Abstract

Clustering is an important part of many modern data analysis pipelines, including network analysis and data retrieval. There are many different clustering algorithms developed by various communities, and it is often not clear which algorithm will give the best performance on a specific clustering task. Similarly, we often have multiple ways to measure distances between data points, and the best clustering performance might require a non-trivial combination of those metrics. In this work, we study data-driven algorithm selection and metric learning for clustering problems, where the goal is to simultaneously learn the best algorithm and metric for a specific application. The family of clustering algorithms we consider is parameterized linkage based procedures that includes single and complete linkage. The family of distance functions we learn over are convex combinations of base distance functions. We design efficient learning algorithms which receive samples from an application-specific distribution over clustering instances and simultaneously learn both a near-optimal distance and clustering algorithm from these classes. We also carry out a comprehensive empirical evaluation of our techniques showing that they can lead to significantly improved clustering performance.

1 Introduction

Overview. Clustering is an important part of many modern data analysis pipelines. For example, we might cluster emails based on content as a pre-processing step for spam detection, or we might cluster individuals in a social network in order to suggest new connections. There are a myriad of different clustering algorithms, and it is not always clear what algorithm will give the best performance on a specific clustering task. Similarly, we often have multiple different ways to measure distances between data points, and it is not obvious which distance metric will lead to the best performance. In this work, we study data-driven algorithm selection and metric learning for clustering problems, where the goal is to use data to simultaneously learn the best algorithm and metric for a specific application such as clustering emails or users of a social network. Each specific application is modeled as a distribution over clustering tasks, we observe an i.i.d. sample of clustering instances drawn from that distribution, and our goal is to choose an approximately optimal algorithm from a parameterized family of algorithms (according to some well-defined loss function). This corresponds to settings where we repeatedly solve clustering instances (e.g., clustering the emails that arrive each day) and we want to use historic instances to learn the best clustering algorithm and metric.

We consider the problem of learning both a clustering algorithm and a distance metric for a specific clustering application domain. The family of clustering algorithms we consider consists of parameterized linkage based procedures and includes single and complete linkage, which are widely used in practice and optimal in many cases [2, 16, 18, 1, 3, 10]. The family of distance metrics we learn over consists of convex combinations of base distance functions. We design efficient learning algorithms that receive samples from an application-specific distribution over clustering instances and simultaneously learn both a near-optimal
distance metric and clustering algorithm from these classes. Our work contributes to a recent line of work that provides learning-theoretical \cite{17} guarantees for data-driven algorithm configuration \cite{11,4,5,7}. These papers analyze the intrinsic complexity of parameterized algorithm families in order to provide sample complexity guarantees, that is, bounds on the number of sample instances needed in order to find an approximately optimal algorithm for a given application domain. Our results build on the work of Balcan et al. \cite{4}, who studied the problem of learning the best clustering algorithm from a class of linkage based procedures, but did not study learning the best metric. In addition to our sample complexity guarantees, we develop a number of algorithmic tools that enable learning application specific clustering algorithms and metrics for realistically large clustering instances. We use our efficient implementations to conduct comprehensive experiments on clustering domains derived from both real-world and synthetic datasets. These experiments demonstrate that learning application-specific algorithms and metrics can lead to significant performance improvements over standard algorithms and metrics.

**Our Results.** We study a parameterized family of linkage-based clustering algorithms that take as input a clustering instance $S$ and output a hierarchical clustering of $S$ represented as a binary cluster tree. Each node in the tree represents a cluster in the data at one level of granularity, with the leaves corresponding to individual data points and the root node corresponding to the entire dataset. Each internal node represents a cluster obtained by merging its two children. Linkage-based clustering algorithms build a cluster tree from the leaves up, starting with each point belonging to its own cluster and repeatedly merging the “closest” pair of clusters until only one remains. The parameters of our algorithm family control both the metric used to measure pointwise distances, as well as how the linkage algorithm measures distances between clusters (in terms of the distances between their points).

This work has two major contributions. Our first contribution is to provide sample complexity guarantees for learning effective application-specific distance metrics for use with linkage-based clustering algorithms. The key challenge is that, if we fix a clustering algorithm from the family we study and a single clustering instance $S$, the algorithm output is a piecewise constant function of our metric family’s parameters. This implies that, unlike many standard learning problems, the loss we want to minimize is very sensitive to the metric parameters and small perturbations to the optimal parameters can lead to high loss. Our main technical insight is that for any clustering instance $S$, we can partition the parameter space of our metric family into a relatively small number of regions such that the ordering over pairs of points in $S$ given by the metric is constant on each region. The clustering output by all algorithms in the family we study only depends on the ordering over pairs of points induced by the metric, and therefore their output is also a piecewise constant function of the metric parameters with not too many pieces. We leverage this structure to bound the intrinsic complexity of the learning problem, leading to uniform convergence guarantees. Moreover, by combining our results with the work of Balcan et al. \cite{4}, we show how to simultaneously learn both an application-specific metric and linkage algorithm.

