expected approximation for cost and moreover it violates the radius constraints by at most a factor of 2γ . See the pseudocode in algorithm 1.

Now we show that our algorithm obtains a constant bicriteria approximation for individually fair k-means.

Our proof uses many ingredients of the proof in Lattanzi and Sohler (2019) with careful modifications to handle the additional constraints imposed by the algorithm. In the remaining part of this section we prove our main theorem focusing on the novel part of our proofs.

3.1 Analysis (Proof of Theorem 1.1)

As in Lattanzi and Sohler (2019), the main observation behind our proof is that every step of our algorithm in expectation reduces the solution cost by a factor $O\left(1-\frac{1}{k}\right)$. In the following, given an input set of points X containing at least 2 distinct points we will let $\Delta = \max_{p,q \in X} \operatorname{dist}(p,q) / \min_{p,q : p \neq q} \operatorname{dist}(p,q)$.

Considering that the cost of the initial solution is at most $\Delta^2 n$, this implies that $O(k \log n\Delta)$ iterations suffice to obtain a constant approximation.

To simplify the exposition we assume that every cluster in the optimal solution has non-zero $\cos t$.³

Next we state two lemmas outlining the algorithm's analysis that are central in our proof of Theorem 1.1. Theorem 1.1 itself is proven in Appendix C.1.

Lemma 3.1. Let X be the set of points from a feasible instance, $\gamma \geq 3$, and S a set of centers with $cost \ cost(X,S) > 2000 \ Opt_k$. With probability $\frac{1}{1000}$, for S' = CONSTRAINEDLOCALSEARCH + (X,S), we have $cost(X,S') \leq (1 - \frac{1}{100k}) \ cost(X,S)$.

Lemma 3.2. Let X be the set of points from a feasible instance, and \hat{S}

a set of centers with $cost(X, \hat{S}) \leq \gamma n \Delta^2$. After running $Z \geq 200000k \log(\gamma n \Delta)$ rounds of Algorithm 2 on \hat{S} outputs a solution S such that $E[cost(X, S)] \in O(Opt_k)$.

3.2 Proof of Lemma 3.1

The proof in this section follows the structure of the proofs in Lattanzi and Sohler (2019) with some fundamental modification to carefully handle the anchor zones constraints.

Before proving the lemma we recall two well-known results. The following lemma is folklore:

Lemma 3.3. Let $X \subseteq \mathbb{R}^d$ be a set of points and let $c \in \mathbb{R}^d$ be a center. Then we have $cost(X, \{c\}) = |X| \cdot ||c - \mu(X)||^2 + cost(X, \mu(X)).$

We will also use the following lemma (rephrased from Corollary 21 in Feldman et al. (2018)).

Lemma 3.4. Let $\epsilon > 0$. Let $p, q \in \mathbb{R}^d$ and let $C \subseteq \mathbb{R}^d$ be a set of k centers. Then $|cost(\{p\}, C) - cost(\{q\}, C)| \le \epsilon \cdot cost(\{p\}, C) + (1 + \frac{1}{\epsilon}) ||p - q||^2$.

We assume that the optimal solution $S^* = \{c_1^*, \ldots, c_k^*\}$ is unique (this can be enforced using proper tie breaking) and use X_1^*, \ldots, X_k^* to denote the corresponding

optimal partition. We will also use $S = \{c_1, \ldots, c_k\}$ to refer to our current clustering with corresponding partitions X_1, \ldots, X_k . When the indices are not relevant, we will drop the index and write, for example, $c \in S$.

We use a notation and proof strategy similar to Kanungo et al. (2002). We start by partitioning the optimal centers into anchor centers, A^* , and unconstrained centers, U^* .

An optimal center is in A^* if it is the closest optimal center to an anchor point (breaking ties arbitrarily), the remaining centers form the set of unconstrained centers. We say that an optimal center $c^* \in U^*$ is *captured* by a center $c \in S$ if c is the nearest center to c^* among all centers in S. Also we say that an optimal center $c^* \in A^*$ with corresponding anchor point a is captured by a center $c \in S$ if c is the nearest center to c^* among all centers in the anchor zone defined by a. Note that a center $c \in S$ may capture more than one optimal center and every optimal center is captured by exactly one center from S (ties are broken arbitrarily). Some centers in c may not capture any optimal center. Similarly to Kanungo et al. (2002) we call these centers *lonely* and we denote them with L. Finally, let H be the index set of centers capturing exactly one cluster. W.l.o.g., we assume that for $h \in H$ we have that $c_h \in S$ captures $c_h^* \in S^*$, i.e., the indices of the clusters with a one-to-one correspondence are identical.

Note that the above definition is slightly different from the classic definition in Kanungo et al. (2002). In fact, an optimal center may not be captured by its closest center but by its closest center in the anchor zone. Nevertheless we can show that it is still possible to recover a similar result to the one in Lattanzi and Sohler (2019) in this setting. Note one useful proposition of our definition, whose proof is deferred to the appendix.

Proposition 3.5. Let $c^* \in A^*$ be an optimal center with corresponding anchor point a, and let c' be the closest point in S to c^* , and let c^* be captured by the center $c \in S$. Then $dist(c^*, c) \leq ((\gamma+1)/(\gamma-1))dist(c^*, c')$

We will use the above definition as in Lattanzi and Sohler (2019). Intuitively, if a center c captures exactly one cluster of the optimal solution, we think of it as a candidate center for this cluster. In this case, if c is far away from the center of this optimal cluster, we argue that with good probability we sample a point close to the center. In order to analyze the change of cost, we will argue that we can assign all points in the cluster of c that are not in the captured optimal cluster to a different center without increasing their contribution by too much. This will be called the reassignment cost and is formally defined in the definition below. We will show that with good probability we sample from a cluster such that the improvement for the points

³Note that this is w.l.o.g., since we can artificially increase the cost of every cluster by adding for each point a copy at distance $\min_{p,q \in X} \operatorname{dist}(p,q)/n$.

in the optimal cluster is significantly bigger than the reassignment cost.

If a center is lonely, we think of it as a center that can be moved to a different cluster. Again, we will argue that with high probability we can sample points from other clusters such that the reassignment cost is much smaller than the improvement for this cluster.

Now we start to analyze the cost of reassignment of the points due to a center swap. We would like to argue that the cost of reassigning the points currently assigned to a cluster center with index from H or L to other clusters is small. As discussed above, for $h \in H$, we will assign all points from X_h that are not in X_h^* to other centers. For $l \in L$ we will consider the cost of assigning all points in X_i to other clusters. We use the following definition to capture the cost of this reassignment introduced in Lattanzi and Sohler (2019).

Definition 3.6. Let $X \subseteq \mathbb{R}^d$ be a point set and $S \subseteq \mathbb{R}^d$ be a set of k cluster centers and let H be the subset of indices of cluster centers from $S = \{c_1, \ldots, c_k\}$ that capture exactly one cluster center of an optimal solution $S^* = \{c_1^*, \ldots, c_k^*\}$. Let $X_i, X_i^*, 1 \leq i \leq k$, be the corresponding clusters. Let $h \in H$ be an index with cluster X_h and w.l.o.g. let X_h^* be the cluster in the optimal solution captured by c_h . The reassignment cost of c_h is defined as

reassign
$$(X, S, c_h) = \cot(X \setminus X_h^*, S \setminus \{c_h\}) - \cot(X \setminus X_h^*, S).$$

For $\ell \in L$ we define the reassignment cost of c_{ℓ} as

 $\operatorname{reassign}(X, S, c_{\ell}) = \operatorname{cost}(X, S \setminus \{c_{\ell}\}) - \operatorname{cost}(X, S).$

We will now prove the following bound on reassignment costs. We note that this proof is similar to the proof in Lattanzi and Sohler (2019) but it includes key differences to handle the fact that optimal centers may not be assigned to the closest center in the current solution. The proof is provided in Appendix C.5.

