Clustering with Diversity

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Abstract

We consider the clustering with diversity problem: given a set of colored points in a metric space, partition them into clusters such that each cluster has at least $\ell$ points, all of which have distinct colors. We give a 2-approximation to this problem for any $\ell$ when the objective is to minimize the maximum radius of any cluster. We show that the approximation ratio is optimal unless $P=NP$, by providing a matching lower bound. Several extensions to our algorithm have also been developed for handling outliers. This problem is mainly motivated by applications in privacy-preserving data publication.

Keywords: Approximation algorithm, k-center, k-anonymity, l-diversity

1 Introduction

Clustering is a fundamental problem with a long history and a rich collection of results. A general clustering problem can be formulated as follows. Given a set of points $P$ in a metric space, partition $P$ into a set of disjoint clusters such that a certain objective function is minimized, subject to some cluster-level and/or instance-level constraints. Typically, cluster-level constraints impose restrictions on the number of clusters or on the size of each cluster. The former corresponds to the classical $k$-center, $k$-median, $k$-means problems, while the latter has recently received much attention from various research communities \cite{17,1,16}. On the other hand, instance-level constraints specify whether particular items are similar or dissimilar, usually based on some background knowledge \cite{26,3}. In this paper, we impose a natural instance-level constraint on a clustering problem, that the points are colored and all points partitioned into one cluster must have distinct colors. We call such a problem clustering with diversity. Note that the traditional clustering problem is a special case of ours where all points have unique colors.

As an illustrating example, consider the problem of choosing locations for a number of factories in an area where different resources are scattered. Each factory needs at least $\ell$ different resources allocated to it and the resource in one location can be sent to only one factory. This problem corresponds to our clustering problem where each kind of resource has a distinct color, and we have a lower bound $\ell$ on the the cluster size.
The main motivation to study clustering with diversity is privacy preservation for data publication, which has drawn tremendous attention in recent years in both the database community [24, 8, 29, 21, 28, 7, 30] and the theory community [1, 22, 2, 12, 11]. The goal of all the studies in privacy preservation is to prevent linking attacks [25]. Consider the table of patient records in Figure 1(a), usually called the microdata. There are three types of attributes in a microdata table. The sensitive attribute (SA), such as “Disease”, is regarded as the individuals’ privacy, and is the target of protection. The identifier, in this case “Name”, uniquely identifies a record, hence must be ripped off before publishing the data. The rest of the attributes, such as “Age”, “Gender”, and “Education”, should be published so that researchers can apply data mining techniques to study the correlation between these attributes and “Disease”. However, since these attributes are public knowledge, they can often uniquely identify individuals when combined together. For example, if an attacker knows (i) the age (25), gender (M), and education level (Master) of Bob, and (ii) Bob has a record in the microdata, s/he easily finds out that Tuple 2 is Bob’s record and hence, Bob contracted HIV. Therefore, these attributes are often referred to as the quasi-identifiers (QI). The solution is thus to make these QIs ambiguous before publishing the data so that it is difficult for an attacker to link an individual from the QIs to his/her SA, but at the same time we want to minimize the amount of information loss due to the ambiguity introduced to the QIs so that the interesting correlations between the QIs and the SA are still preserved.

The usual approach taken to prevent linking attacks is to partition the tuples into a number of QI-groups, namely clusters, and within each cluster all the tuples share the same (ambiguous) QIs. There are various ways to introduce ambiguity. A popular approach, as taken by [1], is to treat each tuple as a high-dimensional point in the QI-space, and then only publish the center, the radius, and the number of points of each cluster. To ensure a certain level of privacy, each cluster is required to have at least k points so that the attacker is not able to correctly identify an individual with confidence larger than 1/k. This requirement is referred to as the k-ANONYMITY principle [1, 22]. The problem, translated to a clustering problem, can be phrased as follows: Cluster a set of points in a metric space, such that each cluster has at least r points. When the objective is to minimize the maximum radius of all clusters, the problem is called r-GATHERING and a 2-approximation is known [1].

However, the k-ANONYMITY principle suffers from the homogeneity problem: A cluster may have too many tuples with the same SA value. For example, in Figure 1(b), all tuples in QI-group 1, 3, and 4 respectively have the the same disease. Thus, the attacker can infer what disease all the people within a QI-group have contracted without identifying any individual record. The above problem has led to the development of many SA-aware principles. Among them, ℓ-DIVERSITY [21] is the most widely deployed [14, 21, 18, 29, 28, 8], due to its simplicity and good privacy guarantee. The principle demands that, in each cluster, at most 1/ℓ of its tuples can have the same SA value. Figure 1(c) shows a 2-diverse version of the microdata. In an ℓ-diverse table, an attacker can figure out the real SA value of the individual with confidence no more than 1/ℓ. Treating the SA values as colors, this problem then exactly corresponds to the clustering with diversity problem defined at the beginning, where we have a lower bound ℓ on the cluster size.

In contrast to the many theoretical results for r-GATHERING and k-ANONYMITY
Figure 1: (a) The microdata; (b) A $2$-anonymous table; (c) An $2$-diverse table;

no approximation algorithm with performance guarantees is known for $\ell$-
DIVERSITY, even though many heuristic solutions have been proposed $[20,14,21]$.

Clustering with instance-level constraints and other related work.  Clustering with
instance-level constraints is a developing area and begins to find many interesting ap-
lications in various areas such as bioinformatics $[5]$, machine learning $[26,27]$, data
cleaning $[4]$, etc. Wagstaff and Cardie in their seminal work $[26]$ considered the follow-
ting two types of instance-level hard constraints: A must-link (ML) constraint dictates
that two particular points must be clustered together and a cannot-link (CL) constraint
requires they must be separated. Many heuristics and variants have been developed
subsequently, e.g. $[27,31]$, and some hardness results with respect to minimizing the
number of clusters were also obtained $[10]$. However, to the best of our knowledge,
no approximation algorithm with performance guarantee is known for any version of
the problem. We note that an $\ell$-diverse clustering can be seen as a special case where
nodes with the same color must satisfy CL constraints.