Our second main contribution is a comprehensive empirical evaluation of our proposed methods, enabled by new algorithmic insights for efficiently learning application-specific algorithms and metrics from sample clustering instances. For any fixed clustering instance, we show that we can use an execution tree data structure to efficiently construct a coarse partition of the joint parameter space so that on each region the output clustering is constant. Roughly speaking, the execution tree compactly describes all possible sequences of merges the linkage algorithm might make together with the parameter settings for the algorithm and metric that lead to that merge sequence. The learning procedure proposed by Balcan et al. \cite{4} takes a more combinatorial approach, resulting in partitions of the parameter space that have many unnecessary regions and increased overall running time. Balcan et al. \cite{3} and Balcan et al. \cite{7} also use an execution tree approach for different algorithm families, however their specific approaches to enumerating the tree are not efficient enough to be used in our setting. We show that using a depth-first traversal of the execution tree leads to significantly reduced memory requirements, since in our setting the execution tree is shallow but very wide.

Using our efficient implementations, we evaluate our approach on several real world and synthetic clustering applications. We learn the best algorithm and metric for clustering applications derived from MNIST, CIFAR-10, Omniglot, and a synthetic rings and disks distribution. Across these different tasks the optimal clustering algorithm and metric vary greatly. Moreover, in most cases we achieve significant improvements in clustering
quality over standard clustering algorithms and metrics.

Related work. Gupta and Roughgarden \[11\] introduced the theoretical framework for analyzing algorithm selection problems that we consider in this work. They provide sample complexity guarantees for greedy algorithms for canonical subset selection problems including the knapsack problem, maximum weight independent set, and machine scheduling.

Some recent works provide sample complexity guarantees for learning application-specific clustering algorithms. Balcan et al. \[4\] consider several parameterized families of linkage based clustering algorithms, one of which is a special case of the family studied in this paper. Their sample complexity results are also based on showing that for a single clustering instance, we can find a partitioning of the algorithm parameter space into regions where the output clustering is constant. The families of linkage procedures they study have a single parameter, while our linkage algorithm and metric families have multiple. Moreover, they suppose we are given a fixed metric for each clustering instance and do not study the problem of learning an application-specific metric. Balcan et al. \[7\] study the related problem of learning the best initialization procedure and local search method to use in a clustering algorithm inspired by Lloyd’s method for $k$-means clustering. Their sample complexity results are again based on demonstrating that for any clustering instance, there exists a partitioning of the parameter space on which the algorithm’s output is constant. The parameter space partitions in both of these related works are defined by linear separators. Due to the interactions between the distance metric and the linkage algorithm, our partitions are defined by quadratic functions.

The procedures proposed by prior work for finding an empirically optimal algorithm for a collection of problem instances roughly fall into two categories: combinatorial approaches and approaches based on an execution-tree data structure. Gupta and Roughgarden \[11\] and Balcan et al. \[4\] are two examples of the combinatorial approach. They show that the boundaries in the constant-output partition of the algorithm parameter space always occur at the solutions to finitely many equations that depend on the problem instance. To find an empirically optimal algorithm, they find all solutions to these problem-dependent equations to explicitly construct a partition of the parameter space. Unfortunately, only a small subset of the solutions are actual boundaries in the partition. Consequently, their partitions contain many extra regions and suffer from long running times. The execution-tree based approaches find the coarsest possible partitioning of the parameter space such that the algorithm output is constant. Balcan et al. \[7\] and Balcan et al. \[6\] both use execution trees to find empirically optimal algorithm parameters for different algorithm families. However, the specific algorithms used to construct and enumerate the execution tree are different from those explored in this paper and are not suitable in our setting.

2 Learning Clustering Algorithms

We begin by formalizing the problem we study. Let $\mathcal{X}$ be a data domain. Each clustering instance consists of a point set $S = \{x_1, \ldots, x_n\} \subset \mathcal{X}$ and an (unknown) target clustering $\mathcal{Y} = (C_1, \ldots, C_k)$, where the sets $C_1, \ldots, C_k$ partition $S$ into $k$ clusters. Linkage-based clustering algorithms output a hierarchical clustering of the input data, represented by a cluster tree. We measure the agreement of a cluster tree $T$ with the target clustering $\mathcal{Y} = (C_1, \ldots, C_k)$ in terms of the Hamming distance between $\mathcal{Y}$ and the closest pruning of $T$ into $k$ clusters (i.e., $k$ disjoint subtrees that contain all the leaves of $T$). More formally, we define the loss

$$\ell(T, \mathcal{Y}) = \min_{P_1, \ldots, P_k} \min_{\sigma \in \mathcal{S}_n} \frac{1}{|S|} \sum_{i=1}^{k} |C_i \setminus P_{\sigma_i}|,$$

where $A \setminus B$ denotes set difference, the first minimum is over all prunings $P_1, \ldots, P_k$ of the cluster tree $T$, and the second minimum is over all permutations of the $k$ cluster indices. This formulation allows us to handle the case where each clustering task has a different number of clusters, and where the desired number might not be known in advance. Our analysis applies to any loss function $\ell$ measuring the quality of the output cluster tree $T$, but we focus on the Hamming distance for simplicity. Given a distribution $\mathcal{D}$ over clustering instances (i.e., point sets together with target clusterings), our goal is to find the algorithm $A$ from a family $\mathcal{A}$ with the lowest expected loss for an instance sampled from $\mathcal{D}$. As training data, we assume that
we are given an i.i.d. sample of clustering instances annotated with their target clusterings drawn from the application distribution $\mathcal{D}$.