Lemma 3.7. For $r \in H \cup L$ we have

$$reassign(X, S, c_r) \le \frac{13}{100} \operatorname{cost}(X_r, S) + 332 \operatorname{cost}(X_r, S^*).$$

Now that we have a good bound on the reassignment cost we make a case distinction. Recall that we assume that for every $h \in H$ the optimal center captured by c_h is c_H^* , i.e., the indices are identical. We first consider the case that $\sum_{h \in H} \operatorname{cost}(X_h^*, S) > \frac{1}{3} \operatorname{cost}(X, S)$.

With the previous lemma at hand, we can focus on the centers $h \in H$ where replacing h by an arbitrary point close to the optimal cluster center of the optimal cluster captured by h greatly improves solution cost. As in Lattanzi and Sohler (2019) we call such clusters good and make this notion precise in the following definition.

Definition 3.8. A cluster index $h \in H$ is called *good* if

$$\operatorname{cost}(X_h^*, S) - \operatorname{reassign}(X, S, c_h) - 9\operatorname{cost}(X_h^*, \{c_h^*\}) > \frac{1}{100k} \cdot \operatorname{cost}(X, S).$$

The above definition estimates the gain of replacing c_h by a point close to the center of X_h^* by considering a clustering that reassigns the points in X_h that do not belong to X_h^* and assigns all points in X_h^* to the new center. Now we want to show that we have a good probability to sample a good cluster. In particular, we first argue that the sum of the cost of good clusters is large. We note that the following proof is a simple adaptation of Lattanzi and Sohler (2019); its proof is deferred to the appendix.

Lemma 3.9. If $3\sum_{h\in H} cost(X_h^*, S) > cost(X, S) \ge 2000 Opt_k$, then

$$\sum_{h \in H, h \text{ is good}} \operatorname{cost}(X_h^*, S) \ge \frac{9}{400} \operatorname{cost}(X, S).$$

Now we present a lemma from Lattanzi and Sohler (2019) that whenever a cluster has high cost w.r.t. C, it suffices to consider the points close to the optimal center to get an approximation of cluster cost. We will then use this fact to argue that we sample with good probability a point close to the center.

Lemma 3.10 (Lemma 6 from Lattanzi and Sohler (2019) restated). Let $Q \subseteq \mathbb{R}^d$ be a point set and let $S \subseteq \mathbb{R}^d$ be a set of k centers and let $\alpha \geq 9$. If $cost(Q, S) \geq \alpha \cdot cost(Q, \{\mu(Q)\})$ then

$$cost(R,S) \ge \left(\frac{\alpha-1}{8}\right) \cdot cost(Q, \{\mu(Q)\}).$$

where $R \subseteq Q$ is the subset of Q at squared distance at $most \frac{2}{|Q|} \cdot cost(Q, \{\mu(Q)\})$ from $\mu(Q)$.

Now we can argue that sampling according to the sum of squared distances will provide us with constant probability with a good center. Consider any index $h \in H$ with h being good. We will apply lemma 3.10 with $Q = X_h^*$ and $\alpha = \operatorname{cost}(Q, S)/\operatorname{cost}(Q, \mu(Q))$. Note that by the definition of good, we have that $\alpha \geq 9$. Now let us define R_h^* to be the set R guaranteed by lemma 3.10. We have $\operatorname{cost}(X_h^*, S) \geq \frac{\alpha-1}{8} \operatorname{cost}(X_h^*, \{c_h^*\}) = \frac{\alpha-1}{8\alpha} \operatorname{cost}(X_h^*, S) \geq \frac{1}{9} \operatorname{cost}(X_h^*, S)$ by our choice of α (observe that c_h^* equals $\mu(X_h^*)$). Since the sum of squared distances of points in good clusters

is at least $9/400 \operatorname{cost}(X, S)$ by lemma 3.9, we conclude that $\sum_{h \in H,h \text{ is good}} \operatorname{cost}(R_h^*, S) \geq \frac{9}{9\cdot400} \operatorname{cost}(X, S)$. Thus, the probability to sample a point from $\sum_{h \in H,h \text{ is good}} \operatorname{cost}(R_h^*, S)$ is more than 1/400. By the definition of good, if we sample such a point $c \in R_h^*$ we can swap it with c_h to get a new clustering of cost at most $\operatorname{cost}(X, S \setminus \{c_h\} \cup \{c\}) \leq \operatorname{cost}(X, S) - \operatorname{cost}(X_h^*, S) +$ reassign $(X, S, \{c_h\}) + \operatorname{cost}(X_h^*, \{c\})$. By lemma 3.3 we know that $\operatorname{cost}(X_h^*, \{c\}) \leq 9\operatorname{cost}(X_h^*, \{c_h^*\})$. Hence, with probability at least 1/400 the new clustering has cost at most

$$\operatorname{cost}(X, S) - (\operatorname{cost}(X_h^*, S) - \operatorname{reassign}(X, H, c_h))$$
$$-9\operatorname{cost}(X_h^*, \{c_h^*\}) \le (1 - \frac{1}{100k}) \cdot \operatorname{cost}(X, S).$$

To check that the swap is feasible we only need to make sure that the swap is feasible if $\{c_h^*\} \in A^*$. Otherwise we already know that the anchor balls are covered by other centers. If $\{c_h^*\} \in A^*$, let *a* be the anchor point corresponding to c_h^* . Note that from the definition of good cluster, $\cos(X_h^*, S) - 9\cos(X_h^*, \{c_h^*\}) > 0$ so by lemma 3.3 we have $d(\{c_h^*\}, S) \ge 9d(\{c_h^*\}, c)$. So given that the radius of the anchor ball is $3\delta(a)$ and the distance between c_h^* and *a* is bounded by $\delta(a)$ by triangle inequality we have that *c* is inside the anchor ball. This proves our lemma in the first case.

In the second case, we have $\sum_{h \in H} \operatorname{cost}(X_h^*, S) < 1/3 \operatorname{cost}(X, S)$. Now let $R = \{1, \ldots, k\} \setminus H$, so we get $\sum_{r \in R} \operatorname{cost}(X_r^*, S) \ge 2/3 \operatorname{cost}(X, S)$. Observe that R equals the index set of optimal cluster centers that were captured by centers that capture more than one optimal center. This is because every optimal center is captured by one center and R does not include H. In this case, if the index of a center of our current solution is in $R \setminus L$ we cannot easily move the cluster center without having impact on other clusters. What we do instead is to use the centers in L as candidate centers for a swap. Note that those swaps are always feasible because inside each anchor ball we also have a center not in L. Similar to the case above we will argue that we can swap a center from L with a point that is close to an optimal center of a cluster X_r^* for some $r \in R$.

