Fairness, Semi-Supervised Learning, and More: A General Framework for Clustering with Stochastic Pairwise Constraints

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Abstract

Metric clustering is fundamental in areas ranging from Combinatorial Optimization and Data Mining, to Machine Learning and Operations Research. However, in a variety of situations we may have additional requirements or knowledge, distinct from the underlying metric, regarding which pairs of points should be clustered together. To capture and analyze such scenarios, we introduce a novel family of stochastic pairwise constraints, which we incorporate into several essential clustering objectives (radius/median/means). Moreover, we demonstrate that these constraints can succinctly model an intriguing collection of applications, including among others Individual Fairness in clustering and Must-link constraints in semi-supervised learning. Our main result consists of a general framework that yields approximation algorithms with provable guarantees for important clustering objectives, while at the same time producing solutions that respect the stochastic pairwise constraints. Furthermore, for certain objectives we devise improved results in the case of Must-link constraints, which are also the best possible from a theoretical perspective. Finally, we present experimental evidence that validates the effectiveness of our algorithms.

1 Introduction

In a generic metric clustering problem, there is a set of points \( C \), requiring service from a set of locations \( F \), where both \( C \) and \( F \) are embedded in some metric space. The sets \( C, F \) do not need to be disjoint, and we may very well have \( C = F \). The goal is then to choose a set of locations \( S \subseteq F \), where \( S \) might have to satisfy additional problem-specific requirements and an assignment \( \phi : C \rightarrow S \), such that a metric-related objective function over \( C \) is minimized.

However, in a variety of situations there may be external and metric-independent constraints imposed on \( \phi \), regarding which pairs of points \( j, j' \in C \) should be clustered together, i.e., constraints forcing a linkage \( \phi(j) = \phi(j') \). In this work, we generalize this deterministic requirement, by introducing a novel family of stochastic pairwise constraints. Our input is augmented with multiple sets \( P_q \) of pairs of points from \( C \) (\( P_q \subseteq \binom{C}{2} \) for each \( q \)), and values \( \psi_q \in [0, 1] \). Given these, we ask for a randomized solution, which ensures that in expectation at most \( \psi_q |P_q| \) pairs of \( P_q \) are separated in the returned assignment. In Sections 1.1-1.2 we discuss how these constraints have enough expressive power to capture a wide range of applications such as extending the notion of Individual Fairness from classification to clustering, and incorporating elements of Semi-Supervised clustering.

Another constraint we address is when \( C = F \) and every chosen point \( j \in S \) must serve as an exemplar of the cluster it defines (the set of all points assigned to it). The subtle difference here, is that an exemplar point should be assigned to its own cluster, i.e., \( \phi(j) = j \) for all \( j \in S \). This constraint is highly relevant in strict classification settings, and is trivially satisfied in vanilla clustering variants where each point is always assigned to its nearest point in \( S \). However, the presence of additional requirements on \( \phi \) makes its satisfaction more challenging. Previous literature, especially in the context of fairness in clustering [Anderson et al. 2020; Esmaeili et al. 2020; Bera et al. 2019; Bercea et al. 2019], does not address this issue, but in our framework we explicitly offer the choice of whether or not to enforce it.

1.1 Formal Problem Definitions

We are given a set of points \( C \) and a set of locations \( F \), in a metric space characterized by the distance function \( d : C \cup F \times C \cup F \to \mathbb{R}_{\geq 0} \), which satisfies the triangle inequality. Moreover, the input includes a concise description of a set \( \mathcal{L} \subseteq 2^F \), that captures the allowable configurations of location openings. The goal of all problems we consider, is to find a set \( S \subseteq F \), with \( S \in \mathcal{L} \), and an efficiently-sampleable distribution \( D \) over assignments \( C \to S \), such that for a randomly drawn \( \phi \sim D \) we have: (i) an objective function being minimized, and (ii) depending on the variant at hand, further constraints are satisfied by \( \phi \). We study two types of additional constraints imposed on \( \phi \).

- **Stochastic Pairwise Constraints (SPC):** We are given a family of sets \( \mathcal{P} = \{P_1, P_2, \ldots\} \), where each \( P_q \subseteq \binom{C}{2} \) is a set of pairs of points from \( C \), and a sequence \( \psi_q = (\psi_1, \psi_2, \ldots) \) with \( \psi_q \in [0, 1] \). We then want \( \sum_{(j, j') \in P_q} \Pr_{\phi \sim D}[\phi(j) \neq \phi(j')] \leq \psi_q |P_q|, \forall P_q \in \mathcal{P} \).

- **Centroid Constraint (CC):** When this is imposed on any of our problems, we must first have \( C = F \). In addition, we should ensure that \( \Pr_{\phi \sim D}[\phi(i) = i] = 1 \) for all \( i \in S \).

**Special Cases of SPC:** When each \( P_q \in \mathcal{P} \) has \( |P_q| = 1 \), we get two interesting resulting variants.
• $\psi_q = 0, \forall q$: For each $P_q = \{ \{ j, j' \} \}$ we must ensure that $j, j'$ have $\Pr_{\phi \sim \mathcal{D}}[d(\phi(j), j) = d(\phi(j'))] = 1$, and hence we call such constraints must-link (ML). Further, since there is no actual randomness involved in these constraints, we assume w.l.o.g. that $|\mathcal{D}| = 1$, and only solve for a single $\phi: \mathcal{C} \mapsto S$ instead of a distribution over assignments.

• $\psi_q \geq 0, \forall q$: For each $P_q = \{ \{ j, j' \} \}$ we must have $\Pr_{\phi \sim \mathcal{D}}[d(\phi(j) \neq \phi(j'))] \leq \psi_q$, and therefore we call this constraint probabilistic-bounded-separation (PBS).

The objective functions we consider are:

• $\mathcal{L}$-center/$\mathcal{L}$-supplier: Here we aim for the minimum $\tau$ ("radius"), such that $\Pr_{\phi \sim \mathcal{D}}[d(\phi(j), j) \leq \tau] = 1$ for all $j \in \mathcal{C}$. Further, in the $\mathcal{L}$-center setting, we have $\mathcal{C} = \mathcal{F}$.

• $\mathcal{L}$-median ($p = 1$/ $\mathcal{L}$-means ($p = 2$)): Here the goal is to minimize $\left( \sum_{j \in \mathcal{C}} \mathbb{E}_{\phi \sim \mathcal{D}}[d(\phi(j), j)^p] \right)^{1/p}$.

There are four types of location specific constraints that we study in this paper. In the first, which we call unrestricted, $\mathcal{L} = 2^\mathcal{F}$ and hence any set of locations can serve our needs. In the second, we have $\mathcal{L} = \{ S \subseteq \mathcal{F} \mid |S| \leq k \}$ for some given positive integer $k$. This variant gives rise to the popular $k$-center/$k$-supplier/k-median/k-means objectives. In the third, we assume that each $i \in \mathcal{F}$ has an associated cost $w_i \geq 0$, and for some given $W \geq 0$ we have $\mathcal{L} = \{ S \subseteq \mathcal{F} \mid \sum_{i \in S} w_i \leq W \}$. In this case the resulting objectives are called knapsack-center/knapsack-supplier/knapsack-median/knapsack-means. Finally, if the input also consists of a matroid $\mathcal{M} = (\mathcal{F}, \mathcal{I})$, where $\mathcal{I} \subseteq 2^\mathcal{F}$ the family of independent sets of $\mathcal{M}$, we have $\mathcal{L} = \mathcal{I}$, and the objectives are called matroid-center/matroid-supplier/matroid-median/matroid-means.