As opposed to the hard constraints imposed on any clustering, the correlation clus-
tering problem $[6]$ considers soft and possibly conflicting constraints and aims at min-
imizing the violation of the given constraints. An instance of this problem can be repre-
sented by a complete graph with each edge labeled (+) or (−) for each pair of vertices,
indicating that two vertices should be in the same or different clusters, respectively.
The goal is to cluster the elements so as to minimize the number of disagreements, i.e.,
(−) edges within clusters and (+) edges crossing clusters. The best known approxima-
tions for various versions of the problem are due to Ailon et al. $[3]$. If the number of
clusters is stipulated to be a small constant $k$, there is a polynomial time approximation
scheme $[15]$. In the Dedupalog project, Arasu et al. $[4]$ considered correlation clustering
together with instance-level hard constraints, with the aim of de-duplicating entity
references.

Approximation algorithms for clustering with outliers were first considered by
Charikar et al. $[9]$. The best known approximation factor for $r$-GATHERING with out-
liers is $4$ due to Aggrawal et al. $[1]$. 

| T-1D(Name) | Age | Gender | Degree | Disease | QI$\lambda$ | Disease | QI$\lambda$ | Disease |
|-----------|-----|--------|--------|---------|------------|---------|------------|---------|
| 1 (Adam)  | 29  | M      | M.Sc.  | HIV     | (center, radius) | HIV     | (center, radius) | HIV     |
| 2 (Bob)   | 25  | M      | M.Sc.  | HIV     | (center, radius) | pneumonia | (center, radius) | bronchitis |
| 3 (Calvin)| 25  | M      | B.Sc.  | pneumonia | (center, radius) | pneumonia | (center, radius) | bronchitis |
| 4 (Daisy) | 29  | F      | B.Sc.  | bronchitis | (center, radius) | bronchitis | (center, radius) | bronchitis |
| 5 (Elam)  | 40  | M      | B.Sc.  | bronchitis | (center, radius) | bronchitis | (center, radius) | bronchitis |
| 6 (Frank) | 45  | M      | B.Sc.  | bronchitis | (center, radius) | bronchitis | (center, radius) | bronchitis |
| 7 (George)| 35  | M      | B.Sc.  | pneumonia | (center, radius) | pneumonia | (center, radius) | pneumonia |
| 8 (Henry) | 37  | M      | B.Sc.  | pneumonia | (center, radius) | pneumonia | (center, radius) | pneumonia |
| 9 (Ivy)   | 50  | F      | Ph.D.  | dyspepsia | (center, radius) | dyspepsia | (center, radius) | pneumonia |
| 10 (Jane) | 60  | F      | Ph.D.  | pneumonia | (center, radius) | pneumonia | (center, radius) | pneumonia |
Our results. In this paper, we give the first approximation algorithms to the clustering with diversity problem. We formally define the problem as follows.

Definition 1 (ℓ-DIVERSITY) Given a set of \(n\) points in a metric space where each of them has a color, cluster them into a set \(C\) of clusters, such that each cluster has at least \(\ell\) points, and all of its points have distinct colors. The goal is to minimize the maximum radius of any cluster.

Our first result (Section 2) is a 2-approximation algorithm for ℓ-DIVERSITY. The algorithm follows a similar framework as in [1], but it is substantially more complicated. The difficulty is mainly due to the requirement to resolve the conflicting colors in each cluster while maintaining its minimum size \(\ell\). To the best of our knowledge, this is first approximation algorithm for a clustering problem with instance-level hard constraints.

Next, we show that this approximation ratio is the best possible by presenting a matching lower bound (Section 3). A lower bound of 2 is also given in [1] for \(r\)-GATHERING. But to carry that result over to ℓ-DIVERSITY, all the points need to have unique colors. This severely limits to applicability of this hardness result. In Section 3 we give a construction showing that even with only 3 colors, the problem is NP-hard to approximate within any factor strictly less than 2. In fact, if there are only 2 colors, we show that the problem can be solved optimally in polynomial time via bipartite matching.

Unlike \(r\)-GATHERING, an instance to the ℓ-DIVERSITY problem may not have a feasible solution at all, depending on the color distribution. In particular, we can easily see that no feasible clustering exists when there is one color that has more than \(\lfloor n/\ell \rfloor\) points. One way to get around this problem is to have some points not clustered (which corresponds to deleting a few records in the ℓ-DIVERSITY problem). Deleting records causes information loss in the published data, hence should be minimized. Ideally, we would like to delete points just enough such that the remaining points admit a feasible ℓ-diverse clustering. In Section 4 we consider the ℓ-DIVERSITY-OUTLIERS problem, where we compute an ℓ-diverse clustering after removing the least possible number of points. We give an \(O(1)\)-approximation algorithm to this problem.

Our techniques for dealing with diversity and cluster size constraints may be useful in developing approximation algorithms for clustering with more general instance-level constraints.

2 A 2-Approximation for ℓ-DIVERSITY

In this section we assume that a feasible solution on a given input always exists. We first introduce a few notations. Given a set of \(n\) points in a metric space, we construct a weighted graph \(G(V, E)\) where \(V\) is the set of points and each vertex \(v \in V\) has a color \(c(v)\). For each pair of vertices \(u, v \in V\) with different colors, we have an edge \(e = (u, v)\), and its weight \(w(e)\) is just their distance in the metric space. For any \(u, v \in V\), let \(\text{dist}_G(u, v)\) be the shortest path distance of \(u, v\) in graph \(G\). For any set \(A \subseteq V\), let \(N_G(A)\) be the set of neighbors of \(A\) in \(G\). For a pair of sets \(A \subseteq V, B \subseteq V\), let \(E_G(A; B) = \{(a, b) \mid a \in A, b \in B, (a, b) \in E(G)\}\). The diameter of a cluster \(C\) of nodes is defined to be \(d(C) = \max_{u, v \in C}(w(e(u, v)))\). Given a cluster \(C\) and
its center \( v \), the radius \( r(C) \) of \( C \) is defined as maximum distance from any node of \( C \) to \( v \), i.e., \( r(C) = \max_{u \in C} w(u, v) \). By triangle inequality, it is obvious to see that \( \frac{1}{2} d(C) \leq r(C) \leq d(C) \).