Recall that we have already bound the cost of reassigning a center in L so we just need to argue that the probability of sampling a good center is high enough.

In particular, we focus on the centers $r \in R$ and swap an arbitrary center $\ell \in L$ with an arbitrary point close to one of the centers in R to improve the cost of the solution. Slightly overloading notation, we call such cluster centers *good* and make this notion precise in the following definition.

Definition 3.11. A cluster with index $i \in \{1, \ldots, k\}$

is called *good*, if there exists a center $\ell \in L$ such that

$$\begin{split} \operatorname{cost}(X_i^*,S) - \operatorname{reassign}(X,S,\ell) &- 9 \mathrm{cost}(X_i^*,\{c_i^*\}) > \\ & \frac{1}{100k} \cdot \operatorname{cost}(X,S). \end{split}$$

The above definition estimates the cost of removing ℓ and inserting a new cluster center close to the center of X_i^* by considering a clustering that reassigns the points in X_i^* and assigns all points in X_i^* to the new center. In the following we will now argue that the sum of cost of good clusters is large, this will be useful to show that the probability of sampling such a cluster is high enough. The proof of the following lemma is deferred to the Appendix.

Lemma 3.12. If $3\sum_{h\in H} cost(X_h^*, S) \leq cost(X, S)$ and $cost(X, S) \geq 2000 Opt_k$ we have

$$\sum_{r \in R, r \text{ is good}} \operatorname{cost}(X_r^*, S) \ge \frac{1}{20} \operatorname{cost}(X, S).$$

Note that also in this case we can now argue similarly as in the other case that sampling according to sum of squared distances will provide us with constant probability with a good center using lemma 3.10. In fact, since the sum of squared distances of points in good centers is at least 1/20cost(X, S) by lemma 3.12, it follows together with lemma 3.10 that we sample a point from a good cluster X_r^* that is within distance two times the average cost of the cluster with probability $\frac{1}{1000}$. By the definition of a good cluster, we know that such a point improves the cost of the current clustering by at least a factor of $(1 - \frac{1}{100k})$. Thus, Lemma 3.1 follows.

4 Empirical analysis

In this section we evaluate empirically the algorithms presented and we compare them with state-of-theart methods from the literature. In our analysis, all datasets used are *publicly available*. We implemented our algorithms, and the other baselines in Python, and we ran each instance of our experiments independently using a single-core from machines within our institution's cloud with x86-64 architecture, 2.25GHz and using less than 32GB of RAM. To foster the reproducibility of our experiments we released our code open source.⁴

Datasets. We used several real-world datasets from the UCI Repository Dheeru and Karra Taniskidou

⁴Our code is available open source at the following link: https://github.com/google-research/ google-research/tree/master/individually_fair_ clustering/.

(2017) and from the SNAP library, that are standard in the clustering literature. This includes: adult Kohavi et al. (1996) n = 32561, d = 6, bank Moro et al. (2014) n = 45211, d = 3, diabetes Dheeru and Karra Taniskidou (2017) n = 101766, d = 2, gowalla Cho et al. (2011), n = 100000, d = 2, skin Bhatt and Dhall (2010), n = 245057, d = 4, shuttle⁵ n = 58000, d = 9, and covertype Blackard and Dean (1999), n = 581012, d = 54. For consistency with prior work, for adult, bank and diabetes we use the same set of columns used in the analysis of Mahabadi and Vakilian (2020). We preprocess each dataset to have zero mean and unit standard deviation in every dimension. All experiments use the Euclidean distance. The effect of the value of k is discussed in Appendix A.

Algorithms. We consider the following algorithms. – VanillaKMeans. Standard non-fair k-means implementation from sklearn. This baseline represents the k-means cost achievable neglecting fairness.

- **ICML20** Mahabadi and Vakilian (2020): We implemented the algorithm following the recommendation of the paper (i.e., using a single swap in the local search and a factor $3\delta(p)$ instead of $6\delta(p)$ in the initialization). We set $\epsilon = 0.01$ in the algorithm.

- NeurIPS21 Chakrabarty and Negahbani (2021): We use the Python code provided by the authors.⁶ We use both the more accurate algorithm NeurIPS21 and the faster algorithm using sparsification (NeurIPS21Sparsify).

- **Greedy**: Similarly to prior work we consider the execution of the greedy seeding algorithm as a baseline.

- **LSPP**: We implemented our local-search algorithm with modifications similar to that of ICML20 (a single swap and $\mu = 3$ factor in seeding algorithm). We also modified the algorithm to run only a fixed number of local-search iterations (namely 500) in all experiments.

Moreover, we also design a fairness preserving Lloyd's method, the F-Lloyd's method, that we add as a postprocessing of our algorithm. In the F-Lloyd's method we assign each point to the nearest center. Then we obtain the mean of the clusters. Notice that the mean minimizes the k-means cost, but it may not be a feasible solution for the distance bound. For this reason, we use the anchor points obtained by our algorithm to find the next center approximating, with binary search, the closest feasible point to the mean (respecting the anchor points constraints), on the line between the current center and the mean. Though this procedure does not alter the theoretical guarantees, it improves the results empirically. We use 20 iterations of the F-Lloyd's method at the end of our algorithm.⁷

Metrics. We focus on three key metrics: the k-means cost of clustering, the average runtime of algorithm and the *bound ratio* $\max_p \frac{\operatorname{dist}(p,S)}{\delta(p)}$ where S is the solution of the algorithm. We repeat each experiment configuration 10 times and report the mean and standard deviation of the metrics.

Comparison with other baselines. In this section we report a comparison of our algorithm with the other baselines. For all experiments, unless otherwise specified, we replicate the setting of individual fairness Mahabadi and Vakilian (2020) for $\delta(p)$, by setting $\delta(p)$ as the distance to the n/k-th nearest point.

Notice that the ICML20 algorithm evaluates, for each iteration of local search, all possible swaps of one center with a non-center while NeurIPS21 and NeurIPS21Sparsify both depend on computing all-pairs distances in $O(dn^2)$ time. This makes these algorithms not scalable to large datasets, unlike our algorithm. Therefore all prior experiments Mahabadi and Vakilian (2020); Chakrabarty and Negahbani (2021) used a subsample of ≈ 1000 elements from the datasets to run their algorithm. In this section we use a similar approach for consistency.

In Figure 1a, 1b, 1c, we report the results of the various algorithms for different sizes of the sample on the gowalla dataset, fixing k = 10.

The main message of the paper is summarized in Figure 1a. We allowed each algorithm to run for up to 1 hour on increasingly large samples of the data. Notice how our algorithm is orders of magnitude faster than all fair baselines including the faster NeurIPS21Sparsify variant. ICML20 does not complete in 1 hour past size ~ 5000 , NeurIPS21 past ~ 7000 , NeurIPS21Sparsify past ~ 25000 while our algorithm's running time is not highly affected by scale. This will allow us to run on 500,000 sized datasets, orders of magnitude larger than SOTA algorithms.

Then we focus on the k-means cost of the solution in Figure 1b. Notice that our algorithm (LSPP) has a cost better (or comparable) than that of all fair baselines and close to the unfair VanillaKMeans.