We study a parameterized family of linkage-based clustering algorithms. These algorithms construct a hierarchical clustering of a point set by starting with each point belonging to a cluster of its own and then repeatedly merge the closest pair of clusters until only one remains. There are two distinct notions of distance at play in linkage-based algorithms: first, the notion of distance between pairs of points (e.g., Euclidean distance between feature vectors, edit distance between strings, or the Jaccard distance between sets). Second, these algorithms must define a distance function between clusters, which we refer to as a merge function to avoid confusion. A merge function $D$ defines the distance between a pair of clusters $A, B \subset \mathcal{X}$ in terms of the pairwise distances given by a metric $d$ between their points. For example, single linkage uses the merge function $D_{\text{min}}(A, B; d) = \min_{a \in A, b \in B} d(a, b)$ and complete linkage uses the merge function $D_{\text{max}}(A, B; d) = \max_{a \in A, b \in B} d(a, b)$. Here, we have made the dependence on the metric $d$ explicit, but when the metric is clear from context it will be omitted.

Our parameterized family of linkage-based clustering algorithms allows us to vary both the metric used to measure distances between points, as well as the merge function used to measure distances between clusters. To vary the metric, we suppose we have access to $L$ metrics $d_1, \ldots, d_L$ defined on our data universe $\mathcal{X}$, and our goal is to find the best convex combination of those metrics. That is, for any parameter vector $\beta \in \Delta_L = \{\beta \in [0, 1]^L | \sum_i \beta_i = 1\}$, we define a metric $d_\beta(x, x') = \sum_{i=1}^L \beta_i \cdot d_i(x, x')$. This definition is suitable across a wide range of applications, since it allows us to learn the best combination of a given set of metrics for the application at hand. Similarly, for varying the merge function, we suppose we have $L'$ merge functions $D_1, \ldots, D_{L'}$. For any parameter $\alpha \in \Delta_{L'}$, define the merge function $D_\alpha(A, B; d) = \sum_{i=1}^{L'} \alpha_i D_i(A, B; d)$. For each pair of parameters $\beta \in \Delta_L$ and $\alpha \in \Delta_{L'}$, we obtain a different clustering algorithm (i.e., one that repeatedly merges the pair of clusters minimizing $D_\alpha(\cdot; d_\beta)$). Pseudocode for this method is given in Algorithm 1. Each cluster is represented as a binary tree whose leaves correspond to the points belonging to that cluster. We slightly abuse notation and use merge functions to measure the distance between two clusters represented this way. For any clustering instance $S \subset \mathcal{X}$, we let $A_{\alpha, \beta}(S)$ denote the cluster tree output by Algorithm 1 when run with parameter vectors $\alpha$ and $\beta$.

**Algorithm 1** Linkage Clustering

**Input:** Metrics $d_1, \ldots, d_L$, merge functions $D_1, \ldots, D_{L'}$, points $x_1, \ldots, x_n \in \mathcal{X}$, parameters $\alpha$ and $\beta$.

1. Let $\mathcal{N} = \{\text{Leaf}(x_1), \ldots, \text{Leaf}(x_n)\}$ be the initial set of nodes (one leaf per point).
2. While $|\mathcal{N}| > 1$
   (a) Let $A, B \in \mathcal{N}$ be the clusters in $\mathcal{N}$ minimizing $D_\alpha(A, B; d_\beta)$.
   (b) Remove clusters $A$ and $B$ from $\mathcal{N}$ and add Node$(A, B)$ to $\mathcal{N}$.
3. Return the cluster tree (the only element of $\mathcal{N}$).

First, we provide sample complexity results that hold for any collection of metrics $d_1, \ldots, d_L$ and any collection of merge functions $D_1, \ldots, D_{L'}$ that belong to the following family:

**Definition 1.** A merge function $D$ is 2-point-based if for any pair of clusters $A, B \subset \mathcal{X}$ and any metric $d$, there exists a pair of points $(a, b) \in A \times B$ such that $D(A, B; d) = d(a, b)$. Moreover, the pair of points defining the merge distance must depend only on the ordering of pairwise distances. More formally, if $d$ and $d'$ are two metrics s.t. for all $a, a' \in A$ and $b, b' \in B$, we have $d(a, b) \leq d(a', b')$ if and only if $d'(a, b) \leq d'(a', b')$, then $D(A, B; d) = d(a, b)$ implies that $D(A, B; d') = d'(a, b)$.

For example, both single and complete linkage are 2-point-based merge functions, since they output the distance between the closest or farthest pair of points, respectively.