To specify the problem at hand, we use the notation Objective-List of Constraints. For instance, $\mathcal{L}$-means-SPC-CC is the $\mathcal{L}$-means problem, where we additionally impose the SPC and CC constraint. We could also further specify $\mathcal{L}$, by writing for example $k$-means-SPC-CC. Moreover, observe that when no constraints on $\phi$ are imposed, we get the vanilla version of each objective, where the lack of any stochastic requirement implies that the distribution $\mathcal{D}$ once more has support of size 1, i.e., $|\mathcal{D}| = 1$, and we simply solve for just an assignment $\phi: \mathcal{C} \mapsto S$.

1.2 Motivation

In this section we present a wide variety of applications, that can be effectively modeled by our newly introduced SPCs.

Fairness: With machine-learning clustering approaches being ubiquitous in everyday decision making, a natural question that arises and has recently captured the interest of the research community, is how to avoid clusterings which perpetuate existing social biases.

The individual approach to fair classification introduced in the seminal work of (Dwork et al. 2012) assumes that we have access to an additional metric, separate from the feature space, which captures the true "similarity" between points (or some approximation of it). This similarity metric may be quite different from the feature space $d$ (e.g., due to redundant encodings of features such as race), and its ultimate purpose is to help "treat similar candidates similarly". Note now that the PBS constraint introduced earlier, can succinctly capture this notion. For two points $j, j'$, we may have $\psi_{j,j'} \in [0, 1]$ as an estimate of their true similarity (with 0 indicating absolute identity), and interpret unfair treatment as deterministically separating these two points in the final solution. Hence, a fair randomized approach would cluster $j$ and $j'$ apart with probability at most $\psi_{j,j'}$.

A recent work that explores individual fairness in clustering is (Anderson et al. 2020). Using our notation, the authors in that paper require a set $S \subseteq \mathcal{L}$, and for all $j \in \mathcal{L}$ a distribution $\phi_j$ that assigns $j$ to each $i \in S$ with probability $\phi_{i,j}$. Given that, they seek solutions that minimize the clustering objectives, while ensuring that for given pairs $j, j'$, their assignment distributions are statistically similar based on some metric $D$ that captures distributional proximity (e.g., total variation and KL-divergence). In other words, they interpret individual fairness as guaranteeing $D(\phi_{j, \cdot}, \phi_{j', \cdot}) \leq \psi_{j, j'}$ for all provided pairs $\{ j, j' \}$ and values $\psi_{j, j'}$. Although this work is interesting in terms of initiating the discussion on individual fair clustering, it has a significant modeling issue. To be more precise, suppose that for $j, j'$ the computed $\phi_{j, \cdot}, \phi_{j', \cdot}$ are both the uniform distribution over $S$. Then according to that paper’s definition a fair solution is achieved. However, the actual probability of placing $j, j'$ apart with probability at most $\psi_{j, j'}$ in different clusters (hence treating them unequally) is almost 1 if we do not consider any correlation between $\phi_{j, \cdot}$ and $\phi_{j', \cdot}$. On the other hand, our definition which instead asks for a distribution $D$ over assignments $\phi: \mathcal{C} \mapsto S$, always provides meaningful results, since it bounds the quantity that really matters, i.e., the probability of separating $j$ and $j'$ in a random $\phi \sim \mathcal{D}$.

Another closely related work in the context of individual fair clustering is (Brubach et al. 2020). The authors of that paper study a special case of PBS, where for each $j, j' \in \mathcal{C}$ we have $\psi_{j, j'} = d(j, j')/\tau^*$, with $\tau^*$ the objective value of the optimal solution. They then provide a log $k$-approximation for the $k$-center objective under the above constraints. Compared to that, our framework 1) can handle the median and means objectives as well, 2) can incorporate further requirements on the set of chosen locations (unrestricted/knapsack/matroid), 3) allows for arbitrary values for the separation probabilities $\psi_{j, j'}$, and 4) provides smaller constant-factor approximations for the objective functions.

Semi-Supervised Clustering: A common example of ML constraints is in the area of semi-supervised learning (Wagstaff et al. 2001; Basu, Davidson, and Wagstaff 2008; Zhu 2006). There we assume that pairs of points have been annotated (e.g., by human experts) with additional information about their similarity (Zhang and Yan 2007), or that some points may be explicitly labeled (Zhu, Ohramanani, and Lafferty 2003; Bilenko, Basu, and Moonen 2004), allowing pairwise relationships to be inferred. Then these extra requirements are incorporated in the algorithmic setting in the form of ML constraints. Further, our SPCs capture the scenario where the labeler generating the constraints is assumed to make some bounded number of errors (by associating each labeler with a set $P_q$ and an accuracy $\psi_q$), and also allow for multiple labelers (e.g., from crowdsourcing labels) with different accuracies. Similar settings have been studied.
by Chang et al. [2017], Luo et al. [2018] as well.

**OTU Clustering:** The field of metagenomics involves analyzing environmental samples of genetic material to explore the vast array of bacteria that cannot be analyzed through traditional culturing approaches. A common practice in the study of these microbial communities is the de novo clustering of genetic sequences (e.g., 16S rRNA marker gene sequences) into Operational Taxonomic Units (OTUs) [Edgar 2013, Westcott and Schloss 2017], that ideally correspond to clusters of closely related organisms. One of the most ubiquitous approaches to this problem involves taking a fixed radius (e.g., 97% similarity based on string alignment [Stackebrandt and Goebel 1994]) and outputting a set of center sequences, such that all points are assigned to a center within the given radius [Edgar 2013, Ghodsi, Liu, and Pop 2011]. In this case, we do not know the number of clusters a priori, but we may be able to generate pairwise constraints based on a distance/similarity threshold as in [Westcott and Schloss 2017] or reference databases of known sequences. Thus, the “unrestricted” variant of our framework is appropriate here, where the number of clusters should be discovered, but radius and pairwise information is known or estimated. Other work in this area has considered conspecific probability, a given probability that two different sequences belong to the same species (easily translated to PBS) and adverse triplets; sets of ML constraints that cannot all be satisfied simultaneously (an appropriate scenario for a set $P_q$ as defined in Section 1 [Edgar 2018]).

**Community Preservation:** There are scenarios where clustering a group/community of points together is beneficial for the coherence and quality of the final solution. Examples of this include assigning students to schools such that students living in the same neighborhood are not placed into different schools, vaccinating people with similar de-
our knowledge we are the first to tackle them purely from a Combinatorial Optimization perspective, with the exception of Davidson, Ravi, and Shamis [2010]. This paper provides a $(1 + \epsilon)$ approximation for $k$-center-ML, but only in the restricted $k = 2$ setting.

1.4 Further Related Work
Clustering problems have been a longstanding area of research in Combinatorial Optimization, with all important settings being thoroughly studied [ Hochbaum and Shmoys 1986; Gonzalez 1985; Harris et al. 2017; Byrka et al. 2017; Ahmadian et al. 2017; Chakrabarty and Nagarbham 2019].

The work that initiated the study of fairness in clustering is [Chierichetti et al. 2017]. That paper addresses a notion of demographic fairness, where points are given a certain color indicating some protected attribute, and then the goal is to compute a solution that enforces a fair representation of each color in every cluster. Further work on similar notions of demographic fairness includes [Bercea et al. 2019; Bera et al. 2019; Esmaeili et al. 2020; Huang, Jiang, and Vishnoi 2019; Backurs et al. 2019; Ahmadian et al. 2019].

Finally, a separation constraint similar to PBS is found in [Davidson, Ravi, and Shamis 2010]. In that paper however, the separation constraint is deterministic and also depends on the underlying distance between two points. Due to their stochastic nature, our PBS constraints allow room for more flexible solutions, and also capture more general separation scenarios, since the $\psi_p$ values can be arbitrarily chosen.