Finally, Figure 1c shows the max ratio of distance of a point p to centers vs $\delta(p)$. We observe that VanillaKMeans has a bound ratio between 60 and 90 (out of the plot scale), confirming the need for fair algorithms. For the remainder of the paper we will ignore VanillaKMeans.

Now we focus on the fair algorithms. Notice that the

⁵Thanks to NASA for releasing the dataset.

⁶The code was obtained from https://github.com/moonin12/individually-fair-k-clustering and adapted.

⁷Later, we discuss the applicability of this improvement to other prior baselines.



Figure 1: Mean completion time, cost, and bound ratio for the algorithms on Gowalla dataset subsampled to different sizes, k = 10. The shades represent the 95% confidence interval (notice that some algorithms are deterministic). Runs that did not complete in 1 hour on the sample are not reported. VanillaKMeans bound ratio is > 60 in all runs and not show in the plot as out of scale).

(much slower) ICML20 has statistically comparable bounds with LSPP (and both significantly better than their worst case guarantees), while NeurIPS21 and NeurIPS21Sparsify have slightly better bounds.

Experiments on the full datasets. The scalability of our algorithm allows us to run it on the full datasets with up to 1/2 million elements. In this section, we run our algorithm and the fast Greedy baseline on all complete datasets, using k = 10. Our algorithm completed all runs in less than 2 hours on the full datasets.

To compare with all the slower baselines we allow ICML20, NeurIPS21 and NeurIPS21Sparsify to run on a subsample of the data containing 4000 points (but we evaluate the solution on the entire dataset). This of course has no theoretical guarantee and can perform especially poorly in case of outliers. In the supplementary material we report the standard deviation for the metrics in Table 1.

For this large-scale experiment, the input bound $\delta(p)$ for each point p is set using the n/k-th closest point in a random sample of 1000 elements.

In all but one dataset, our algorithm has a significantly lower k-means cost than that of all other baselines. Similarly to the above results, our algorithm has a similar or better ratio bound than that of ICML20 (with the sampling heuristic), while the ratio bound of NeurIPS21 and NeurIPS21Sparsify is sometimes lower. In any instance our algorithm has a much better ratio that the worst-case theoretical guarantees. The results are reported in Table 1.

Finally, we focus on the impact of our novel F-Lloyd's

dataset	algorithm	k-means cost	bound ratio
adult	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 1.56\mathrm{E}{+}05\\ 6.59\mathrm{E}{+}04\\ 1.14\mathrm{E}{+}05\\ 1.02\mathrm{E}{+}05\\ \textbf{6.14}\mathrm{E}{+}\textbf{04}\end{array}$	1.8 1.4 1.2 1.2 1.4
bank	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 8.57\mathrm{E}{+}04\\ 3.23\mathrm{E}{+}04\\ 5.68\mathrm{E}{+}04\\ 5.70\mathrm{E}{+}04\\ \textbf{3.02E}{+}\textbf{04}\end{array}$	1.9 1.6 1.2 1.2 1.6
covtype	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	3.33E+07 2.84E+07 2.76E+07 2.80E+07 2.50E+07	1.3 1.1 1.1 1.1 1.1
diabetes	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	$\substack{\begin{array}{c} 6.60 {\rm E}+04 \\ 3.00 {\rm E}+04 \\ {\rm N/A} \\ 3.36 {\rm E}+04 \\ \textbf{2.66 {\rm E}+04 \end{array}}$	2.7 1.3 N/A 1.2 1.4
gowalla	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 1.17\mathrm{E}{+}04\\ \mathrm{N/A}\\ 8.65\mathrm{E}{+}03\\ 1.63\mathrm{E}{+}04\\ \textbf{6.93E}{+}\textbf{03}\end{array}$	1.6 N/A 1.1 1.2 1.6
shuttle	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 4.89E{+}05\\ 1.91E{+}05\\ 2.60E{+}05\\ 2.72E{+}05\\ \textbf{1.79E{+}05}\end{array}$	2.3 2.0 1.0 1.1 2.1
skin	Greedy ICML20 NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 1.80 {\rm E}{+}05 \\ \textbf{7.47 E}{+}\textbf{04} \\ 9.36 {\rm E}{+}04 \\ 1.03 {\rm E}{+}05 \\ 9.27 {\rm E}{+}04 \end{array}$	2.1 1.8 1.1 1.1 3.1

Table 1: Mean Cost and max bound ratio for all fullsized datasets and k=10 with ICML20, NeurIPS21 and NeurIPS21Sparsify ran on a sample of 4000 points. fair improvement method. We observe that this step can only be applied to algorithms based on anchor points (like ours and ICML20) and that (of course) cannot improve the efficiency of the slow ICML20 baseline. For this reason we tested ICML20 with our F-Lloyd method on a sample of size 1000 points where such an algorithm can run. The full analysis is reported in the supplemental material and confirms all prior experiments. We observe that adding F-Lloyd steps improves the cost of ICML20 baseline as well, but does not change the overall trend reported, i.e., that our algorithm has comparable (or better cost) than all fair baselines while scaling to orders of magnitude larger datasets. We believe that the F-Lloyd algorithm could benefit other work in the future.

5 Conclusions and Future Works

We present a new scalable algorithm for individually fair clusters, with strong theoretical guarantees and good experimental performances. An interesting open question is to use the more recent analysis of LOCALSEARCH++ by Choo et al. (2020) to improve the running time of our algorithm to $O(dnk^2)$. However, it is not clear how to obtain the necessary strong guarantees similar to the one in Lemma 12 of Choo et al. (2020).

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Checklist

- 1. For all models and algorithms presented, check if you include:
 - (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model.
 [Yes]
 - (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm. [Yes]
 - (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries. [Yes]
- 2. For any theoretical claim, check if you include:
 - (a) Statements of the full set of assumptions of all theoretical results. [Yes]
 - (b) Complete proofs of all theoretical results. [Yes]
 - (c) Clear explanations of any assumptions. [Yes]
- 3. For all figures and tables that present empirical results, check if you include:
 - (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL).
 [Yes]
 - (b) All the training details (e.g., data splits, hyperparameters, how they were chosen). [Not Applicable]
 - (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). [Yes]
 - (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). [Yes]
- 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
 - (a) Citations of the creator If your work uses existing assets. [Yes]
 - (b) The license information of the assets, if applicable. [Not Applicable]
 - (c) New assets either in the supplemental material or as a URL, if applicable. [Not Applicable]
 - (d) Information about consent from data providers/curators. [Not Applicable]
 - (e) Discussion of sensible content if applicable, e.g., personally identifiable information or offensive content. [Not Applicable]

- 5. If you used crowdsourcing or conducted research with human subjects, check if you include:
 - (a) The full text of instructions given to participants and screenshots. [Not Applicable]
 - (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. [Not Applicable]
 - (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. [Not Applicable]

A Additional experimental results

Small scale datasets and effect of F-Lloyd improvement The results observed before are confirmed in all datasets, as shown in Table 2, where we report the cost and bound ratio for all datasets, subsampled to 1000 elements, and k = 10.

In this experiment we report as well the results of using our novel F-Lloyd's fair improvement method on top of the ICML20 baseline (recall that this step can only be applied to algorithms based on anchor points such as LSPP and ICML20). Even with this improvement, the picture remains unchanged LSPP has always the lowest cost (or close to lowest cost, achieved by the improved ICML20+F-Lloyd) to all fair algorithms while scaling to 2 orders of magnitude larger datasets than ICML20 (even without the additional running time of F-Lloyd which only makes ICML20 slower). For this reason, for the remainder of the paper we focus on the ICML20 baseline as introduced by the authors.