A star forest is a forest where each connected component is a star. A spanning star forest is a star forest spanning all vertices. The cost of a spanning forest \( F \) is the length of the longest edge in \( F \). We call a star forest semi-valid if each star component contains at least \( \ell \) colors and valid if it is semi-valid and each star is polychromatic, i.e., each node in the star has a distinct color. Note that a spanning star forest with cost \( R \) naturally defines a clustering with largest radius \( R \). Denote the radius and the diameter of the optimal clustering by \( r^* \) and \( d^* \), respectively.

We first briefly review the 2-approximation algorithm for the \( r \)-Gathering problem [1], which is the special case of our problem when all the points have distinct colors. Let \( e_1, e_2, \ldots \) be the edges of \( G \) in a non-decreasing order of their weights. The general idea of the \( r \)-Gathering algorithm [1] is to first guess the optimal radius \( R \) by considering each graph \( G_i \) formed by the first \( i \) edges \( E_i = \{ e_1, \ldots, e_i \} \), as \( i = 1, 2, \ldots \). It is easy to see that the cost of a spanning star forest of \( G_i \) is at most \( w(e_i) \). For each \( G_i \) (1 \( \leq i \leq m \)), the following condition is tested (rephrased to fit into our context):

(I) There exists a maximal independent set \( I \) such that there is a spanning star forest in \( G_i \) with the nodes in \( I \) being the star centers, and each star has at least \( r \) nodes.

It is proved [1] that the condition is met if the length of \( e_i \) is \( d^* \). The condition implies the radius of our solution is at most \( d^* \) which is at most \( 2r^* \). Therefore, we get an 2-approximation. In fact, the independent set \( I \) can be chosen greedily and finding the spanning star forest can be done via a network flow computation.

Our 2-approximation for the \( \ell \)-diversity problem follows the same framework, that is, we check each \( G_i \) in order and test the following condition:

(II) There exists a maximal independent set \( I \) such that there is a valid spanning star forest in \( G_i \) with the nodes in \( I \) being the star centers.

The additional challenge is of course that, while condition (I) only puts a constraint on the size of each star, condition (II) requires both the size of each star to be at least \( \ell \) and all the nodes in a star have distinct colors. Below we first give a constructive algorithm that for a given \( G_i \), tries to find an \( I \) such that condition (II) is met. Next we show that when \( w(e_i) = d^* \), the algorithm is guaranteed to succeed. The approximation ratio of 2 then follows immediately.

To find an \( I \) to meet condition (II), the algorithm starts with an arbitrary maximal independent set \( I \), and iteratively augments it until the condition is met, or fails otherwise. In each iteration, we maintain two tests. The first one, denoted by flow test F-Test\((G_i, I)\), checks if there exists a semi-valid spanning star forest in \( G_i \) with nodes in \( I \) being star centers. If \( I \) does not pass this test, the algorithm fails right away. Otherwise we go on to the second test, denoted by matching test M-Test\((G_i, I)\), which tries to find a valid spanning star forest. If this test succeeds, we are done; otherwise the failure of this test yields a way to augment \( I \) and we proceed to the next iteration. The algorithm is outlined in Algorithm [1].
for all the colors, we say that the M-T class does not guarantee that the cardinality constraint is preserved. The crucial fact here together give a spanning star forest such that each star is polychromatic. However, this exists a valid spanning star forest with nodes in \( B \). We do so by a bipartite matching test M-T problem. As the name suggests, we conduct the test using a network flow computation.

We first create a source \( s \) and a sink \( t \). For each node \( v \in V \), we add an edge \((s, v)\) with capacity 1, and for each node \( o_j \in I(1 \leq j \leq |I|) \), we create a vertex \( o_j \) and add an outgoing edge \((o_j, t)\) with capacity lower bound \( \ell \). For each node \( o_j \in I \) and each color \( c \), we create a vertex \( p_{j,c} \) and an edge \((p_{j,c}, o_j)\) with capacity upper bound 1. For any \( v \in V \) such that \((v, o_j) \in E_i \) or \( v = o_j \), and \( v \) has color \( c \), we add an edge from \( v \) to \( p_{j,c} \) without capacity constraint. Finally, we add one new vertex \( o_j' \) for each \( o_j \in I \), connect all \( v \in V \) to \( o_j' \) without capacity constraint if \((v, o_j) \in E_i \) or \( v = o_j \), and connect \( o_j' \) to \( t \) without capacity constraint. The capacity upper bound of \((p_{j,c}, o_j)\) forces at most one node with color \( c \) to be assigned to \( o_j \). Therefore, all nodes assigned to \( o_j \) have distinct colors. The capacity lower bounds of \((o_j, t)\)'s require that each cluster has at least \( \ell \) nodes. Nodes \( o_j' \)'s are used to absorb other unassigned nodes. It is not difficult to see that there exists a semi-valid spanning star forest with nodes in \( I \) being star centers in \( G_i \) if an \( n \)-units flow can be found. In this case we say that the F-Test is passed. See Figure 2 for an example. Note that a network flow problem with both capacity lower bounds and upper bounds is usually referred to as the circulation problem, and is polynomially solvable [19].