1.5 An LP-Rounding Subroutine
We present an important subroutine developed by Kleinberg and Tardos [2002], which we repeatedly use in our results, and call it KT-Round. Suppose we have a set of elements $V$, a set of labels $L$, and a set of pairs $E \subseteq \binom{V}{2}$. Consider the following Linear Program (LP).

\[
\sum_{v \in V} x_{i,v} = \begin{cases} 1 & \text{if } i \in L \\ 0 & \text{otherwise} \end{cases} \quad \forall v \in V \tag{1}
\]

\[
z_{e} \geq x_{i,v} - x_{l,w}, & \forall e = \{v, w\} \in E, \forall l \in L \tag{2}
\]

\[
z_{e} = \frac{1}{2} \sum_{l \in L} z_{e,l}, & \forall e = \{v, w\} \in E \tag{3}
\]

\[
0 \leq x_{i,v}, z_{e}, z_{e,l} \leq 1, & \forall v \in V, \forall e \in E, \forall l \in L \tag{5}
\]

Theorem 7. [Kleinberg and Tardos 2002] Given a feasible solution $(x, z)$ of (1)-(5), there exists a randomized rounding approach KT-Round$(V, L, E, x, z)$, which in polynomial expected time assigns each $v \in V$ to a label $\phi(v) \in L$, such that:

1. $Pr[\phi(v) \neq \phi(w)] \leq 2z_{e}, \forall e = \{v, w\} \in E$
2. $Pr[\phi(v) = l] = x_{i,v}, \forall v \in V, \forall l \in L$

2 A General Framework for Approximating Clustering Problems with SPCs
In this section we show how to achieve approximation algorithms with provable guarantees for $\mathcal{L}$-center-SPC/$\mathcal{L}$-supplier-SPC/$\mathcal{L}$-median-SPC/$\mathcal{L}$-means-SPC using a general two-step framework. At first, let $P_{c}$ denote any of the vanilla versions of the objective functions we consider, i.e., $P_{c} \in \{\mathcal{L}$-center, $\mathcal{L}$-supplier, $\mathcal{L}$-median, $\mathcal{L}$-means$\}$.

To tackle a $P_{c}$-SPC instance, we begin by using on it any known $\rho$-approximation algorithm $A_{P_{c}}$ for $P_{c}$. This gives a set of locations $S_{P_{c}}$, and an assignment $\phi_{P_{c}}$, which yield an objective function cost of $\tau_{P_{c}}$ for the corresponding $P_{c}$ instance. In other words, we drop the SPC constraints from the $P_{c}$-SPC instance, and simply treat it as its vanilla counterpart. Although $\phi_{P_{c}}$ may not satisfy the SPCs, we are going to use the set $S_{P_{c}}$ as our chosen locations. The second step in our framework would then consist of constructing the appropriate distribution over assignments. Toward that end, consider the following LP, where $P' = \cup_{p \in P} P_{p}$.

\[
\sum_{i \in S_{P_{c}}} x_{i,j} = 1 \quad \forall j \in \mathcal{C} \tag{6}
\]

\[
z_{e} \geq \min x_{i,j} - x_{i,j'}, \forall e = \{j, j'\} \in P', \forall i \in S_{P_{c}} \tag{7}
\]

\[
z_{e,i} \geq x_{i,j} - x_{i,j'}, \forall e = \{j, j'\} \in P', \forall i \in S_{P_{c}} \tag{8}
\]

\[
z_{e} = \frac{1}{2} \sum_{i \in S_{P_{c}}} z_{e,i} \quad \forall e \in P' \tag{9}
\]

\[
\sum_{i \in S_{P_{c}}} z_{e} \leq \psi_{p}|P_{p}| \quad \forall \psi_{p} \in \mathcal{P} \tag{10}
\]

\[
0 \leq x_{i,j}, z_{e}, z_{e,i} \leq 1 \quad \forall i \in S_{P_{c}}, \forall j \in \mathcal{C}, \forall e \in P' \tag{11}
\]

The variable $x_{i,j}$ can be interpreted as the probability of assigning point $j$ to location $i \in S_{P_{c}}$. To understand the meaning of the $z$ variables, it is easier to think of the integral setting, where $x_{i,j} = 1$ iff $j$ is assigned to $i$ and 0 otherwise. In this case, $z_{e,i}$ is 1 for $e = \{j, j'\}$ exactly one of $j$ and $j'$ are assigned to $i$. Thus, $z_{e,i}$ is 1 iff $j$ and $j'$ are separated. We will later show that in the fractional setting $z_{e,i}$ is a lower bound on the probability that $j$ and $j'$ are separated. Therefore, constraint (9) simply states that every point must be assigned to a center, and given the previous discussion, (10) expresses the provided SPCs.

Depending on which exact objective function we optimize, we must augment LP (1)-(11) accordingly.

- **$\mathcal{L}$-center ($\alpha = 1$)/$\mathcal{L}$-supplier ($\alpha = 2$):** Here we assume w.l.o.g. that the optimal radius $\tau^{*}_{SPC}$ of the original $P_{c}$-SPC instance is known. Observe that this value is always the distance between some point and some location, and hence there are only polynomially many alternatives for it. Thus, we execute our algorithm for each of those, and in the end keep the outcome that resulted in a feasible solution of minimum value. Given now $\tau^{*}_{SPC}$, we add the following constraint to the LP.

\[
x_{i,j} = 0, \forall i, j : d(i, j) > \tau_{P_{c}} + \alpha \cdot \tau^{*}_{SPC} \tag{12}
\]

- **$\mathcal{L}$-median ($p = 1$)/$\mathcal{L}$-means ($p = 2$):** In this case, we augment the LP with the following objective function.

\[
\min \sum_{j \in \mathcal{C}} \sum_{i \in S_{P_{c}}} x_{i,j} \cdot d(i, j)^{p} \tag{13}
\]

The second step of our framework begins by solving the appropriate LP for each variant of $P_{c}$, in order to acquire a
Algorithm 1: Approximating \( P_{L\text{-SPC}} \)

1. \((S_{P_L}, \phi_{P_L}) \leftarrow A_{P_L}(\mathcal{C}, F, L, C)\)
2. Solve LP (6)–(11) with (12) for \( L\text{-center}/L\text{-supplier} \)
   and with (13) for \( L\text{-median}/L\text{-means} \), and get a fractional solution \((\bar{x}, \bar{z})\); 
3. \( \phi \leftarrow \text{KT-Round}(\mathcal{C}, S_{P_L}, P', \bar{x}, \bar{z})\);

fractional solution \((\bar{x}, \bar{z})\) to the LP. Finally, the distribution \( \mathcal{D} \) over assignments \( \mathcal{C} \mapsto S_{P_L} \) is constructed by running KT-Round \((\mathcal{C}, S_{P_L}, P', \bar{x}, \bar{z})\). Notice that this will yield an assignment \( \phi \sim \mathcal{D} \), where \( \mathcal{D} \) results from the internal randomness of KT-Round. Our overall approach for solving \( P_{L\text{-SPC}} \) is presented in Algorithm 1.

**Theorem 8.** Let \( \tau_{SPC}^* \) the optimal value of the given \( P_{L\text{-SPC}} \) instance. Then Algorithm 1 guarantees that \( S_{P_L} \in \mathcal{C}, \sum_{(i,j) \in E} \text{Pr}_{\phi \sim \mathcal{D}}[\phi(j) \neq \phi(j') | \phi(j)] \leq 2 \sqrt{p} |P_q| \forall P_q \in \mathcal{P} \) and

1. \( P_L \) is \( L\text{-center}(\alpha = 1)/L\text{-supplier}(\alpha = 2) \): Here we get \( \text{Pr}_{\phi \sim \mathcal{D}}[\phi(j) = i'] \leq \alpha \cdot \tau_{SPC}^* + \tau_{PC} \) for all \( j \in \mathcal{C} \).
2. \( P_L \) is \( L\text{-median}(p = 1)/L\text{-means}(p = 2) \): Here we get \( \sum_{(i,j) \in E} \text{Pr}_{\phi \sim \mathcal{D}}[\phi(j) = i']^{1/p} \leq 2 \tau_{SPC}^* + \tau_{PC} \).