Effect of k A similar overall picture appears in Figure 2a, 2b, where we report the results of the various algorithms for different k's on a sample of 1000 elements in the adult dataset. Notice that our algorithm has lower or comparable cost to all fair baselines in cost in Figure 2a and the comparable or slightly higher bound ratio in Figure 2b.



Figure 2: Mean completion cost and bound ratio for the algorithms on the adult dataset subsampled to 1000 elements and different k's. The shades represent the 95% confidence interval.

Additional results on large-scale datasets As we mentioned before, our algorithm is the only one that runs on the big datasets within reasonable time (and memory).

To compare with all the slower baselines we allow ICML20, NeurIPS21 and NeurIPS21Sparsify to run on a subsample of the data containing 4000 points (but we evaluate the solution on the entire dataset). This of course has no theoretical guarantee and can perform especially poorly in case of outliers.

For this large-scale experiment, the input bound $\delta(p)$ for each point p is set using the n/k-th closest point in a random sample of 1000 elements.

The results in Table 1 shows that in all but one dataset, our algorithm has a significantly lower k-means cost than that of all other baselines. Similarly to the above results, our algorithm has a similar or better ratio bound than that of ICML20 (with the sampling heuristic), while the ratio bound of NeurIPS21 and NeurIPS21Sparsify is sometimes lower. In any instance our algorithm has a much better ratio that the worst-case theoretical guarantees.

dataset	algorithm	k-means cost	bound ratio
adult	Greedy ICML20 ICML20+F-Lloyd NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 3832.6 () \\ 1854.9 () \\ 1733.2 () \\ 2744.3 () \\ 2745.5 () \\ 1726.0 (9.4) \end{array}$	$\begin{array}{c} 2.0 \ () \\ 1.2 \ () \\ 1.3 \ () \\ 1.1 \ () \\ 1.2 \ () \\ 1.2 \ (0) \end{array}$
bank	Greedy ICML20 ICML20+F-Loyd NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 1081.8 \ () \\ 568.4 \ () \\ 517.9 \ () \\ 784.2 \ () \\ 761.2 \ () \\ 510.5 \ (6.9) \end{array}$	$\begin{array}{c} 1.8 () \\ 1.4 () \\ 1.5 () \\ 1.2 () \\ 1.2 () \\ 1.4 (0.1) \end{array}$
covtype	Greedy ICML20 ICML20+F-Lloyd NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 50629.8 \ () \\ 42121.5 \ () \\ \textbf{35211.3} \ () \\ 47810.6 \ () \\ 46078.6 \ () \\ 35860.4 \ (569) \end{array}$	$\begin{array}{c} 1.3 (-) \\ 1.1 (-) \\ 1.0 (-) \\ 1.1 (-) \\ 1.1 (-) \\ 1.0 (0.0) \end{array}$
diabetes	Greedy ICML20 ICML200+F-Loyd NeurIPS21 NeurIPS21Sparsify LSPP	522.3 () 266.4 () 231.8 () N/A 299.8 () 248.5 (8.5)	2.1 () 1.1 () 1.1 () N/A 1.1 () 1.2 (0.2)
gowalla	Greedy ICML20 ICML200+F-Lloyd NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 41.4 () \\ 18.6 () \\ 17.3 () \\ 44.3 () \\ 68.6 () \\ 20.3 (1.6) \end{array}$	1.6 () 1.0 () 1.0 () 1.0 () 1.0 () 1.3 (0.1)
shuttle	Greedy ICML20 ICML200+F-Lloyd NeurIPS21 NeurIPS21Sparsify LSPP	$\begin{array}{c} 2647.4 () \\ 1335.0 () \\ 1272.1 () \\ 2494.8 () \\ 2477.1 () \\ 1219.1 (31.3) \end{array}$	$\begin{array}{c} 2.0 () \\ 1.8 () \\ 1.8 () \\ 1.0() \\ 1.2 () \\ 1.8 (0.1) \end{array}$
skin	Greedy ICML20 ICML200+F-Lloyd NeurIPS21 NeurIPS21Sparsify LSPP	584.3 (-) $292.8(-)$ $276.2 (-)$ $379.4 (-)$ $384.1 (-)$ $314.3 (27.7)$	$\begin{array}{c} 2.7 (-) \\ 2.3 (-) \\ 2.4 (-) \\ 1.1 (-) \\ 1.1 (-) \\ 2.5 (0.1) \end{array}$

Table 2: Cost and max bound ratio for all datasets subsampled for 1000 elements and k = 10 (stddev in parentheses for the LSPP randomized algorithm). N/A indicates that the algorithm did not complete in 2 hours. In this table we also report experiments with the F-Lloyd heuristic applied to ICML20.

dataset	algorithm	$\cos t \ stddev$	bound ratio stddev
adult	ICML20	$6.81E{+}02$	1.00E-01
	NeurIPS21	$1.34E{+}04$	$0.00\mathrm{E}{+00}$
	NeurIPS21Sparsify	$7.65\mathrm{E}{+}03$	$0.00\mathrm{E}{+00}$
	LSPP	$8.84\mathrm{E}{+02}$	$0.00\mathrm{E}{+00}$
bank	ICML20	$1.04E{+}03$	1.00E-01
	NeurIPS21	$5.95\mathrm{E}{+03}$	$0.00\mathrm{E}{+00}$
	NeurIPS21Sparsify	$6.57\mathrm{E}{+}03$	$0.00\mathrm{E}{+00}$
	LSPP	$6.85\mathrm{E}{+02}$	1.00E-01
covtype	ICML20	$2.23\mathrm{E}{+}05$	$0.00\mathrm{E}{+00}$
	NeurIPS21	$1.85\mathrm{E}{+}05$	$0.00\mathrm{E}{+00}$
	NeurIPS21Sparsify	$3.83\mathrm{E}{+}05$	$0.00\mathrm{E}{+00}$
	LSPP	$4.51\mathrm{E}{+}05$	$0.00\mathrm{E}{+00}$
diabetes	ICML20	$8.19\mathrm{E}{+02}$	2.00E-01
	NeurIPS21	N/A	N/A
	NeurIPS21Sparsify	$1.22\mathrm{E}{+03}$	1.00E-01
	LSPP	$9.58\mathrm{E}{+02}$	1.00E-01
gowalla	ICML20	N/A	N/A
	NeurIPS21	$2.07\mathrm{E}{+}03$	$0.00\mathrm{E}{+00}$
	NeurIPS21Sparsify	$4.05\mathrm{E}{+}03$	1.00E-01
	LSPP	$1.32\mathrm{E}{+03}$	$0.00\mathrm{E}{+00}$
shuttle	ICML20	$1.25\mathrm{E}{+}04$	2.00E-01
	NeurIPS21	$6.57\mathrm{E}{+}03$	$0.00\mathrm{E}{+00}$
	NeurIPS21Sparsify	$1.37\mathrm{E}{+}04$	$0.00\mathrm{E}{+00}$
	LSPP	$1.05\mathrm{E}{+}04$	3.00E-01
skin	ICML20	$3.51E{+}03$	3.00E-01
	NeurIPS21	$1.60\mathrm{E}{+}03$	1.00E-01
	NeurIPS21Sparsify	$1.31E{+}04$	$0.00\mathrm{E}{+00}$
	LSPP	$4.80\mathrm{E}{+}02$	2.00E-01

Table 3: Standard deviation of cost and max bound ratio for all full-sized datasets and k=10 with ICML20, NeurIPS21 and NeurIPS21Sparsify ran on a sample of 4000 points .