**Theorem 1.** Fix any metrics $d_1, \ldots, d_L$, 2-point-based merge functions $D_1, \ldots, D_{L'}$, and distribution $\mathcal{D}$ over clustering instances with at most $n$ points. For any parameters $\epsilon > 0$ and $\delta > 0$, let $(S_1, Y_1), \ldots, (S_N, Y_N)$ be an i.i.d. sample of $N = O\left(\left(\frac{L' + L}{\epsilon^2}\right) \log\left(\frac{n}{\delta}\right)\right)$ clustering instances with target clusterings drawn from $\mathcal{D}$. Then
with probability at least \(1 - \delta\) over the draw of the sample, we have

\[
\sup_{(\alpha, \beta) \in \Delta_L \times \Delta_L} \left| \frac{1}{N} \sum_{i=1}^N \ell(A_{\alpha, \beta}(S_i), Y_i) - \mathbb{E}_{(S, Y) \sim \mathcal{D}} \left[ \ell(A_{\alpha, \beta}(S), Y) \right] \right| \leq \epsilon.
\]

The key step in the proof of Theorem 1 is to show that we can partition the joint parameter space \(\Delta_L' \times \Delta_L\) into \(T\) regions \(Z_1, \ldots, Z_T\) such that \(\log(T) = O((L' + L)^3 \log(Nn))\) and, for all regions \(Z_j\) and clustering instances \(S_i\), the output of Algorithm 1 run on instance \(S_i\) is constant for \((\alpha, \beta) \in Z_j\). This implies that when restricted to the region \(Z_j\), the loss functions \((\alpha, \beta) \mapsto \ell(A_{\alpha, \beta}(S_i), Y_i)\) for \(i \in [N]\) are all constant. We use this fact to bounds the empirical Rademacher complexity of these functions in terms of \(\log(T)\), the log number of regions, leading to uniform convergence guarantees. The proof of Theorem 1 is given in Appendix A. In the remainder of this section, we prove the key structural property.

Before proving this structural result, we introduce notation for describing the kind of partition we will construct. We let \(\zeta = (\alpha, \beta) \in \Delta_L' \times \Delta_L\) denote a pair of parameter vectors for Algorithm 1 viewed as a vector in \(\mathbb{R}^{L' + L}\). Our parameter space partition will be induced by the sign-pattern of \(M\) quadratic functions.

**Definition 2** (Sign-Pattern Partition). The sign-pattern partition of \(\mathbb{R}^p\) induced by a collection of \(M\) real-valued functions \(f_1, \ldots, f_M : \mathbb{R}^p \to \mathbb{R}\) is defined as follows: Let \(F : \mathbb{R}^p \to \{\pm 1\}^M\) be the function \(F(\zeta) = (\text{sign}(f_1(\zeta)), \ldots, \text{sign}(f_M(\zeta)))\). Two points \(\zeta, \zeta' \in \mathbb{R}^p\) belong to the same region in the partition iff \(F(\zeta) = F(\zeta')\). Each region is of the form \(Z = \{\zeta \in \mathbb{R}^p | F(\zeta) = b\}\), for some sign-pattern vector \(b \in \{\pm 1\}^M\).

Our analysis depends crucially on the number of regions in the sign-pattern partition induced by a collection of functions. Based on the work of Buck [9], we know that when the functions \(f_1, \ldots, f_M\) are linear, then the number of regions is at most \((3M)^p\)—a substantial improvement over the naïve bound of \(2^M\). We can also leverage this result to bound the number of regions by \((3M)^{p^2 + p}\) when the functions are quadratic by viewing each quadratic function as a linear function on a \((p^2 + p)\)-dimensional space. The following result summarizes these facts and is proved in Appendix A.

**Lemma 1.** Let \(T\) be the number of regions in the sign-pattern partition of \(\mathbb{R}^p\) induced by \(f_1, \ldots, f_M : \mathbb{R}^p \to \mathbb{R}\).

1. If the functions are linear, i.e., \(f_i(\zeta) = w_i^\top \zeta + r_i\) for \(w_i \in \mathbb{R}^p\) and \(r_i \in \mathbb{R}\), then \(T \leq (3M)^p\).
2. If the functions are quadratic, i.e., \(f_i(\zeta) = \zeta^\top Q_i \zeta + w_i^\top \zeta + r_i\) for \(Q_i \in \mathbb{R}^{p \times p}\), \(w_i \in \mathbb{R}^p\), and \(r_i \in \mathbb{R}\), then \(T \leq (3M)^{p^2 + p}\).

First, we prove a structural property for the parameterized family of metrics. We show that for any fixed metrics \(d_1, \ldots, d_L\) and clustering instance \(S = \{x_1, \ldots, x_n\} \subset \mathcal{X}\), we can find a sign-pattern partitioning of \(\Delta_L\) induced by linear functions such that, on each region, the ordering over pairs of points in \(S\) induced by the metric \(d_\beta\) is constant. For our purposes, the most important consequence of this result is that for each region \(Z\) in this partitioning of \(\Delta_L\), the following holds: For any 2-point-based merge function \(D\) and any pair of clusters \(A, B \subset S\), there exists a pair of points \((a, b) \in A \times B\) such that \(D(A, B; d_\beta) = d_\beta(a, b)\) for all \(\beta \in Z\). In other words, restricted to \(\beta\) parameters belonging to \(Z\), the same pair of points \((a, b)\) defines the \(D\)-merge distance for the clusters \(A\) and \(B\).