Once \( G_i \) and \( I \) pass F-Test, we try to redistribute those vertices that cause color conflicts. We do so by a bipartite matching test M-T \((G_i, I)\) which returns two vertex sets \( S \) and \( S' \) that are useful later. Concretely, we test whether there exists a matching in the bipartite graph \( B(I - C, C - I; E_{G_i}(I - C; C - I)) \) for each color class \( C \) such that all vertices in \( C - I \) are matched. If such matchings can be found for all the colors, we say that the M-Test is passed. Note that all these matchings together give a spanning star forest such that each star is polychromatic. However, this does not guarantee that the cardinality constraint is preserved. The crucial fact here is that \( I \) passes both F-Test and M-Test. In Lemma 2 we formally prove that there exists a valid spanning star forest with nodes in \( I \) as star centers if and only if \( G_i \) and \( I \) pass both F-Test and M-Test. To actually find a valid spanning star forest, we can again use the network flow construction in F-Test but without the \( o_j' \) nodes. If M-Test fails, we know that for some color class \( C \), there exists a subset \( S' \subseteq C - I \) such that

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**Algorithm 1:** Algorithm to find an \( I \) in \( G_i \) to meet condition (II)

1. Let \( I \) be an arbitrary maximal independent set in \( G_i \);
2. while F-Test\((G_i, I)\) is passed do
   3. \((S, S') \leftarrow M-Test(G_i, I) \) /* \( S \subseteq V, S' \subseteq I \) */
   4. if \( S = \emptyset \) then
      5. Succeed;
   6. else
      7. \( I \leftarrow I - S' + S \);
      8. Add nodes to \( I \) until it is a maximal independent set;
9. Fail;

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the size of its neighbor set $|N_B(S)|$ is less than $|S|$ by Hall’s theorem [19]. In this case, M-Test returns $(S, N_B(S))$; such a set $S$ can be found by a maximum matching algorithm. Then we update the independent set $I ← I − N_B(S) + S$; we show that $I$ is still an independent set in Lemma 1. Finally, we add nodes to $I$ arbitrarily until it becomes a maximal independent set. Then, we start the next iteration with the new $I$. Since $|S| > |N_B(S)|$, we increase $|I|$ by at least one in each iteration. So the algorithm terminates in $≤ n$ iterations.

Before proving that Algorithm 1 is guaranteed to succeed when $w(e) = d^*$, we prove the two lemmas left in the description of our algorithm. The first lemma ensures that $I$ is always an independent set.

**Lemma 1** The new set $I ← I − S' + S$ obtained in each update is still an independent set in $G_i$.

**Proof:** Since all vertices in $S$ have the same color, there is no edge among them. Therefore, we only need to prove that there is no edge between $I − S'$ and $S$, which is trivial since $S' = N_B(S)$. □

The second lemma guarantees that we find a feasible solution if both tests are passed.

**Lemma 2** Given $G_i = G(V, E_i)$ and $I$, a maximal independent set of $G_i$, both F-Test$(G_i, I)$ and M-Test$(G_i, I)$ are passed if and only if there exists a valid spanning star forest in $G_i$ with nodes in $I$ being star centers.

**Proof:** The “if” part is trivial. We only prove the “only if” part. Suppose $G_i$ and $I$ pass both F-Test$(G_i, I)$ and M-Test$(G_i, I)$. Consider a semi-valid spanning star forest obtained in $G_i$ after F-Test. We delete a minimal set of leaves to make it a valid star (not necessarily spanning) forest $F$. Consider the bipartite graph $B(I − C; C − I, E_{G_i}(I − C; C − I))$ for each color class $C$. We can see $F ∩ B$ is a matching in $B$. Since $I$ passes M-Test, we know that there exists a maximum matching such that all nodes in $C − I$ can be matched. If we use the Hungarian algorithm to compute a maximum matching with $F ∩ B$ as the initial matching, the nodes in $I − C$ which are originally matched will still be matched in the maximum matching due to the property of the alternating...
Therefore, the following invariants are maintained: each star is polychromatic and has at least $\ell$ colors. By applying the above maximum matching computation for each color class, we obtain a valid spanning star forest in $G_i$. □

Finally, we prove that Algorithm 1 is guaranteed to succeed on $G_i$ for the maximal index $i^*$ such that $w(e_i) = d^*$, where $d^*$ is the optimal cluster diameter of any valid spanning star forest of $G$.

**Lemma 3** Algorithm 1 will succeed on $G_{i^*}$.

**Proof:** Suppose $C^* = \{C^*_1, \ldots, C^*_k\}$ is the set of clusters in the optimal clustering with cluster diameter $d^*$. Since $G_{i^*}$ include all edges of weights no more than $d^*$, each $C^*_j$ induces a clique in $G_{i^*}$ for all $1 \leq j \leq k^*$, thus it contains at most one node in any independent set. Therefore, any maximal independent set $I$ in $G_{i^*}$ can pass $F$-Test($G_{i^*}, I$), and we only need to argue that $I$ will also pass $M$-Test($G_{i^*}, I$). Each update to the independent set $I$ increases the size of $I$ by at least 1 and the maximum size of $I$ is $k^*$. When $|I| = k^*$, each $C^*_j$ contains exactly one node in $I$ and this $I$ must be able to pass $M$-Test($G_{i^*}, I$). So Algorithm 1 must succeed in some iteration. □

By Lemma 3, the cost of the spanning star forest found by Algorithm 1 is at most $d^*$. Since the cost of the optimal spanning forest is at least $d^*/2$, we obtain a 2-approximation.

**Theorem 1** There is a polynomial-time 2-approximation for $\ell$-DIVERSITY.

## 3 The Lower Bound

In this section, we show that $\ell$-DIVERSITY is NP-hard to approximate within a factor less than 2 even when there are only three colors. Therefore the approximation ratio given in the Section 2 for $\ell$-DIVERSITY is tight. Note that if there are two colors, the problem is polynomially solvable. Indeed, if there are only two colors we can use the following simple algorithm to obtain an optimal solution. We start with an empty graph and add edges one by one in an increasing order of their weights (as before, we just add those edges whose endpoints’ colors are different), getting a series of threshold graphs $G_i (1 \leq i \leq m)$. For each graph $G_i$, we try to find a perfect matching between the two color classes. It is easy to see $w(e_i)$ is the optimal solution where $i$ is the smallest such that a perfect matching in $G_i$ exists.