Standard deviation of the metrics in large datasets. In Table 3 we report the standard deviation for the metrics in Table 1. Notice that in this experiment, the input to ICML20, NeurIPS21 and NeurIPS21Sparsify algorithms are run on a random subsample, so this makes the algorithm non-deterministic. Notice that our algorithm has statistically significantly lower cost than the other baselines in almost all datasets.

Effect of the normalization of the points. In our experiments, we applied two preprocessing steps that are common in the clustering literature Borassi et al. (2020): each point in the dataset is shifted so that the dataset has zero mean; and each dimension is scaled to have unit standard deviation. We have observed that such pre-processing has no significant effect on the experimental conclusion of our work. In Table 4 we report results for the same experiments previously reported in Table 1, this time executed on the adult dataset without normalization.

As observed before, our algorithm has a significantly lower (or comparable) k-means cost than that of other baselines, better ratio than the worst-case theoretical guarantees and a much faster runtime than all fair algorithms.

B Seeding Strategy for Local Search

We describe the seeding procedure outlined in algorithm 3 to initialize our local-search approach. The proof of this lemma can be found in Section B.

		k-means-cost	\max -fairness-cost
dataset	algorithm		
adult (no norm.)	Greedy	$5.0 E{+}13$	$2.9\mathrm{E}{+00}$
	ICML20	$1.2\mathrm{E}{+13}$	$1.8\mathrm{E}{+00}$
	NeurIPS21	N/A	N/A
	NeurIPS21Sparsify	$5.2\mathrm{E}{+13}$	$1.8\mathrm{E}{+00}$
	LSPP	$1.3\mathrm{E}{+13}$	$2.3\mathrm{E}{+00}$

Table 4: Mean Cost and max bound ratio for all full-sized datasets and k=10 with ICML20, NeurIPS21 and NeurIPS21Sparsify ran on a sample of 4000 points on the Adult datasets without normalization.

Lemma B.1. If the problem is feasible, Algorithm 3 with parameter $\gamma > 2$ returns a set of points S of size at most k such that each point p is at distance at most $\gamma\delta(p)$ from the closest point in S, i.e., $\forall p \in A : dist(p, S) \leq \gamma\delta(p)$.

Proof of Lemma B.1. The proof is similar to the proof of correctness of Gonzales' algorithm for k-center Gonzalez (1985) and of Hochbaum and Shmoys' algorithm Hochbaum and Shmoys (1985). Observe first that by feasibility, there cannot be k + 1 points p'_1, \ldots, p'_{k+1} such that the balls $\delta(p'_i)$ are all pairwise disjoint (since otherwise the optimum solution would need k + 1 centers to satisfy the $\delta(p')$ constraints).

Let p_1, \ldots, p_{k^*} be the sequence of points picked by the algorithm. We have that $\delta(p_i) \leq \delta(p_j)$ for any $i \leq j$. Note that at the end of the algorithm, each point p is at distance at most $\gamma\delta(p)$ from one of p_1, \ldots, p_{k^*} so what remains to be shown is that $k^* \leq k$. We claim that the collection of balls centered at the p_i and of radii $\delta(p_i)$ are all pairwise disjoint and so if the problem is feasible, the algorithm does not return more than k points (i.e.: $k^* \leq k$). Consider a pair i, j and without loss of generality i > j. We have that p_i is at distance at least $\gamma\delta(p_i)$ from p_j by the definition of the algorithm. Since $\gamma > 2$ and $\delta(p_i) \geq \delta(p_j)$, we have that $\delta(p_i) + \delta(p_j) \leq 2\delta(p_i) < \gamma\delta(p_i) \leq \text{dist}(p_i, p_j)$ and so the ball of radius $\delta(p_j)$ around p_j cannot intersect the ball of radius $\delta(p_i)$ around p_j .

C Proof of Section 3

The proof in this section follows closely the structure of the proofs in Lattanzi and Sohler (2019) with some modification to carefully handle the anchor zones constraints.

C.1 Proof of Theorem 1.1

Proof of Theorem 1.1. Observe that the dimension can be reduced to $O(\log k/\varepsilon^{-2})$ using the Johnson-Lindenstrauss transform Becchetti et al. (2019); Makarychev et al. (2019). Hence, in $\tilde{O}(nd)$ time one can find a projection to a space of dimension $O(\log k)$ that preserves the k-means cost of all solutions up to an O(1) factor and execute the algorithm in this space. The claimed running time then follows immediately.

The algorithm returns infeasible only if it finds k + 1 disjoint individual fairness balls. But in that case, the problem is infeasible (their fairness constraints cannot be satisfied with k points).

Let \hat{S} be the set S before calling CONSTRAINEDLOCALSEARCH++. In this set, every point p has distance at most $\gamma\delta(p)$ from a center so $\cos(X, \hat{S}) \leq \gamma n \Delta^2$. lemma 3.2 then shows that after Z calls to CONSTRAINEDLO-CALSEARCH++, we obtain a constant approximation.

Now we show that at any point in time during the execution of the algorithm $\max_{p \in X} \operatorname{dist}(p, S) \leq 2\gamma \delta(p)$. The algorithm guarantees to keep at least one point in every anchor ball. Moreover every point p is at distance at most $\gamma \delta(p)$ from an anchor point p' with $\delta(p) > \delta(p')$. The anchor ball B(p') must have a center $c \in S$, so $\operatorname{dist}(c, p') \leq \gamma \delta(p')$. Thus by triangle inequality $\operatorname{dist}(c, p) \leq 2\gamma \delta(p)$.

It takes O(dnk) time to compute the initial set \hat{S} . To implement the local search, we need to compute the cost of swapping the new sample point with an old center. This requires iterating over all clusters and for each cluster we

need to compute the distance to all other centers and to check that there is at least one center in each anchor ball. Thus, a local search step requires O(dkn + dk) time in the worst case, resulting in a total runtime of O(dnkZ). The Theorem follows.

C.2 Proof of Lemma 3.2

Proof. By Lemma 3.1 we know that if before any call of CONSTRAINEDLOCALSEARCH++ the cost of the centers is bigger than 2000Opt_k then with probability $\frac{1}{1000}$ we reduce the cost by a $(1 - \frac{1}{100k})$ multiplicative factor.

Now consider another random process Y with initial value equal to $\cot(X, \hat{S})$, which for $Z = 100000k \log n\Delta(X)^2$ iterations, it reduces the value by a $\left(1 - \frac{1}{100k}\right)$ multiplicative factor with probability 1/1000, and finally increases the value by an additive $2000 \operatorname{Opt}_k$. It is not hard to see that the final value of Y stochastically dominates the cost of the solution our algorithm produces.