**Lemma 2.** Fix any metrics \(d_1, \ldots, d_L\) and a clustering instance \(S \subset \mathcal{X}\). There exists a set \(\mathcal{H}\) of \(O(|S|^4)\) linear functions mapping \(\mathbb{R}^L\) to \(\mathbb{R}\) with the following property: if two metric parameters \(\beta, \beta' \in \Delta_L\) belong to the same region in the sign-pattern partition induced by \(\mathcal{H}\), then the ordering over pairs of points in \(S\) given by \(d_\beta\) and \(d_\beta'\) are the same. That is, for all points \(a, b, a', b' \in S\) we have \(d_\beta(a, b) \leq d_\beta(a', b')\) iff \(d_\beta'(a, b) \leq d_\beta'(a', b')\).

**Proof.** Let \(S\) be any clustering instance and fix points \(a, b, a', b' \in S\). For any parameter \(\beta \in \Delta_L\), by definition of \(d_\beta\), we have that

\[
d_\beta(a, b) \leq d_\beta(a', b') \iff \sum_{i=1}^L \beta_i d_i(a, b) \leq \sum_{i=1}^L \beta_i d_i(a', b') \iff \sum_{i=1}^L \beta_i (d_i(a, b) - d_i(a', b')) \leq 0.
\]
Define the linear function $h_{a,b,a',b'}(\beta) = \sum_{i=1}^{L} \beta_i (d_i(a, b) - d_i(a', b'))$. Then we have that $d_{\beta}(a, b) \leq d_{\beta}(a', b')$ if $h_{a,b,a',b'}(\beta) \leq 0$ and $d_{\beta}(a, b) > d_{\beta}(a', b')$ if $h_{a,b,a',b'}(\beta) > 0$.

Let $\mathcal{H} = \{h_{a,b,a',b'} | a, b, a', b' \in S\}$ be the collection of all such linear functions collected over all possible subsets of 4 points in $S$. Now suppose that $\beta$ and $\beta'$ belong to the same region in the sign-pattern partition induced by $\mathcal{H}$. For any points $a, b, a', b' \in S$, we are guaranteed that $\text{sign}(h_{a,b,a',b'}(\beta)) = \text{sign}(h_{a,b,a',b'}(\beta'))$, which by the above arguments imply that $d_{\beta}(a, b) \leq d_{\beta}(a', b')$ if $d_{\beta'}(a, b) \leq d_{\beta'}(a', b')$, as required.

Building on Lemma 2, we now prove the main structural property of Algorithm 1. We argue that for any clustering instance $S \subset X$, we can find a sign-pattern partition induced by quadratic functions of $\Delta_L \times \Delta_L \subseteq \mathbb{R}^{L+L}$ over $\alpha$ and $\beta$ into regions such that on each region, the ordering over all pairs of clusters according to the merge distance is fixed. This implies that for all $(\alpha, \beta)$ in one region of the partition, the output of Algorithm 1 when run on $S$ is constant, since the algorithm output only depends on the ordering over pairs of clusters in $S$ given by $D_\alpha(\cdot, \cdot; d_{\beta})$.

**Lemma 3.** Fix any metrics $d_1, \ldots, d_L$, any 2-point-based merge functions $D_1, \ldots, D_{L'}$, and clustering instance $S \subset X$. There exists a set $Q$ of $O(3^L |S|^{4L+L})$ quadratic functions defined on $\mathbb{R}^{L+L}$ so that if parameters $(\alpha, \beta)$ and $(\alpha', \beta')$ belong to the same region of the sign-pattern partition induced by $Q$, then the ordering over pairs of clusters in $S$ given by $D_\alpha(\cdot, \cdot; d_{\beta})$ and $D_\alpha'(\cdot, \cdot; d_{\beta'})$ is the same. That is, for all clusters $A, B, A', B' \subseteq S$, we have that $D_\alpha(A, B; d_{\beta}) \leq D_\alpha'(A', B'; d_{\beta'})$ iff $D_\alpha(A, B; d_{\beta}) \leq D_\alpha'(A', B'; d_{\beta'})$.

**Proof.** From Lemma 2 we know we can find a set $\mathcal{H}$ of $O(|S|^L)$ linear functions defined on $\mathbb{R}^L$ that induce a sign-pattern partition of the $\beta$ parameter space $\Delta_L \subseteq \mathbb{R}^L$ into regions where the ordering over pairs of points according to the $d_{\beta}$ distance is constant. From the first statement in Lemma 1 we know that this partition has at most $O((3|\mathcal{H}|)^L) = O(3^L |S|^{4L})$ regions.