**Proof.** At first, notice that since \( S_{P_L} \) results from running \( A_{P_L} \), it must be the case that \( S_{P_L} \subseteq \mathcal{C} \).

Focus now on LP (6)–(11) with either (12) or (13), depending on the underlying objective. In addition, let \( S \subseteq \mathcal{C} \) and \( \mathcal{D}^* \) be the set of locations and the distribution over assignments \( \mathcal{C} \mapsto S^* \), that constitute the optimal solution of \( P_{L\text{-SPC}} \).

Given those, let \( x_{i,j} = \text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j) = i] \) for all \( i \in S^* \) and \( j \in \mathcal{C} \). Moreover, for every \( i' \in S^* \) let \( \kappa(i') = \arg \min_{i \in S_{P_L}} \text{d}(i, i') \) by breaking ties arbitrarily. Finally, for all \( i \in S_{P_L} \) we define \( N(i) = \{ i' \in S^* | i = \kappa(i') \} \), and notice that the sets \( N(i) \) form a partition of \( S^* \).

Consider now the vectors \( \hat{x}_{i,j} = \sum_{i' \in N(i)} x_{i',j} \) for every \( i \in S_{P_L} \) and \( j \in \mathcal{C} \), and \( \hat{x}_{i,j} = |\hat{x}_{i,j} - \bar{x}_{i,j}| \) for every \( e = \{j, j'\} \in P' \) and \( i \in S_{P_L} \). We first show that the above vectors constitute a feasible solution of LP (6)–(11). Initially, notice that constraints (7), (8), (9), (11) are trivially satisfied. Regarding constraint (6), for any \( j \in \mathcal{C} \) we have:

\[
\sum_{i \in S_{P_L}} \hat{x}_{i,j} = \sum_{i \in S_{P_L}} \sum_{i' \in N(i)} x_{i',j} = \sum_{i' \in S^*} x_{i',j} = 1
\]

The second equality follows because the sets \( N(i) \) induce a partition of \( S^* \). The last equality is due to the optimal solution \( D^*, S^* \) satisfying \( \sum_{i \in S} \text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j) = i] = 1 \).

To show satisfaction of constraint (10) focus on any \( e = \{j, j'\} \in P' \) and \( i \in S_{P_L} \). Then we have:

\[
\hat{z}_{e,i} = \left| \sum_{i' \in N(i)} \left( x_{i',j} - x_{i',j'} \right) \right| \leq \sum_{i' \in N(i)} |x_{i',j} - x_{i',j'}|
\]

Therefore, we can easily upper bound \( \hat{z}_{e,i} \) as follows:

\[
\hat{z}_{e,i} = \frac{1}{2} \sum_{i \in S_{P_L}} \hat{z}_{e,i} \leq \frac{1}{2} \sum_{i \in S_{P_L}} \sum_{i' \in N(i)} |x_{i',j} - x_{i',j'}|
\]

To move one, notice that:

\[
\text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j') = i'] = \sum_{i \in S^*} \text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j) = i' \land \phi(j') = i'] \leq \min_{i \in S^*} \{x_{i',j}, x_{i',j'}\} \tag{15}
\]

To relate (14) and (15) consider the following trick.

\[
\sum_{i \in S^*} \min\{x_{i',j}, x_{i',j'}\} + \frac{1}{2} \sum_{i \in S^*} |x_{i',j} - x_{i',j'}| =
\]

\[
\sum_{i \in S^*} \left( \min\{x_{i',j}, x_{i',j'}\} + \frac{|x_{i',j} - x_{i',j'}|}{2} \right) =
\]

\[
\sum_{i \in S^*} x_{i',j} + x_{i',j'} = \frac{2}{2} = 1 \tag{16}
\]

Finally, combining (14), (15), (16) we get:

\[
\hat{z}_{e,i} \leq 1 - \sum_{i \in S^*} \min\{x_{i',j}, x_{i',j'}\} \leq \text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j) \neq \phi(j')]
\]

Given the above, for every \( P_q \in \mathcal{P} \) we have:

\[
\sum_{e \in S_q} \hat{z}_{e,i} \leq \sum_{j \in \mathcal{C}} \sum_{P_q \in \mathcal{P}} \text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j) \neq \phi(j')] \leq \text{Pr}_{\phi \sim \mathcal{D}^*}[\phi(j) \neq \phi(j')]
\]

where the last inequality follows from optimality of \( \mathcal{D}^* \).

Now that we know that \( (\hat{x}, \hat{z}) \) is a feasible solution for (6)–(11), we proceed by considering how this solution affects the objective function of each underlying problem.

**L-center** (\( \alpha = 1 \))/**L-supplier** (\( \alpha = 2 \)): The objective here is captured by the additional constraint (12). Hence, we also need to show that \( \hat{x} \) satisfies (12), i.e., that for all \( i \in S_{P_L}, j \in \mathcal{C} \) for which \( d(i, j) > \tau_{PC} + \alpha \cdot \tau_{SPC} \), we have \( \hat{x}_{i,j} = 0 \).

Suppose for the sake of contradiction that there exists a \( j \in \mathcal{C} \) and an \( i \in S_{P_L} \) such that \( d(i, j) > \tau_{PC} + \alpha \cdot \tau_{SPC} \) and \( \hat{x}_{i,j} > 0 \). Since \( \hat{x}_{i,j} = \sum_{i' \in N(i)} x_{i',j} \), this implies that there exists \( i' \in N(i) \) with \( x_{i',j} > 0 \), which consecutively implies \( d(i', j) \leq \tau_{SPC}^* \) by the triangle inequality we get:

\[
d(i, j) \leq d(i, i') + d(i', j) \leq d(i, i') + \tau_{SPC}^*
\]

In **L-center**, because \( i' \in N(i) \) we also have \( d(i, i') \leq \tau_{PC} \), and so we reach a contradiction. In **L-supplier** we have:

\[
d(i, i') \leq d(i', \phi_{PC}(j)) \leq d(i', j) + d(\phi_{PC}(j), j) \leq \tau_{SPC}^* + \tau_{PC}
\]

Combining (17), (18) gives the desired contradiction for the case of **L-supplier** as well.