So the final expected value of Y is larger than the expected value of cost(X, S) conditioned on the initial clustering \hat{S} . Furthermore,

$$\begin{split} E[Y] &= 2000 \text{Opt}_k + \text{cost}(X, \hat{S}) \cdot \sum_{i=0}^{Z} {\binom{Z}{i}} \left(\frac{1}{1000}\right)^i \left(\frac{999}{1000}\right)^{Z-i} \left(1 - \frac{1}{100k}\right)^i \\ &= \text{cost}(X, \hat{S}) \left(1 - \frac{1}{10000k}\right)^Z + 2000 \text{Opt}_k \\ &\leq \frac{\text{cost}(X, \hat{S})}{n\Delta(X)^2} + 2000 \text{Opt}_k. \end{split}$$

This implies that $E[\operatorname{cost}(X,S)|\hat{S}] \leq \frac{\operatorname{cost}(X,\hat{S})}{n\Delta(X)^2} + 2000\operatorname{Opt}_k$. Our upper-bound on the cost of \hat{S} is deterministic, hence $E[\operatorname{cost}(X,S)] \leq \frac{\operatorname{cost}(X,\hat{S})}{n\Delta(X)^2} + 2000\operatorname{Opt}_k \leq 2001\operatorname{Opt}_k$. \Box

This section contains the proofs of the lemmas of Section 3.

C.3 Proof of Lemma 3.2

The proof in this section follows closely the structure of the proofs in Lattanzi and Sohler (2019) and we include it for completeness.

Proof of Lemma 3.2. By Lemma 3.1 we know that if before any call of CONSTRAINEDLOCALSEARCH++ the cost of the centers is bigger than 2000Opt_k then with probability $\frac{1}{1000}$ we reduce the cost by a $(1 - \frac{1}{100k})$ multiplicative factor.

We next use another random process Y to handle dependencies between rounds. In this way we can have a coupling with an independent process that is easier to analyze. We let Y be a random process with initial value equal to $\cot(X, \hat{S})$, which for $Z = 100000k \log n\Delta^2$ iterations, it reduces the value by a $\left(1 - \frac{1}{100k}\right)$ multiplicative factor with probability 1/1000, and finally increases the value by an additive $20000 \operatorname{pt}_k$. It is not hard to see that the final value of Y stochastically dominates the cost of the solution our algorithm produces. So the final expected value of Y is larger than the expected value of $\cos(X, S)$ conditioned on the initial clustering \hat{S} . Furthermore,

$$\begin{split} E[Y] &= 2000 \text{Opt}_k + \text{cost}(X, \hat{S}) \cdot \sum_{i=0}^{Z} {\binom{Z}{i}} \left(\frac{1}{1000}\right)^i \left(\frac{999}{1000}\right)^{Z-i} \left(1 - \frac{1}{100k}\right)^i \\ &= \text{cost}(X, \hat{S}) \left(1 - \frac{1}{100000k}\right)^Z + 2000 \text{Opt}_k \\ &\leq \frac{\text{cost}(X, \hat{S})}{n\Delta^2} + 2000 \text{Opt}_k. \end{split}$$

This implies that $E[\cot(X, S)|\hat{S}] \leq \frac{\cot(X, \hat{S})}{n\Delta^2} + 2000 \text{Opt}_k$. Our upper-bound on the cost of \hat{S} is deterministic, hence $E[\cot(X, S)] \leq \frac{\cot(X, \hat{S})}{n\Delta^2} + 2000 \text{Opt}_k \leq 2001 \text{Opt}_k$. \Box

C.4 Proof of Proposition 3.5

Proof of Proposition 3.5. If c' is within distance $\gamma\delta(a)$ to a, the lemma follows from dist $(c^*, c) = \text{dist}(c^*, c')$ by definition of c and anchor ball. Otherwise we know that c^* is at distance at most δ from a, c is at distance at most $\gamma\delta$ from a, and c' is at distance at least $\gamma\delta$ from a. The lemma follows the triangle inequality.

C.5 Proof of Lemma 3.7

Proof of Lemma 3.7. We only present the case $r \in H$. The case $r \in L$ is almost identical (in fact, simpler). We observe that reassign $(X, S, c_r) = \cot(X_r \setminus X_r^*, S \setminus \{r\}) - \cot(X_r \setminus X_r^*, S)$ since vertices in clusters other than X_r will still be assigned to their current center. If $r \in H$, we assign every point in $X_r \cap X_i^*$, $i \neq r$, to the center that captured the center of X_i^* . While this assignment may not be optimal, its cost provides an upper bound on the cost of reassigning the points: We move every point in $X_r \cap X_i^*$, $i \neq r$, to the center of X_i^* . Now the closest center of S to these points is a center with distance close to the one that captured the center of X_i^* , which, for points not in X_r^* , cannot be r, since r is in H. The fact that the squared moved distance of each point equals its contribution to the optimal solution allows us to get an upper bound on the cost change using lemma 3.4. After this, we move the points back to their original location while keeping their cluster assignments fixed. Again we can use the bound on the overall moved distance together with lemma 3.4 to obtain a bound on the change of cost. Combining the two gives an upper bound on the increase of cost that comes from reassigning the points. Details follow.

Let Q_r be the (multi)set of points obtained from $X_r \setminus X_r^*$ by moving each point in $X_i^* \cap X_r$, $i \neq r$, to c_i^* . We apply lemma 3.4 with $\epsilon = 1/100$ to get an upper bound for the change of cost with respect to S that results from moving the points to Q_r . For $p \in X_r \setminus X_r^*$ let $q_p \in Q_r$ be the point of Q_r to which p has been moved. We have:

$$|\operatorname{cost}(\{p\}, S) - \operatorname{cost}(\{q_p\}, S)| \le \frac{1}{100} \operatorname{cost}(\{p\}, S) + 101 \cdot \operatorname{cost}(\{p\}, S^*).$$

Summing up over all points in $X_r \setminus X_r^*$ yields

$$\left|\operatorname{cost}(X_r \setminus X_r^*, S) - \operatorname{cost}(Q_r, S)\right| \le \frac{1}{100} \operatorname{cost}(X_r \setminus X_r^*, S) + 101 \cdot \operatorname{cost}(X_r \setminus X_r^*, S^*).$$

Let $Q_{r,i}$ be the points in Q_r that are nearest to center $c_i \in S$ and let $X_{r,i}$ be the set of their original locations. For $p \in X_{r,i}$ that has been moved to $q_p \in Q_{r,i}$ with q_p let c'_i be the closest point to q_p not equal to r. Note that the only case in which $c_i \neq c'_i$ is when $c_i = r$. Furthermore, q_p is not captured by r because r captures c^*_r and is in H. So by proposition 3.5 we know $\cos(\{q_p\}, \{c'_i\}) \leq \frac{\mu+1}{\mu-1} \cos(\{q_p\}, \{c_i\})$. Thus we have:

$$\begin{aligned} |\operatorname{cost}(\{q_p\}, \{c_i\}) - \operatorname{cost}(\{p\}, \{c'_i\})| \\ &= |\operatorname{cost}(\{q_p\}, \{c_i\}) - \operatorname{cost}(\{q_p\}, \{c'_i\})| + |\operatorname{cost}(\{q_p\}, \{c'_i\}) - \operatorname{cost}(\{p\}, \{c'_i\})| \\ &\leq \frac{2}{\mu - 1} \operatorname{cost}(\{q_p\}, \{c_i\}) + \frac{1}{100} \operatorname{cost}(\{q_p\}, \{c'_i\}) + 101 \cdot \operatorname{cost}(\{p\}, \{q_p\}) \\ &\leq \frac{1}{\mu - 1} \left(2 + \frac{\mu + 1}{100}\right) \operatorname{cost}(\{q_p\}, \{c_i\}) + 101 \cdot \operatorname{cost}(\{p\}, \{q_p\}), \end{aligned}$$

where in the first inequality we used lemma 3.4 with $\epsilon = 1/100$.