Now let $Z \subseteq \Delta_L$ be any region of the sign-pattern partition of $\Delta_L$ induced by $\mathcal{H}$. From Lemma 2 we know that for all parameters $\beta \in Z$, the ordering over pairs of points in $S$ according to $d_{\beta}$ is fixed. For any 2-point-based merge function, the pair of points used to measure the distance between a pair of clusters depends only on ordering of pairs of points according to distance. Therefore, since $D_1, \ldots, D_{L'}$ are 2-point-based, we know that for any pair of clusters $(A, B)$ and each merge function index $i \in [L']$, there exists a pair of points $(a_i, b_i) \in A \times B$ such that $D_i(A, B; d_{\beta}) = d_{\beta}(a_i, b_i)$ for all $\beta \in Z$. In other words, all of the merge functions measure distances between $A$ and $B$ using a fixed pair of points for all values of the metric parameter $\beta$ in the region $Z$. Similarly, let $A', B' \subseteq S$ be any other pair of clusters and $(a_i', b_i') \in A' \times B'$ be the pairs of points defining $D_i(A', B'; d_{\beta})$ for each $i \in [L']$. Then for all $\beta \in Z$, we have that

$$D_\alpha(A, B; d_{\beta}) \leq D_\alpha(A', B'; d_{\beta}) \iff \sum_{i=1}^{L'} \alpha_i D_i(A, B; d_{\beta}) \leq \sum_{i=1}^{L'} \alpha_i D_i(A, B; d_{\beta})$$

$$\iff \sum_{i=1}^{L'} \alpha_i \sum_{j=1}^{L} \beta_j d_j(a_i, b_i) \leq \sum_{i=1}^{L'} \alpha_i \sum_{j=1}^{L} \beta_j d_j(a_i', b_i')$$

$$\iff \sum_{i=1}^{L'} \sum_{j=1}^{L} \alpha_i \beta_j (d_j(a_i, b_i) - d_j(a_i', b_i')) \leq 0.$$

Now define the quadratic function

$$q_{A,B,A',B'}(\alpha, \beta) = \sum_{i=1}^{L'} \sum_{j=1}^{L} \alpha_i \beta_j (d_j(a_i, b_i) - d_j(a_i', b_i')).$$

For all $\beta \in Z$, we are guaranteed that $D_\alpha(A, B; d_{\beta}) \leq D_\alpha(A', B'; d_{\beta})$ if and only if $q_{A,B,A',B'}(\alpha, \beta) \leq 0$. Notice that the coefficients of $q_{A,B,A',B'}$ only depend on $4L'$ points in $S$, which implies that if we collect these quadratic functions over all quadruples of clusters $A, B, A', B' \subseteq S$, we will only obtain $O(|S|^{4L'})$ different
quadratic functions. These $O(|S|^{4L'})$ functions induce a sign-pattern partition of $\Delta_{L'} \times Z$ for which the desired conclusion holds.

In order to obtain the result for the entire joint parameter space $\Delta_{L'} \times \Delta_L$, let $Q \subseteq H$ (viewed as quadratic functions over $\mathbb{R}^{L'+L}$) by placing a zero coefficient on all quadratic terms and terms depending on $\alpha$, as well as the $O(|S|^{4L'})$ quadratic functions obtained from each region $Z$ in the sign-pattern partition of $H$ described above. Since each of the $O(3^L|S|^{4L'})$ regions in the sign-pattern partition of $H$ contribute $O(|S|^{4L'})$ quadratic functions to $Q$, the total size of $Q$ is $|Q| = O(3^L|S|^{4L'+L})$.

Now suppose that $(\alpha', \beta')$ and $(\alpha, \beta)$ belong to the same region of the sign-pattern partition of $\Delta_{L'} \times \Delta_L \subseteq \mathbb{R}^{L'+L}$ induced by the quadratic functions $Q$. Since $Q$ contains $H$, this implies that $\beta$ and $\beta'$ belong to the same region in the sign-pattern partition induced by $H$. Moreover, since $Q$ contains all the quadratic functions defined in (2) for that region, it follows that $D_{\alpha}(A, B; d_{\beta}) \leq D_{\alpha'}(A', B'; d_{\beta'})$ if and only if $D_{\alpha}(A, B; d_{\beta}) \leq D_{\alpha}(A', B'; d_{\beta'})$, as required.

\[ \Box \]

3 Efficient Algorithm Selection

In this section we provide efficient algorithms for learning low-loss clustering algorithms for application-specific distributions $D$ defined over clustering instances. We focus on two special cases of the general family introduced in Section 2. At the end of the section, we discuss how to generalize our techniques to other cases. In the first case, we fix the merge function to be complete linkage, $D_{\text{merge}}(A, B; d) = \max_{a \in A, b \in B} d(a, b)$, and any pair of metrics $d_0$ and $d_1$ and consider the algorithm family that interpolates between the metrics $d_0$ and $d_1$ (i.e., $L' = 1$ and $L = 2$). To simplify notation, in this case we consider a single parameter $\beta \in [0, 1]$ and define $d_{\beta}(x, x') = (1 - \beta)d_0(x, x') + \beta d_1(x, x')$. For any clustering instance $S$, we let $A_{\beta, \text{metric}}(S; d_0, d_1)$ denote the output cluster tree of running the algorithm with parameter $\beta$ on instance $S$ and let $A_{\beta, \text{merge}}(d_0, d_1)$ denote the family of all such algorithms. When the pair of metrics is clear from context, we omit them.