**L-median** (\( p = 1 \))/**L-means** (\( p = 2 \)): Here the overall objective function for \( \hat{x} \) is given by:

\[
\left( \sum_{j \in \mathcal{C}} \sum_{i \in S_{P_L}} \hat{x}_{i,j} d(i, j)^p \right)^{\frac{1}{p}} =
\]

\[
\left( \sum_{j \in \mathcal{C}} \sum_{i \in S_{P_L}} \sum_{i' \in N(i)} x_{i',j} d(i, j)^p \right)^{\frac{1}{p}} \tag{19}
\]
In addition, for \( i' \in N(i) \) we also get:
\[
d(i, j) \leq d(i, i') + d(i', j) \leq d(i', \phi_{P_L}(j)) + d(i', j) \\
\leq 2d(i', j) + d(\phi_{P_L}(j), j)
\]
Combining (19), (20) and the fact that the median and means objectives are monotone norms, we get (19) \( \leq A + B \), where:
\[
A = \left( \sum_{j \in C} \sum_{i' \in S_{P_L}} \sum_{i \in N(i)} 2x_{i', j}^* d(i', j)^p \right)^{\frac{1}{p}} \\
= 2 \left( \sum_{j \in C} \sum_{i' \in S_{\phi}} \sum_{i \in N(i)} x_{i', j}^* d(i', j)^p \right)^{\frac{1}{p}} \leq 2 \tau_{S_{\phi}}^2
\]
\[
B = \left( \sum_{j \in C} \sum_{i' \in S_{P_L}} \sum_{i \in N(i)} \sum_{i' \in S_{\phi}} x_{i', j}^* \sum_{i' \in S_{\phi}} d(\phi_{P_L}(j), i)^p \right)^{\frac{1}{p}} \\
= \left( \sum_{j \in C} \sum_{i' \in S_{\phi}} d(\phi_{P_L}(j), i)^p \sum_{i' \in S_{\phi}} \sum_{i' \in S_{\phi}} x_{i', j}^* \right)^{\frac{1}{p}} \\
= \left( \sum_{j \in C} \sum_{i' \in S_{\phi}} d(\phi_{P_L}(j), i)^p \right)^{\frac{1}{p}} = \tau_{P_L}
\]
Combining (21), (22) we finally get (19) \( \leq 2 \tau_{S_{\phi}}^2 + \tau_{P_L} \).
Since \((\bar{x}, \bar{z})\) is a feasible solution to the appropriate version of the assignment LP, step 2 of Algorithm 1 is well-defined, and thus can compute a solution \((\bar{x}, \bar{z})\) that satisfies (6)-(11) and additionally: i)
\[
\bar{x}_{i,j} = 0, \quad \forall i,j : d(i,j) > \tau_{P_L} + \alpha \cdot \tau_{S_{\phi}}^2
\]
for \( L\text{-center}(\alpha = 1)/L\text{-supplier}(\alpha = 2) \), and ii)
\[
\left( \sum_{j \in C} \sum_{i' \in S_{P_L}} \bar{x}_{i,j} d(i,j)^p \right)^{\frac{1}{p}} \leq \left( \sum_{j \in C} \sum_{i' \in S_{P_L}} \bar{x}_{i,j} d(i,j)^p \right)^{\frac{1}{p}} \leq 2 \tau_{S_{\phi}} + \tau_{P_L}
\]
for \( L\text{-median}(p = 1)/L\text{-means}(p = 2) \).

Since \((\bar{x}, \bar{z})\) satisfies (6)-(11) and the second property of Theorem 7, we know that a point \( \bar{z} \in C \) will never be assigned to a location \( i \in S_{P_L} \), such that \( d(i,j) > \tau_{P_L} + \alpha \cdot \tau_{S_{\phi}}^2 \). Therefore, \( \Pr_{\phi \sim D}[d(\phi(j) \neq \phi(j'))] \leq 2\bar{z}_{e_c} \), \( \forall e_c = (j,j') \in P' \). Hence, for every \( P_q \in P' \):
\[
\sum_{(j,j') \in P_q} \Pr_{\phi \sim D}[d(\phi(j) \neq \phi(j'))] \leq 2 \bar{z}_{e_c} \leq 2 \psi_q|P_q|
\]
The last inequality is due to \( \bar{z} \) satisfying (10).

Regarding all the different objective functions, we have the following. For \( L\text{-center}(\alpha = 1)/L\text{-supplier}(\alpha = 2) \), because of (23) and the second property of Theorem 7, we know that a point \( \bar{z} \in C \) will never be assigned to a location \( i \in S_{P_L} \), such that \( d(i,j) > \tau_{P_L} + \alpha \cdot \tau_{S_{\phi}}^2 \). Therefore, \( \Pr_{\phi \sim D}[d(\phi(j) \neq \phi(j'))] \leq 2 \tau_{P_L} + \alpha \cdot \tau_{S_{\phi}}^2 \) for all \( j \in C \). As for the \( L\text{-median}(p = 1)/L\text{-means}(p = 2) \) objectives, the second property of Theorem 7 ensures:
\[
\left( \sum_{j \in C} d(\phi(j), j)^p \right)^{\frac{1}{p}} = \left( \sum_{j \in C} d(\phi(j), j)^p \right)^{\frac{1}{p}} \leq 2 \tau_{S_{\phi}} + \tau_{P_L}
\]
where the last inequality follows from (24).

Since \( P_L \) is a less restricted version of \( P_{C-S}\), the optimal solution value \( \tau_{P_L} \) for \( P_L \) in the original instance where we dropped the SPCs, should satisfy \( \tau_{P_L} \leq \tau_{S_{\phi}} \). Therefore, because \( A_{P_L} \) is a \( \rho \)-approximation algorithm for \( P_L \), we get \( \tau_{P_L} \leq \rho \cdot \tau_{S_{\phi}} \). The latter implies the following.

**Corollary 9.** The approximation ratio achieved through Algorithm 1 is \((\rho + 1)\) for \( L\text{-center}-SPC \), and \( (\rho + 2) \) for \( L\text{-supplier}-SPC/L\text{-median}-SPC/L\text{-means}-SPC \).

**Tighter analysis for the unrestricted \((C = 2^F)\) case:** For this case, a more careful analysis leads to the following.

**Theorem 10.** When \( L = 2^F \), Algorithm 1 achieves an objective value of at most \( \tau_{S_{\phi}}^* \) for all objectives we study (center/supplier/median/means).

**Proof.** Note that the first step of our framework will choose \( S_{P_L} = F \), and hence \( \tau_{P_L} = 0 \). In addition, a closer examination of our analysis for the supplier/median/means settings reveals the following. Focus on (17) and (20), and note that because \( S_{P_L} = F \), we get \( d(i,i') = 0 \) for each \( i' \in S^\phi \). Hence, \( d(i,j) \leq d(i', j) \) which leads to an objective function value of at most \( \tau_{S_{\phi}}^* \) for all problems.

### 3 Addressing the Centroid Constraint

In this section we present results that incorporate the Centroid Constraint (CC) to a variety of the settings we study. Moreover, recall that for this case \( C = F \), and hence the supplier objective reduces to the center one.

#### 3.1 Approximating \( k \)-center-SPC-CC

Our approach for solving this problem heavily relies on Algorithm 1 with two major differences.

The first difference compared to Algorithm 1 lies in the assignment algorithm \( A_k \) used to tackle \( k \)-center. For \( k \)-center there exists a 2-approximation which gives a target radius \( \tau \), it either returns a solution where each \( j \in C \) gets assigned to a location \( i \in S_{P_L} \) with \( d(i,j) \leq 2\tau \), or outputs an "infeasible" message, indicating that there exists no solution of radius \( \tau \) \((Hochbaum and Shmoys 1986)\).

Recall now that w.l.o.g. the optimal radius \( \tau_{C}^* \) for the \( k \)-center-SPC-CC instance is known. In the first step of our framework we will use the variant of \( A_k \) mentioned earlier with \( \tau_{C}^* \) as its target radius, and get a set of chosen locations...
Algorithm 2: Approximating $k$-center-SPC-CC
1 $(S_k, \phi_k) \leftarrow A_k(C, F, L, \tau^*_C)$;
2 Solve LP (6)-(1) with (12), (15) and $S_k$ as the chosen locations, and get a solution $(\bar{x}, \bar{z})$;
3 $\phi \leftarrow KT$-Round$(C, S_k, P', \bar{x}, \bar{z})$;

$S_k$. The second step is then the same as in Algorithm 1 with the addition of the next constraint to the assignment LP:

$$x_{i,i} = 1, \forall i \in S_k$$

(25)

The overall process is presented in Algorithm 2.