**Theorem 2** There is no polynomial-time approximation algorithm for $\ell$-DIVERSITY that achieves an approximation factor less than 2 unless $P = NP$.

To prove the NP-hardness for three colors, we show first the following problem is NP-hard: Given a 3-colorable graph $G = (V, E)$ and a feasible 3-coloring, decide

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1Recall that an augmenting path $P$ (with respect to matching $M$) is a path starting from unmatched node, alternating between unmatched and matched edges and ending also at an unmatched node (for example, see [23]). By taking the symmetric difference of $P$ and $M$, which we call augmenting on $P$, we can obtain a new matching with one more edge.
if $V$ can be partitioned into subsets of size three such that the three vertices in each subset are connected and the colors of them are all different. We call such a partition a $P(ath)_3$-partition of $G$. Note that the NP-hardness of the $P_3$-partitioning problem directly leads to the fact that $ℓ$-DIVERSITY cannot be approximated within a factor less than 2, since if we assign the weights of all edges in $G$ to be 1 and consider the metric completion\(^2\) of $G$, then the optimal solution of $ℓ$-DIVERSITY on $G$ is 1 if $G$ admits a $P_3$-partitioning and at least 2 otherwise.

We reduce from the well-known 3-dimensional matching problem\(^{13}\) to the $P_3$-partition problem. Recall that in a 3-dimensional matching instance, we are given a tripartite hyper-graph $G = (X \cup Y \cup Z, E)$ with color classes $X, Y, Z$ such that $|X| = |Y| = |Z|$. Each hyper-edge is of the form $(x, y, z), x \in X, y \in Y, z \in Z$. A perfect matching is a set $M \subseteq E$ of hyper-edges such that each vertex is incident to exactly one edge in $M$. Given a 3-dimensional matching instance $G(V, E)$, we construct a 3-colorable graph $G'$ as well as a feasible 3-coloring such that $G$ has a perfect matching if and only if $G'$ can be $P_3$-partitioned.

The key component of our reduction is the gadget depicted in Figure 3. $G'$ has a copy of the vertices of $G$. We color the vertices in $X, Y$ and $Z$ with colors 1, 2 and 3, respectively. For each hyperedge $e = (x, y, z) \in E(G)$, we attach a distinct gadget to $G'$ by identifying $x, y, z$ with the three corner nodes of the gadget, respectively (corner nodes are those in thick circles in Figure 3(a)). The gadget has the following nice property.

**Property 1** If $G'$ can be $P_3$-partitioned, then any $P_3$-partition of $G'$ restricted in one gadget can only take one of the two forms shown in Figure 3(b).

The proof of the property is graphically obvious owing to the structure of the gadget. One can easily make it rigorous by a case by case analysis. To relate the partition of each gadget to the 3-dimensional matching problem, we use the following reduction. We take $e(x, y, z)$ as a matching edge if and only if the $P_3$-partition on $G'$ restricted in the corresponding gadget takes the first form in Figure 3(b). It is easy to see that $G$ has a perfect matching if and only if $G'$ can be $P_3$-partitioned.

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\(^2\)The metric completion of $G(V, E)$ is a complete graph with vertex set $V$ and the weight of edge $(u, v)$ defined by the shortest path distance between $u$ and $v$ in $G$ for every $u, v \in V$.\(^{13}\)
4 Dealing with Unqualified Inputs

For the \( \ell \text{-DIVERSITY} \) problem, a feasible solution may not exist depending on the input color distribution. The following simple lemma gives a necessary and sufficient condition for the existence of a feasible solution.

**Lemma 4** There exists a feasible solution for \( \ell \text{-DIVERSITY} \) if and only if the number of nodes with the same color \( c \) is at most \( \lfloor \frac{n}{\ell} \rfloor \) for each color \( c \).

**Proof:** The “only if” part is trivial. We only show the “if” part. Suppose the color class \( C \) contains the most number of nodes. We create \(|C|\) empty clusters, and process color classes one after another. For each node \( v \), we put it into the cluster currently containing the least number of nodes provided that the cluster does not contain a node having the same color as \( v \). Note that during the process, it can be easily shown that the sizes of clusters differ by at most one by induction. Therefore, each cluster contains at least \( \left\lfloor \frac{n}{|C|} \right\rfloor \geq \ell \) nodes at the end of the process. \( \square \)

To cluster an instance without a feasible solution, we must exclude some nodes as outliers. The following lemma characterizes the minimum number of outliers.

**Lemma 5** Let \( C_1, C_2, \ldots, C_k \) be the color classes sorted in the non-increasing order of their sizes.

1. Let \( p \) be the maximum integer satisfying \( \sum_{i=1}^{k} \min (p, |C_i|) \geq p\ell \). The minimum number of outliers is given by \( q = \sum_{i=1}^{k} \max (0, |C_i| - p) \) and \( p \) is the number of clusters when we exclude \( q \) outliers.

2. \( p\ell \leq n - q < p(\ell + 1) \).

**Proof:** Let \( p^* \) be the maximum number of clusters in any feasible solution. It is easy to see that we must exclude at least \( \sum_{i=1}^{k} \max (0, |C_i| - p^*) \) outliers. Thus the number of points left is at most

\[
\sum_{i=1}^{k} (|C_i| - \max (0, |C_i| - p^*)) = \sum_{i=1}^{k} \min (p^*, |C_i|),
\]

which should be at least \( p^*\ell \). Since we pick \( p \) to be the maximum integer such that \( \sum_{i=1}^{k} \min (p, |C_i|) \geq p\ell \), we have \( p \geq p^* \). Thus \( q \) is a lower bound on the number of outliers. Moreover, if we delete \( \max (0, |C_i| - p) \) nodes from \( C_i \), the remainders admit a feasible clustering from Lemma 4. Therefore, \( q \) is also an upper bound, and the proof of part 1 is completed.