Next, we consider the case where we fix any metric $d_0$ and any pair of merge functions $D_0$ and $D_1$ and consider the algorithm family that interpolates between the given merge functions (i.e., $L' = 2$ and $L = 1$). Again, we use a single parameter $\alpha \in [0, 1]$ to parameterize this family, defining the merge function $D_{\alpha}(A, B; d) = (1 - \alpha)D_0(A, B; d) + \alpha D_1(A, B; d)$. We let $A_{\alpha, \text{merge}}(S; D_0, D_1)$ denote the cluster tree produced by the algorithm with parameter $\alpha$ and $A_{\alpha, \text{merge}}(D_0, D_1)$ denote this algorithm family. Again, when $D_0$ and $D_1$ are clear from context, we omit them.

Our goal is to design efficient procedures for finding the algorithm in these families that has the lowest average loss on a sample of labeled clustering instances $(S_1, Y_1), \ldots, (S_N, Y_N)$ where $Y_i = (C_{i,1}^{(i)}, \ldots, C_{i,k}^{(i)})$ is the target clustering for instance $S_i$. Recall that the loss function $\ell(T, Y)$ defined in (1) computes the Hamming distance between the target clustering $Y$ and the closest pruning of the cluster tree $T$. Formally, our goal is to solve the following optimization problems:

\[
\arg\min_{\alpha \in [0, 1]} \frac{1}{N} \sum_{i=1}^{N} \ell(A_{\alpha, \text{merge}}(S_i; D_0, D_1), Y_i), \quad \text{and} \quad \arg\min_{\beta \in [0, 1]} \frac{1}{N} \sum_{i=1}^{N} \ell(A_{\beta, \text{metric}}(S_i; d_0, d_1), Y_i).
\]

The key challenge of these optimization problems is that, for a fixed clustering instance $S$ and any of our algorithm families, we can partition the parameter space $[0, 1]$ into finitely many intervals such that for each interval $I$, the cluster tree output by the algorithm is the same for every parameter in $I$. It follows that the loss function is a piecewise constant function of the algorithm parameter. Therefore, both optimization problems are non-convex and the loss derivative is zero wherever it is defined, rendering gradient descent and similar algorithms ineffective.

We solve the optimization problems by explicitly computing the piecewise constant loss function for each instance $S_i$. That is, for clustering instance $i$ we find a collection of discontinuity locations $0 = c_0^{(i)} < \cdots < c_M^{(i)} = 1$ and values $v_0^{(i)}, \ldots, v_M^{(i)} \in \mathbb{R}$ so that for each $j \in [M]$, running the algorithm on instance $S_i$ with a parameter in $[c_j^{(i)}, c_{j+1}^{(i)})$ has loss equal to $v_j^{(i)}$. Given this representation of the loss functions for all $N$ instances, finding the parameter with minimal average loss can be done in $O(M \log(M))$ time, where $M = \sum_i M_i$ is the total number of discontinuities from all $N$ loss functions. To do this, sort the set of all
discontinuities from all $N$ loss functions and then enumerate the corresponding partition of $\mathbb{R}$ keeping a running average of the loss on each interval, while remembering the lowest loss interval encountered. The bulk of the computational cost is incurred by computing the piecewise constant loss functions, which we focus on for the rest of the section.

Our efficient optimization procedures exploit a more powerful structural property of the algorithm families we study: for a clustering instance $S$, not only is the output cluster tree a piecewise constant function of the algorithm parameter, but for any length $t$, the sequence of first $t$ merges performed by the algorithm is a piecewise constant function of the parameter. For length $t = 0$, the partition is a single region containing all parameters in $[0, 1]$, since every algorithm trivially starts with the empty sequence of merges. For each length $t > 0$, the piecewise constant partition for the first $t$ merges is a refinement of the partition for $t - 1$ merges. We can represent this sequence of partitions using a partition tree, which is a tree where each node is labeled by an interval, for all depths $t$ the nodes at depth $t$ partition $[0, 1]$, and edges represent subset relationships. The tree described above represents all possible execution paths for the algorithm family when run on the instance $S$ as we vary the algorithm parameter. In particular, each path from the root node to a leaf corresponds to one possible sequence of merges. We therefore call this tree the execution tree of the algorithm family when run on $S$. Figure 1 shows an example execution tree for the family $A_{\text{merge}}(D_{\text{min}}, D_{\text{max}})$. To find the piecewise constant loss function for a clustering instance $S$, we perform a depth-first traversal of the leaves of the execution tree and compute the loss for the cluster tree produced at each leaf.

**Optimizing the Merge Function.** In this section we show that for any merge functions $D_0$ and $D_1$ and any clustering instance $S$, the execution tree of $A_{\text{merge}}(D_0, D_1)$ when run on $S$ is well defined. Moreover, we give an efficient algorithm for finding the children of any node in the tree. Finally, we show how to compute the piecewise constant loss function for $A_{\text{merge}}(D_0, D_1)$ on the instance $S$ by performing a depth-first traversal of the execution tree.