Theorem 11. Let $\tau^*_C$ be the optimal value of the given $k$-center-SPC-CC instance and $D$ the distribution over assignments given by KT-Round. Then Algorithm 2 guarantees $|S_k| \leq k, \sum_{(i,j') \in P} Pr_{\phi \rightarrow D}[\phi(j) \neq \phi(j')] \leq 2\psi_D |P_q| \forall P_q \in P$, and $Pr_{\phi \rightarrow D}[d(\phi(i),j) \leq 3\tau^*_C] = 1$ for all $j \in C$, and $Pr_{\phi \rightarrow D}[\phi(i) = i] = 1$ for all $i \in S_k$.

Proof. At first, notice that since $S_k$ results from running $A_k$, it must be the case that $|S_k| \leq k$.

Furthermore, because the optimal value of the $k$-center instance is less than $\tau^*_C$, $A_k(C, F, L, \tau^*_C)$ will not return “infeasible”, and $(S_k, \phi_k)$ has an objective value $\tau_k \leq 2\tau^*_C$.

Given this, the reasoning in the proof of Theorem 10 yields $\sum_{(i,j') \in P} Pr_{\phi \rightarrow D}[\phi(j) \neq \phi(j')] \leq 2\psi_D |P_q| \forall P_q \in P$, and $Pr_{\phi \rightarrow D}[d(\phi(i),j) \leq 3\tau^*_C] = 1$ for all $j \in C$, if the $\bar{x}$ defined in that proof also satisfies (25). Hence, the latter statement regarding $\bar{x}$ is all we need to verify.

A crucial property of $A_k$ when executed with a target radius $\tau^*_C$, is that for all $i, \ell \in S_k$ with $i \neq \ell$ we have $d(i, \ell) > 2\tau^*_C$ (Hochbaum and Shmoys, 1986). Due to this, for all $i \in S_k$ and $i' \in S^*$ with $d(i, i') \leq \tau^*_C$, we have $i' \in N(i)$. Suppose otherwise, and let $i' \in N(\ell)$ for some other $\ell \in S_k$. By definition this gives $d(i, \ell) \leq d(i, i') \leq \tau^*_C$. Thus, $d(i, \ell) \leq d(i, i') + d(i', \ell) \leq 2\tau^*_C$. Finally, note that due to $\tau^*_C$, being the optimal value of $k$-center-SPC-CC, we have $\sum_{i' \in S^*} d(i, i') \leq \tau^*_C x_{i,i} = 1$ for all $i \in S_k$. Since $\{i' \in S^* : d(i, i') \leq \tau^*_C\} \subseteq N(i)$, we finally get $x_{i,i} = 1$.

To conclude, we show that $Pr_{\phi \rightarrow D}[\phi(i) = i] = 1$ for every $i \in S_k$. However, this is obvious, because of the second property of Theorem 10 and $\bar{x}$ satisfying (6), (25). $\square$

3.2 A Reassignment Step for the Unrestricted and $k$-Constrained Location Setting

We now demonstrate a reassignment procedure that can be used to correct the output of Algorithm 1 in a way that satisfies the CC. Again, let $P_L$ be any of the vanilla objective functions, and consider Algorithm 3.

Algorithm 3: Approximating $P_L$-SPC-CC
1 Run Algorithm 1 to solve $P_L$-SPC, and get $S \subseteq C$ and an assignment $\phi : C \rightarrow S$ in return;
2 while there exists $i \in S$ with $\phi(i) \neq i$ do
3 $S \leftarrow S \setminus \{i\}$;
4 $i' \leftarrow \arg \min_{j \in C, \phi(j) = i} d(i, j)$;
5 $S \leftarrow S \cup \{i'\}$;
6 for all $j \in C$ with $\phi(j) = i$ do
7 $\phi(j) \leftarrow i'$;

Proof. To show that Algorithm 3 preserves the SPC guarantees, it suffices to prove that the following invariant is maintained throughout the reassignment. For any $j, j'$ that are assigned by Algorithm 1 to the same location, at the end of the while loop we should still have $\phi(j) = \phi(j')$. Suppose now that we initially had $\phi(j) = \phi(j') = i$. If $\phi(i) = i$, then no change will occur, and in the end we still have $\phi(j) = \phi(j') = i$. If on the other hand $\phi(i) \neq i$, we choose an $i' \in \{j' \in C : \phi(j') = i\}$ and then set $\phi(j) = \phi(j') = i'$. Note that this assignment will not change, since the modification also ensures $\phi(i') = i'$. The latter also guarantees that CC holds at termination.

Moreover, notice that when $L = \{S' \subseteq C : |S'| \leq k\}$, the cardinality constraint is not violated. The reason for this is that every time we possibly add a new location to $S$, we have already removed another one from there.

Finally, we need to reason about the approximation ratio of Algorithm 3. At first, let $i$ the location to which $j \in C$ was assigned to by Algorithm 1. As we have already described, $j$ can only be reassigned once, and let $i'$ be its new assignment. Then $d(i', j) \leq d(i, i') + d(i, j) \leq 2d(i, j)$, where the second inequality follows because $i' = \arg \min_{j' \in C, \phi(j') = i} d(i, j')$. Hence, we see that the covering distance for every point at most doubles, and since the optimal value of $P_L$-SPC-CC is not larger than that of $P_L$-SPC-CC, we get an approximation ratio of $2\lambda$ for $P_L$-SPC-CC. Notice that this holds regardless of the specific objective). $\square$

4 Improved Results for Problems with Must-Link Constraints

Since must-link constraints (ML) are a special case of SPCs, Algorithm 1 provides approximation results for the former as well (also note that due to $\psi_D = 0 \forall p$, we have no pairwise constraint violation when using Algorithm 1 purely for ML). However, in this section we demonstrate how we can get improved approximation guarantees for some of the problems we consider. Specifically, we provide a $2/3/3/3$-approximation for $k$-center-ML/knapsack-center-ML/k-supplier-ML/knapsack-supplier-ML, which constitutes a clear improvement over the $3/4/5/5$-approximation, given when Algorithm 1 is executed using the best approximation algorithm for the corresponding vanilla variant.

First of all, recall that in the ML case we are only looking for a set of locations $S$ and an assignment $\phi : C \rightarrow S$, and not for a distribution over assignments. Also, notice that the
Algorithm 4: Approximating ML Constraints

1. \( C \leftarrow \emptyset, S \leftarrow \emptyset \);
2. Initially all \( C_1, C_2, \ldots, C_t \) are considered uncovered;
3. while there exists an uncovered \( C_q \) do
   4. Pick an uncovered \( C_q \);
   5. Pick an arbitrary point \( j_q \in C_q \);
   6. \( C \leftarrow C \cup \{ j_q \} \);
   7. \( C_q \) and all neighboring cliques \( C_p \) of it, are now considered covered;
8. for all \( j_q \in C \) do
   9. if k-center/k-supplier then
      10. \( i_q \leftarrow \arg \min_{i \in F} d(i, j_q) \);
      11. \( S \leftarrow S \cup \{ i_q \} \);
   12. if knapsack-center/knapsack-supplier then
      13. \( i_q \leftarrow \arg \min_{i \in F, d(i, j_q) \leq \tau^*} w_i \);
      14. \( S \leftarrow S \cup \{ i_q \} \);
15. for all \( j \in C \) do
16. \( \phi(j) \leftarrow i_q \);

must-link relation is transitive. If for \( j, j' \) we want \( \phi(j) = \phi(j') \), and for \( j', j'' \) we also require \( \phi(j') = \phi(j'') \), then \( \phi(j) = \phi(j'') \) is necessary as well. Given that, we view the input as a partition \( C_1, C_2, \ldots, C_t \) of the points of \( C \), where all points in \( C_q \), with \( q \in \{1, \ldots, t\} \), must be assigned to the same location of \( S \). We call each part \( C_i \) of this partition a clique. Finally, for the problems we study, we can once more assume w.l.o.g. that the optimal radius \( \tau^* \) is known.