\( n - q \geq p\ell \) is obvious. The \( n - q < p(\ell + 1) \) can be seen as follows. Suppose it is not true. We have

\[
n - \sum_{i=1}^{k} \max(0, |C_i| - p) = \sum_{i=1}^{k} (|C_i| - \max(0, |C_i| - p)) = \sum_{i=1}^{k} \min(p, |C_i|) \geq (p+1)\ell.
\]

Thus, \( \sum_{i=1}^{k} \min(p + 1, |C_i|) \geq (p + 1)\ell \) which contradicts the maximality of \( p \). \( \square \)
With lemma 5 at hand, it is natural to consider the following optimization problem: find an \( \ell \)-DIVERSITY solution by clustering \( n - q \) points such that the maximum cluster radius is minimized. We call this problem \( \ell \)-DIVERSITY-OUTLIERS. From Lemma 5 we can see that \( p \) is independent on the metric and can be computed in advance. In addition, implicit from Lemma 5 is that the number of outliers of each color is also fixed, but we need to decide which points should be chosen as outliers.

In the fortunate case where we have a color class \( C \) with exactly \( p \) nodes, we know that there is exactly one node of \( C \) in each cluster of any feasible solution. By using a similar flow network construction used in F-TEST, we can easily get a 2-approximation using \( C \) as the cluster centers. However, the problem becomes much more difficult when the sizes of all color classes are different from \( p \). Loosely speaking, our difficulty is two-fold: exponentially many choices of outliers and cluster centers.

### 4.1 A Constant Approximation

We first define some notations. We call color classes of size larger than \( p \) popular colors and nodes having such colors popular nodes. Other color classes have at most \( p \) nodes, and these nodes are unpopular. We denote the set of popular nodes by \( P \) and the set of unpopular nodes by \( N \). Note that after removing the outliers, each popular color has exactly \( p \) nodes and each cluster will contain the same number of popular nodes. Let \( z \) be the number of popular nodes each cluster contains. We denote by \( G^d \) the power graph of \( G \) in which two vertices \( u, v \) are adjacent if there is a path connecting \( u \) and \( v \) with at most \( d \) edges. The length of the edge \((u, v)\) in \( G^d \) is set to be \( \text{dist}_{C}(u, v) \).

Before describing the algorithm, we need the following simple lemma.

**Lemma 6** For any connected graph \( G \), \( G^3 \) contains a Hamiltonian cycle which can be found in linear time.

**Proof:** Let \( T \) be any spanning tree of \( G \). It suffices to prove \( T^3 \) contains a Hamiltonian cycle. We root \( T \) at an arbitrary vertex \( r \) and denote the depth of a vertex \( v \) by \( \text{depth}(v) \) (\( \text{depth}(r) = 1 \)). Let \( T_v \) be the subtree rooted at \( v \) and \( Ch(v) \) be the set of children of \( v \). Consider the Algorithm Traverse\((r)\). Clearly, the algorithm runs in linear time.

Suppose the order obtained is \( \{v_1, v_2, \ldots, v_n\} \). We claim \( \text{dist}_T(v_i, v_{i+1}) \leq 3 \) for \( 1 \leq i \leq n - 1 \) and \( \text{dist}_T(v_1, v_n) \leq 1 \). Note that the claim immediately implies the lemma. We prove the claim by induction on the size of the tree. Suppose \( \text{depth}(v) \) is odd (the other case can be proved similarly) and \( Ch(v) = \{u_1, \ldots, u_k\} \). Let \( O_i = \{v_1, v_2, \ldots, v_{i+1}\} \) be the traverse order of \( T_{u_i} \). It is easy to see the order produced by Traverse\((v)\) is \( v, O_1, O_2, \ldots, O_k \). It is also not hard to see that

\[
\text{dist}_T(v, v_{1,1}) \leq \text{dist}_T(v, u_1) + \text{dist}_T(u_1, v_{1,1}) = \text{dist}_T(v, u_1) + \text{dist}_T(v_{1,|O_1|}, v_{1,1}) \leq 2
\]

and
\[
\text{dist}_T(v_{k,|O_k|}, v) = \text{dist}_T(u_k, v) = 1
\]

since \( u_i \) is last vertex in order \( O_i \). We can also see that

\[
\text{dist}_T(v_{i,|O_i|}, v_{i+1,1}) \leq \text{dist}_T(u_i, v) + \text{dist}_T(v, u_{i+1}) + \text{dist}_T(u_{i+1}, v_{i+1,1}) \leq 3.
\]

By induction hypothesis, the proof is completed. \( \square \)
Algorithm 2: Traverse($v$)

1. if depth($v$) is odd then
2. visit($v$);
3. for each ($u \in Ch(v)$) Traverse($u$);
4. else
5. for each ($u \in Ch(v)$) Traverse($u$);
6. visit($v$);

The algorithm still adopts the thresholding method, that is, we add edges one by one to get graphs $G_i = (V, E_i = \{e_1, e_2, \ldots, e_i\})$, for $i = 1, 2, \ldots$, and in each $G_i$, we try to find a valid star forest that spans $G_i$ except outliers. Let $d^*$ be the diameter of the optimal solution that clusters $n - q$ points, and $i^*$ be the maximum index such that $w(e_i) = d^*$. Let $G_i[N]$ be the subgraph of $G_i$ induced by all unpopular nodes. We define the ball of radius $r$ around $v$ to be $B(v, r) = \{u \in N \mid \text{dist}_{G}(v, u) \leq r\}$. For each $G_i$, we run the Algorithm: $\ell$-DIVERSITY-OUTLIERS($G_i$) (see below). We proceed to $G_{i+1}$ when the algorithm claims failure.