Summing up over all points in $X_r \setminus X_r^*$ and the corresponding points in Q_r yields

$$\begin{aligned} |\operatorname{cost}(Q_r, S) - \sum_{i} \operatorname{cost}(X_{r,i}, S \setminus \{r\})| \\ &\leq \frac{1}{\mu - 1} \left(2 + \frac{\mu + 1}{100} \right) \operatorname{cost}(Q_r, S) + 101 \cdot \operatorname{cost}(X_r \setminus X_r^*, S^*) \\ &\leq \frac{26}{25} \left(\frac{11}{100} \operatorname{cost}(X_r \setminus X_r^*, S) + 101 \cdot \operatorname{cost}(X_r \setminus X_r^*, S^*) \right) + \\ &\quad 101 \cdot \operatorname{cost}(X_r \setminus X_r^*, S^*) \\ &\leq \frac{3}{25} \operatorname{cost}(X_r, S) + 231 \cdot \operatorname{cost}(X_r, S^*), \end{aligned}$$

where the second inequality uses the bound on $\mu \geq 3$. Hence,

$$\operatorname{reassign}(X, S, c_r) = |\operatorname{cost}(X_r \setminus X_r^*, S) - \sum_i \operatorname{cost}(X_{r,i}, S \setminus \{r\})|$$

$$\leq |\operatorname{cost}(X_r \setminus X_r^*, S) - \operatorname{cost}(Q_r, S)| + |\operatorname{cost}(Q_r, S) - \sum_i \operatorname{cost}(X_{r,i}, S \setminus \{r\})|$$

$$\leq \frac{13}{100} \operatorname{cost}(X_r, S) + 332 \operatorname{cost}(X_r, S^*). \quad \Box$$

C.6 Proof of Lemma 3.9

Proof of Lemma 3.9. We have $\sum_{h \in H} \operatorname{cost}(X_h^*, C) \geq \frac{1}{3} \operatorname{cost}(X, S)$ and by the definition of good and lemma 3.7

$$\sum_{h \in H,h \text{ is not good}} \operatorname{cost}(X_h^*, S) \leq \sum_{h \in H} \operatorname{reassign}(X, S, c_h) + 9\operatorname{Opt}_k + \frac{1}{100} \operatorname{cost}(X, S) \leq \frac{14}{100} \operatorname{cost}(X, S) + 341\operatorname{Opt}_k.$$

Using that $cost(X, S) \ge 2000 \text{Opt}_k$ we obtain that

$$\sum_{h \in H, h \text{ is not good}} \operatorname{cost}(X_h^*, S) \le \frac{621}{2000} \cdot \operatorname{cost}(X, S).$$

So $\sum_{h \in H,h \text{ is good}} \operatorname{cost}(X_h^*, S) \ge \frac{9}{400} \cdot \operatorname{cost}(X, S)$. The lemma follows.

C.7 Proof of Lemma 3.12

Proof of Lemma 3.12. We have $\sum_{r \in R} \operatorname{cost}(X_r^*, S) \ge 2/3\operatorname{cost}(X, S)$. Note that $|R| \le 2|L|$. By the definition of good and lemma 3.7

$$\sum_{r \in R, r \text{ is not good}} \operatorname{cost}(X_r^*, S)$$

$$\leq 2|L| \min_{\ell \in L} \operatorname{reassign}(X, S, \ell) + 9\operatorname{Opt}_k + \frac{1}{100} \operatorname{cost}(X, S)$$

$$\leq 2 \sum_{\ell \in L} \operatorname{reassign}(X, S, \ell) + 9\operatorname{Opt}_k + \frac{1}{100} \operatorname{cost}(X, S)$$

$$\leq \frac{27}{100} \operatorname{cost}(X, S) + 673\operatorname{Opt}_k.$$

Using that $\sum_{i \in \{1,...,k\}} \operatorname{cost}(X_i^*, S) \ge 2000 \operatorname{Opt}_k$ we obtain that

$$\sum_{r \in R, r \text{ is not good}} \operatorname{cost}(X_r^*, S) \leq \frac{1213}{2000} \operatorname{cost}(X, S)$$

Now the bound follows by combining the previous inequality with $\sum_{r \in R} \operatorname{cost}(X_r^*, S) \ge 2/3 \operatorname{cost}(X, S)$.

D Further Theoretical Considerations

Our algorithms can be used to obtain an O(1)-approximation for the case where $C \not\subseteq X$, using the following argument. Given an instance A, C where $C \not\subseteq X$, consider running our algorithm on the instance A, C' where C' := A – hence looking at the metric induced by the points in A and falling back to the setting considered in our paper. This will give a solution whose centers are in A. We show that we can then transform this solution into a solution whose centers are in C without losing much in the approximation guarantee. To do this, we need to show the following two statements: (1) the cost of the optimum solution in the instance A, C' is at most O(1) times the cost of the optimum solution in the instance A, C; and (2) the cost of turning the solution for A, C'into a solution for A, C only loses a constant factor in the approximation guarantee.

(1) Take the optimum solution OPT for the instance A, C and turn it into a solution for the instance A, C' of cost at most O(1) times higher. Replace each center in Opt with the closest element in A. This yields a solution for A, C' (since C' = A). Note that by the triangle inequality, replacing each element in Opt with the closest point in A only increases the cost by a factor 4. Thus, the cost of the optimum solution for A, C' is only 4 times higher than the cost of Opt. Hence, running our algorithm on the instance A, C' yields a solution of cost O(Opt). We next show how to convert the solution obtained for A, C' to a solution for A, C.

(2) Let's now show that we can transform any α -approximate solution for the instance A, C' to a solution for A, C without losing more than a constant factor. Indeed, for each cluster S of the solution for A, C', pick the center u_S in C that is the closest to S current center c' in A'. For each cluster S, the cost obtained is by triangle inequality is at most $\sum_{s \in S} \operatorname{dist}(s, u_S) \leq \sum_{s \in S} \operatorname{dist}(s, c') + \operatorname{dist}(c', u_S) \leq \sum_{s \in S} \operatorname{dist}(s, c') + |S| \operatorname{dist}(c', u_S)$. Moreover, by the choice of u_S and the triangle inequality, we have that $\operatorname{dist}(c', u_S) \leq (1/|S|) \sum_{s \in S} \operatorname{dist}(s, c') + \operatorname{OPT}_s)$, where OPT_s is the cost of s in the optimum solution for A, C. Thus the overall cost is bounded by $\sum_{s \in S} (2\operatorname{dist}(s, c') + \operatorname{OPT}_s)$. Summing over all clusters, we have that the total cost is at most $(18\alpha + 1)$ times higher than the optimum cost for the instance A, C. Since we prove that our algorithm is an O(1)-approx, the resulting solution is an O(1)-approx too.