**Definition 13.** Two cliques \( C_q, C_p \) are called neighboring if \( \forall j \in C_q, \forall j' \in C_p \) we have \( d(j, j') \leq 2\tau^* \).

Algorithm 4 captures k-center-ML, knapsack-center-ML, k-supplier-ML and knapsack-supplier-ML at once, yielding improved approximations for each of them.

**Theorem 14.** Algorithm 4 is a 2/3/3/3-approximation algorithm for k-center-ML/knapsack-center-ML/k-supplier-ML/knapsack-supplier-ML.

**Proof.** Initially, observe that the must-link constraints are satisfied. When the algorithm chooses a location \( i_q \) based on some \( j_q \in C_q \), all the points in \( C_q \) are assigned to \( i_q \). Also, for the neighboring cliques of \( C_q \) that got covered by it, their whole set of points ends up assigned to \( i_q \) as well.

We now argue about the achieved approximation ratio. For one thing, it is clear that for every \( j, j' \in C_q \) we must have \( d(j, j') \leq 2\tau^* \), and therefore \( C_q \) is a neighboring clique of itself. We thus have the following two cases:

- **k-center-ML:** Here for each \( j_q \in C_q \), we end up placing \( j_q \) in \( S \) as well. Also, all points \( j \) assigned to \( j_q \) belong to neighboring cliques of \( C_q \), and therefore \( d(j, j_q) \leq 2\tau^* \).

- **In all other problems:** for each \( j_q \in C_q \) we choose a location \( i_q \) such that \( d(i_q, j_q) \leq \tau^* \). Also, all points \( j \) assigned to \( i_q \) belong to neighboring cliques of \( C_q \), and therefore \( d(i_q, j) \leq d(i_q, j_q) + d(j_q, j) \leq 3\tau^* \).

Finally, we need to show that either the cardinality or the knapsack constraint on the set of chosen locations is satisfied. Toward that end, notice that if \( C_q \) and \( C_p \), belong in the same cluster in the optimal solution, then they are neighboring. Say \( i^* \) is the location they are both assigned to. Then for all \( j \in C_q \) and \( j' \in C_p \) we get \( d(j, i^*) \leq \tau^* \) and \( d(j', i^*) \leq \tau^* \). Hence, by the triangle inequality for all \( j \in C_q \) and \( j' \in C_p \) we have \( d(j, j') \leq 2\tau^* \).

Given the previous observation, it must be the case that for every \( j_q \in C_q \), the optimal solution assigns it to a location \( i_q^* \), such that for every other \( j_q \in C \) we have \( i_q^* \neq i_q^* \).

Therefore, in the presence of a cardinality constraint:

\[
|S| \leq |C| = \sum_{i_q^* \in C} 1 \leq k
\]

and in the presence of a knapsack constraint:

\[
\sum_{i \in S} w_i \leq \sum_{j \in C} \min_{i \in F, d(i, j) \leq \tau^*} w_i \leq \sum_{j \in C} w_{i_q^*} \leq W
\]

where the last inequality in both cases follows from the optimal solution satisfying the corresponding constraint.

**Observation 15.** Algorithm 4 is a 2/3-approximation for k-center-ML-CC/knapsack-center-ML-CC. This directly follows from steps 10, 13 and 17 of it.

**Observation 16.** Due to known hardness results for the vanilla version of the corresponding problems ([Hochbaum and Shmoys 1986](#hochbaum1986)), Algorithm 4 gives the best possible approximation ratios, assuming that \( P \neq NP \).

## 5 Experimental Evaluation

We implement our algorithms in Python 3.8 and run our experiments on AMD Opteron 6272 @ 2.1 GHz with 64 cores and 512 GB 1333 MHz DDR3 memory. We focus on fair clustering applications with PBS constraints and
evaluate against the most similar prior work. Comparing to (Anderson et al. 2020) using $k$-means-PBS, shows that our algorithm violates fewer constraints while achieving a comparable cost of fairness. Similarly, our comparison with (Brubach et al. 2020) using $k$-center-PBS-CC (that prior algorithm also satisfies the CC constraint) reveals that we are better able to balance fairness constraints and the objective value. Our code is publicly available at https://github.com/chakrabarti/pairwise_constrained_clustering.

Datasets: We use 3 datasets from the UCI ML Repository (Dua and Graff 2017): (1) Bank-4,521 points (Moro, Cortez, and Rita 2014), (2) Adult-32,561 points (Kohavi 1996), and (3) Creditcard-30,000 points (Yeh and Lien 2009).

Algorithms: In all of our experiments, $C = \mathcal{F}$ at first. When solving $k$-means-PBS, we use Lloyd’s algorithm in the first step of Algorithm 1 and get a set of points $L$. The set of chosen locations $S$ is constructed by getting the nearest point in $C$ for every point of $L$. This is exactly the approach used in (Anderson et al. 2020), where their overall algorithm is called ALG-IF. To compare Algorithm 1 to ALG-IF, we use independent sampling for ALG-IF, in order to fix the assignment of each $j \in C$ to some $i \in S$, based on the distribution $\phi_i$ produced by ALG-IF. For $k$-center-PBS-CC, we use Algorithm 2 with a binary search to compute $t^*_\phi$.

Fairness Constraints: We consider three similarity metrics ($F_1, F_2, F_3$) for generating PBS constraints. We use $F_1$ for $k$-center-PBS-CC and $F_2, F_3$ for $k$-means-PBS. $F_1$ is the metric used for fairness in the simulations of (Brubach et al. 2020) and $F_2, F_3$ are the metrics used in the experimental evaluation of the algorithms in (Anderson et al. 2020).

$F_1$ involves setting the separation probability between a pair of points $j$ and $j'$ to $d(j,j')/R_{Scr}$, where $R_{Scr}$ is the radius given by running the Scr algorithm (Mihelic and Robic 2005) on the provided input.

$F_2$ is defined so that the separation probability between a pair $j,j'$ is given by $d(j,j')$, scaled linearly to ensure all such probabilities are in $[0, 1]$. Adopting the approach taken by (Anderson et al. 2020) when using this metric, we only consider pairwise constraints between each $j$ and its closest $m$ neighbors. For our experiments, we set $m = 100$.

Again in order to compare our Algorithm 1 with (Anderson et al. 2020), we need the metric $F_3$. For any $j \in C$, let $r_j$ the minimum distance such that $|j' \in C : d(j,j') \leq r_j| \geq |C|/k$. Then the separation probability between $j$ and any $j'$ such that $d(j,j') \leq r_j$ is set to $d(j,j')/r_j$.

Implementation Details: As performed in (Anderson et al. 2020) and (Brubach et al. 2020), we uniformly sample $N$ points from each dataset and run all algorithms on those sets, while only considering a subset of the numerical attributes and normalizing the features to have zero mean and unit variance. In our comparisons with (Anderson et al. 2020) we use $N = 1000$, while in our comparisons with (Brubach et al. 2020) $N$ is set to 250. For the number of clusters $k$, we study the values $\{4, 6, 8, 10\}$ when comparing to (Anderson et al. 2020), and $\{10, 20, 30, 40, 50, 60\}$ when comparing to (Brubach et al. 2020). Theoretical Algorithm 1 is better for larger $k$.

Finally, to estimate the empirical separation probabilities and the underlying objective function cost, we run 5000 trials for each randomized assignment procedure, and then compute averages for the necessary performance measures we are interested in.