The high level idea of the algorithm is as follows: Our goal is to show that the algorithm can find a valid star forest spanning $n - q$ nodes in $G_{i^*}^{28}$. It is not hard to see that this gives us an approximation algorithm with factor $28 \times 2 = 56$. First, we notice that F-TEST can be easily modified to work for the outlier version by excluding all $o'_j$ nodes and testing whether there is a flow of value $n - q$. However, the network flow construction needs to know in advance the set of candidates of cluster centers. For this purpose, we attempt to attach a set $U$ of $p$ new nodes which we call virtual centers to $G_i$ which serve as the candidates of cluster centers in F-TEST. In the ideal case, if these virtual centers can be distributed such that each of them is attached to a distinct optimal cluster, F-TEST can easily produce a 2-approximation. Since the optimal clustering is not known, this is very difficult in general. However, we show that there is way to carefully distribute the virtual centers such that there is a perfect matching between these virtual centers and the optimal cluster centers and the longest matching edge is at most $27d^*$. This implies that there is a valid spanning star forest in $G_{i^*}^{28}$ (each star is formed by an optimal cluster together with the virtual center that matches the cluster center). Also, it is easy to see that each virtual center is at most $27d^* + d^*$ away from any other node in the same star. Therefore, it suffices to just run F-TEST($G_{i^*}^{28}, U$) to find a feasible solution.

**Algorithm:** $\ell$-DIVERSITY-OUTLIERS($G_i$).

1. If $G_i[N]$ contains a connected component with less than $\ell - z$ nodes, we declare failure.

2. Pick an arbitrary unpopular node $v$ such that $|B(v, w(e_i))| \geq \ell - z$ and delete all vertices in this ball; repeat until no such node exists. Then, pick an arbitrary unpopular node $v$ and delete all vertices in $B(v, w(e_i))$; repeat until no unpopular node is left. Let $B_1, B_2, \ldots, B_k$ be the balls created during the process. If a ball
contains at least \( \ell - z \) unpopular nodes, we call it \textit{big}. Otherwise, we call it \textit{small}.

3. In \( G_i[N] \), shrink each \( B_j \) into a single node \( b_j \). A node \( b_j \) is \textit{big} if \( B_j \) is big and \textit{small} otherwise. We define the weight of \( b_j \) to be \( \mu(b_j) = \frac{|B_j|}{2} \). Let the resulting graph with vertex set \( \{b_j\}_{j=1}^k \) be \( D_i \).

4. For each connected component \( C \) of \( D_i \), do

   (a) Find a spanning tree \( T_C \) of \( C^3 \) such that all small nodes are leaves. If this is not possible, we declare failure.

   (b) Find (by Lemma 6) a Hamiltonian cycle \( P = \{b_1, b_2, \ldots, b_h, b_h+1 = b_1\} \) over all non-leaf nodes of \( C \) such that \( \text{dist}_{D_i}(b_j, b_{j+1}) \leq 9w(e_i) \).

5. We create a new color class \( U \) of \( p \) nodes which will serve as “virtual centers” of the \( p \) clusters. These virtual centers are placed in \( G_i \) “evenly” as follows. Consider each connected component \( C \) in \( D_i \) and the corresponding spanning tree \( T_C \) of \( C^3 \). For each non-leaf node \( b_j \) in \( T_C \), let \( L(b_j) \) be the set of leaves connected to \( b_j \) in \( T_C \), and let \( \eta(b_j) = \mu(b_j) + \sum_{b_x \in L(b_j)} \mu(b_x) \) and \( \delta_j = \sum_{i=1}^{\ell} \eta(b_x) \). We attach \( \lfloor \delta_i \rfloor - \lfloor \delta_{i-1} \rfloor \) virtual centers to the center of \( B_i \) by zero weight edges. If the total number of virtual centers used is not equal to \( p \), we declare failure. Let \( H_i \) be the resulting graph (including all popular nodes, unpopular nodes and virtual centers).

6. Find a valid star forest in \( H_i^{28} \) using \( U \) as centers, which spans \( n - q \) nodes (not including the nodes in \( U \)) by using F-Test. If succeeds, we return the star forest found, otherwise we declare failure.

### 4.2 Analysis of the algorithm

We show that the algorithm succeeds on \( G_i \). Since we perform F-Test on \( H_i^{28} \) in which each edge is of length \( \leq 28d^* \), the radius of each cluster is at most \( 28d^* \leq 56r^* \). Therefore, the approximation ratio is 56.

Let \( H_i \) be the graph obtained by adding virtual centers to \( G_i \) as described above. Let \( C^* = \{C_1^*, \ldots, C_p^*\} \) be the optimal clustering. Let \( I^* = \{\nu_1^*, \ldots, \nu_p^*\} \) be the set of cluster centers of \( C^* \) where \( \nu_i^* \) is the center of \( C_i^* \). We denote the balls grown in step 2 by \( B_1, \ldots, B_k \). Let \( \nu_i \) be the center of \( B_i \).

The algorithm may possibly fail in step 1, step 4(a), step 5 and step 6. Obviously \( G_i \) can pass step 1. Therefore, we only check the other three cases.

Step 4(a) : We prove that the subgraph induced by all big nodes are connected in \( C^3 \). Indeed, we claim that each small node is adjacent to at least one big node in \( C \) from which the proof follows easily. Now we prove the claim. Suppose \( b_j \) is a small node and all its neighbors are small. We know that in \( G_i[N], \nu_j \) has at least \( \ell - z - 1 \) neighbors because \( \nu_j \) is an unpopular node and thus belongs to some optimal cluster. So we could form a big ball around \( \nu_j \), thus contradicting to the fact that \( \nu_j \) is in a small ball. To find a spanning tree with all small nodes as leaves, we first assign each
small node to one of its adjacent node arbitrarily and then compute a tree spanning all the big nodes.