Comparison with (Anderson et al. 2020): In Tables 1 and 2 we show what percentage of fairness constraints are violated by ALG-IF and our algorithm, for the fairness constraints induced by $F_2$ and $F_3$, allowing for an $\epsilon = 0.05$ threshold on the violation of a separation probability bound;
we only consider a pair’s fairness constraint to be violated if the empirical probability of them being separated exceeds that set by the fairness metric by more than $\epsilon$. It is clear that our algorithm outperforms ALG-IF consistently across different values of $k$, different datasets, and both types of fairness constraints considered by (Anderson et al. 2021).

In order to compare the objective value achieved by both algorithms, we first compute the average connection costs over the 5000 runs. Since the cost of the clustering returned by Lloyd’s algorithm contributes to both Algorithm 1 and ALG-IF, we utilize that as an approximation of the cost of fairness. In other words, we divide the objective value of the final solutions by the cost of the clustering produced by Lloyd, and call this quantity cost of fairness. The corresponding comparisons are presented in Tables 2-4. The cost of fairness for both algorithms is very similar, demonstrating a clear advantage of Algorithm 1 since it dominates ALG-IF in the percentage of fairness constraints violated.

Comparison with (Brubach et al. 2020): In Table 5 we show what percentage of fairness constraints are violated by the algorithm of (Brubach et al. 2020) (named Alg-F) and Algorithm 2 using an $\epsilon = 0$; if the empirical probability of separation of a pair exceeds the bound set by the fairness metric by any amount, it is considered a violation. We run ALG-F with two different choices of the scale parameter used in that prior work: $\frac{1}{2}\Scr_{cr}$ (Alg-F(A)) and $\frac{1}{2}\Scr_{cr}$ (Alg-F(B)), where $\Scr_{cr}$ is the value achieved using the $\Scr$ algorithm. The reason for doing so is that (Brubach et al. 2020) consider multiple values for the separation probabilities, and we wanted to have a more clear comparison of our results against all of those. Alg-F(A) leads to 0 violations, while our algorithm produces a small number of violations in a few cases, and Alg-F(B) leads to a significant number of violations. In Table 6 we show the cost of the clusterings produced by ALG-F and Algorithm 2 measured in the normalized metric space by taking the average of the maximum radius of any cluster over the 5000 runs. Alg-F(b) leads to the lowest objective, followed relatively closely by our algorithm, and then finally Alg-F(A) has significantly higher objective values.

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Ethics Statement

Our primary contribution is general and theoretical in nature, so we do not foresee any immediate and direct negative ethical impacts of our work. That said, one use case of our framework—that we highlight prominently both in the general discussion of theoretical results as well as through experimental results performed on standard and commonly-used datasets—is as a tool to operationalize notions of fairness in a broad range of clustering settings. Formalization of fairness as a mathematical concept, while often grounded in legal doctrine (see, e.g., Feldman et al. 2015, Barocas, Hardt, and Narayanan 2019), is still a morally laden and complicated process, and one to which there is no one-size-fits-all “correct” approach.

Our method supports a number of commonly-used fairness definitions; thus, were tools built based on our framework that operationalized those definitions of fairness, then the ethical implications—both positive and negative—of that decision would also be present. Our framework provides strong theoretical guarantees that would allow decision-makers to better understand the performance of systems built based on our approach. Yet, we also note that any such guarantees should, in many domains, be part of a larger conversation with stakeholders—one including understanding the level of comprehension (e.g., Saha et al. 2020, Saxena et al. 2020) and specific wants of stakeholders (e.g., Holstein et al. 2019, Madaio et al. 2020).

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A Omitted Details

Proof of Theorem 3

Proof. Our reduction is based on the $k$-cut problem, in which we are given an undirected graph $G(V, E)$, $k$ distinct nodes $u_1, u_2, \ldots, u_k \in V$ and a $\gamma \in \mathbb{N}_{\geq 0}$. Then we want to know whether or not there exists a cut $S \subseteq E$ with $|S| \leq \gamma$, such that in $G(V, E \setminus S)$ the nodes $u_1, u_2, \ldots, u_k$ are separated (each of them is placed in a different connected component).

Supplier/Median/Means: We now describe the construction of an instance for the clustering problem. For each of the $k$ distinct nodes $u_f$, we create a location $i_{uf}$, and for every two different locations $i_{uf}, i_{uj}$, we set $d(i_{uf}, i_{uj}) = 2$. Then, again for each of the $k$ distinct nodes $u_f$ we create a point $j_{uf}$, that is co-located with $i_{uf}$. In addition, for each of the $|V| - k$ remaining nodes $u$ of the graph we create a point $j_u$, such that $d(i_{uf}, j_u) = 1$ for every previously created location $i_{uf}$, and all those new points are co-located. This construction constitutes a valid metric space. As for the stochastic pairwise constraints, we only have one connected component in $G$. Moreover, each separated pair of all locations $i$ will be upper bounded by $\sqrt{|V| - k}$.

We now claim that the clustering problem has a solution of objective value at most $\frac{1}{|V| - k}/\sqrt{|V| - k}$ in the constructed instance for supplier/median/means iff there exists a $k$-cut of size at most $\gamma$ in $G(V, E)$. Before we proceed, notice that this claim for the median and means objectives implies that there is no actual randomness in the assignment cost. This is true because $|V| - k$, $\sqrt{|V| - k}$ are the least possible values for the corresponding objectives, resulting deterministically from the assignment of the $|V| - k$ points that do not correspond to nodes that need to be separated.

Therefore, suppose at first that there exists a $k$-cut $S$ of size at most $\gamma$. We construct a clustering solution as follows. Open all locations $i_{uf}$ of the instance. Then for each $u \in V$ with corresponding point $j_u$, assign $j_u$ to $i_{uf}$, such that $u$ is in the same connected component in $G(V, E \setminus S)$ as $u_f$. This clearly achieves deterministically the desired objective value cost for each case. Moreover, each separated pair of $P$ corresponds to an edge of $S$, and hence in the end the number of separations in this clustering solution will be upper bounded by $|S| \leq \gamma$.

On the other hand, assume that there exists a solution to the clustering instance of cost at most $\frac{1}{|V| - k}/\sqrt{|V| - k}$. This immediately implies that all available locations are opened. Furthermore, since on expectation at most $\gamma$ pairs are separated, there must be an assignment $\phi$ that separates less than $\gamma$. Given this assignment, we construct a $k$-cut as follows. Remove from $E$ all edges $\{u, v\}$ such that the corresponding points $j_u, j_v$ have $\phi(j_u) \neq \phi(j_v)$. This clearly removes at most $\gamma$ edges from $E$.

To see that two of the special nodes $u_f, u_f'$ will be separated after the above edge removal, note that their respective points in the metric space are assigned to different clusters. Also, the corresponding node of each point in a cluster cannot have an edge to the corresponding node of a point in a different cluster, and hence $u_f, u_f'$ are definitely in distinct connected components.

Center: To handle this objective function, we use an instance similar to that constructed for the supplier objective, with just one difference. This difference will make sure that we can only open locations that correspond to points coinciding with the locations used earlier. So in the previous instance, for each $j_{uf}$ corresponding to a special node $u_f$ we create another point $h_{uf}$, such that $d(j_{uf}, h_{uf}) = 1$, $d(j_u, h_{uf}) = 2$ for all $j_u \neq j_{uf}$ with $j_u$ resulting from some $u \in V$, and $d(h_{uf}, h_{uf'}) = 2$ for every $h_{uf'}$ resulting from $u_f' \neq u_f$. Then, the arguments for the supplier case go through in the exact same manner, since the only locations that can be considered for opening when aiming for a solution of radius 1, are the points $j_{uf}$.