Step 5: We can see that in each connected component \( C \) (with big nodes \( b_1, \ldots, b_h \)) in \( D_{1^*} \), the total number of virtual centers we have placed is \( \sum_{i=1}^{h} (|\delta_i| - |\delta_{i-1}|) = |\delta_h| = |\sum_{x=1}^{h} \eta(b_x)| = |\sum_{b_j \in C} \mu(b_j)| = \left\lfloor \frac{|C|}{p} \right\rfloor \) where \( |C| = \sum_{b_j \in C} |B_j| \), the number of nodes in the connected component of \( G_{1^*}^{\eta}(\mathcal{N}) \) corresponding to \( C \). This is at least the number of clusters created for the component \( C \) in the optimal solution. Therefore, we can see the total number of virtual centers created is at least \( p \). On the other hand, from Lemma 5(2), we can see that \( |\delta| = |\sum_{x=1}^{h} \eta(b_x)| = |\sum_{b_j \in C} \mu(b_j)| = \left\lfloor \frac{|C|}{p} \right\rfloor \). Hence, \( p = \left\lfloor \frac{|\mathcal{N}|}{p} \right\rfloor = \left\lfloor \sum_{b_j \in C} \frac{|C|}{p} \right\rfloor \geq \sum_{b_j \in C} \frac{|C|}{p} \), where the summation is over all connect components. So, we prove that exactly \( p \) virtual centers were placed in \( G_{1^*}^{\eta} \).

Step 6: According to the high level idea discussed before, we only need to show that there is a perfect matching \( M \) between \( U \) and the set of optimal centers \( I^* \) in \( H_{1^*}^{27u} \). We consider the bipartite subgraph \( Q(U, I^*, E_{H_{1^*}^{27u}}(U, I^*)) \). From Hall’s theorem, it suffices to show that \( |N_Q(S)| \geq |S| \) for any \( S \subseteq U \), which can be implied by the following lemma.

**Lemma 7** For any \( S \subseteq U \), the union of the balls of radius \( 27d^* \) around the nodes of \( S \), i.e., \( \bigcup_{u \in S} B(u, 27d^*) \), intersects at least \( |S| \) optimal clusters in \( C^* \).

**Proof:** We can assume w.l.o.g. all nodes of \( S \) are in a single connected component of \( G_{1^*}^{\eta}(\mathcal{N}) \). The generalization to several connected components is straightforward. Let \( P = \{b_1, b_2, \ldots, b_h\} \) be the Hamiltonian cycle (found in Step 4(b)) for such a component (actually, the component after shrinking balls). Let \( \tilde{P} \) be the set of nodes \( b_j \in P \) such that at least one virtual center in \( S \) is attached to \( B_j \).

We first assume \( |\tilde{P}| \leq h - 2 \). In this case, we claim that \( |\bigcup_{u \in S} B(u, 27d^*)| > (|S|+1)(\ell-z) \). We know by definition that the number of nodes in each big ball \( B_j \) plus nodes in those small balls \( B_j \) attached to it (that is, \( b_x \in L(b_j) \)) is \( \eta(b_j)(\ell-z) \). \( \tilde{P} \) can be seen as a collection of subpaths of \( P \). For each of those subpaths, say \( \{b_j, \ldots, b_{j'}\} \), the number of nodes in \( S \) attached to it is at most

\[
\sum_{x=j}^{j'} (|\delta_x| - |\delta_{x-1}|) = |\delta_{j'}| - |\delta_{j-1}| - \sum_{x=1}^{j-1} \eta(b_x^*) - |\sum_{x=1}^{j} \eta(b_x^*)| \leq |\delta_{j'}| - |\delta_{j-1}| + 1
\]

On the other hand, we can see that \( B(\nu_x, 27d^*) \) contains all nodes in \( B_{j-1}, B_j \) and \( B_{j+1} \) and all nodes in the small balls attached to \( B_j \). This is because \( \text{dist}_{D_{1^*}}(b_j, b_{j+1}) \leq 9d^* \) and each \( b_j \) is obtained by shrinking a ball of radius at most \( d^* \). Therefore,

\[
\sum_{x=j}^{j'+1} \eta(b_x^*)(\ell-z) \geq (|\delta_{j'}| - |\delta_{j-1}| + 1)(\ell-z)
\]

\[\mathbf{B_0 = B_h, B_{h+1} = B_1.}\]
where the second inequality holds since $\eta(b_j) \geq 1$ for any big node $b_j$. Summing up all the subpaths of $\tilde{P}$ proves the claim. From Lemma 5.2 and the fact that each cluster has exactly $z$ popular nodes, we can see $|S|$ optimal clusters contains less than $(\ell - z)(|S| + 1)$ unpopular nodes. Therefore, the lemma holds.

If $|\tilde{P}| > h - 2$, then $\bigcup_{u \in S} B(u, 27d^*)$ contains all unpopular nodes in this component. The lemma also follows. □

**Theorem 3** There is a polynomial-time algorithm for $\ell$-DIVERSITY-OUTLIERS that produces a 56-approximation.

## 5 Further Directions

This work results in several open questions. First, as in [1], we could also try to minimize the sum of the radii of the clusters. However, this seems to be much more difficult, and we leave it as an interesting open problem. Another open problem is to design constant approximations for the problem with any fixed number of outliers, that is, for a given number $k$, find an optimal clustering if at most $k$ outliers can be removed.

As mentioned in the introduction, our work can be seen as a stab at the more general problem of clustering under instance-level hard constraints. Although arbitrary CL (cannot-link) constraints seems hard to approximate with respect to minimizing the number of clusters due to the hardness of graph coloring [10], other objectives and special classes of constraints, e.g. diversity constraints, may still admit good approximations. Besides the basic ML and CL constraints, we could consider more complex constraints like the rules proposed in the Dedupalog project [4]. One example of such rules says that whenever we cluster two points $a$ and $b$ together, we must also cluster $c$ and $d$. Much less is known for incorporating these types of constraints into traditional clustering problems and we expect it to be an interesting and rich further direction.

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