**Lemma 4.** For any merge functions $D_0$ and $D_1$ and any clustering instance $S$, the execution tree for $A_{\text{merge}}(D_0, D_1)$ when run on $S$ is well defined. That is, there exists a partition tree s.t. for any node $v$ at depth $t$, the same sequence of first $t$ merges is performed by $A_{\alpha}^{\text{merge}}$ for all $\alpha$ in node $v$’s interval.

Next, we provide an efficient algorithm for finding the children of a node in the execution tree. Given the node’s parameter interval $I = [\alpha_{\text{lo}}, \alpha_{\text{hi}}]$ and the set of clusters $C_1, \ldots, C_m$ resulting from that node’s merge sequence, we use a sweep-line algorithm to determine all possible next merges and the corresponding parameter intervals. First, we calculate the merge for $\alpha = \alpha_{\text{lo}}$ by enumerating all pairs of clusters. Suppose clusters $C_i$ and $C_j$ are the optimal merge for $\alpha = \alpha_{\text{lo}}$. We then determine the largest value $\alpha'$ for which we will still merge these clusters by solving the linear equation $D_\alpha(C_i, C_j) = D_\alpha(C_k, C_l)$ for all other pairs of clusters $C_k$ and $C_l$, keeping track of the minimal solution larger than $\alpha$. Denote the minimal solution larger than $\alpha$ by $c \in I$. We are guaranteed that $A_{\alpha'}^{\text{merge}}$ will merge clusters $C_i$ and $C_j$ for all $\alpha' \in [\alpha, c)$. We repeat this procedure starting from $\alpha = c$ to determine the next merge and corresponding interval, and so on, sweeping through the $\alpha$ parameter space until $\alpha \geq \alpha_{\text{hi}}$. Pseudocode is given in Algorithm 2. Figure 2 shows an example of the operation of Algorithm 2. Our next result bounds the running time of this procedure.

![Figure 1: An example of the execution tree of $A_{\text{merge}}(D_{\text{min}}, D_{\text{max}})$ for a clustering instance with 4 points. We also show the clustering of the points produced by the sequence of merges associated with each node in the tree. Each colored rectangle represents a cluster.](image)
Figure 2: This diagram shows the operation of Algorithm 2 when given three clusters, \( C_1, C_2, \) and \( C_3 \). Each colored line depicts the \( D_\alpha \)-distance between one pair of cluster as a function of the parameter \( \alpha \). On the first iteration, Algorithm 2 determines that clusters \( C_2 \) and \( C_3 \) are the closest for the parameter \( \alpha = \alpha_{lo} \).

Next, it calculates the critical parameter values \( c_{12} \) and \( c_{13} \), shown on the \( \alpha \)-axis. Finally, the algorithm advances \( \alpha \) to the closest critical value, \( c_{13} \) shown.

Repeating the process results in the final output shown.

**Lemma 5.** Let \( C_1, \ldots, C_m \) be a collection of clusters, \( D_0 \) and \( D_1 \) be any pair of merge functions, and \([\alpha_{lo}, \alpha_{hi}]\) be a subset of the parameter space. If there are \( M \) distinct cluster pairs \( C_i, C_j \) that minimize \( D_\alpha(C_i, C_j) \) for values of \( \alpha \in [\alpha_{lo}, \alpha_{hi}] \), then the running time of Algorithm 2 is \( O(Mn^2K) \), where \( K \) is the cost of evaluating the merge functions \( D_0 \) and \( D_1 \).

**Algorithm 2** Find all merges for \( A_{merge}(D_0, D_1) \)

**Input:** Set of clusters \( C_1, \ldots, C_m \), merge functions \( D_0, D_1 \), parameter interval \([\alpha_{lo}, \alpha_{hi}]\).

1. Let \( M = \emptyset \) be the initially empty set of possible merges.
2. Let \( I = \emptyset \) be the initially empty set of parameter intervals.
3. Let \( \alpha = \alpha_{lo} \).
4. While \( \alpha < \alpha_{hi} \):
   (a) Let \( C_i, C_j \) be the pair of clusters minimizing \((1 - \alpha) \cdot D_0(C_i, C_j) + \alpha \cdot D_1(C_i, C_j)\).
   (b) For each \( k, l \in [m] \), let \( c_{kl} = \Delta_0 / (\Delta_0 - \Delta_1) \), where \( \Delta_0 = D_p(C_i, C_j) - D_p(C_k, C_l) \) for \( p \in \{0, 1\} \).
   (c) Let \( c = \min\{c_{kl} \mid c_{kl} > \alpha\} \cup \{\alpha_{hi}\} \).
   (d) Add merge \((C_i, C_j)\) to \( M \) and \((\alpha, c)\) to \( I \).
   (e) Set \( \alpha = c \).
5. Return \( M \) and \( I \).

With this, our algorithm for computing the piecewise constant loss function for an instance \( S \) performs a depth-first traversal of the leaves of the execution tree for \( A_{merge}(D_0, D_1) \), using Algorithm 2 to determine the children of each node. When we reach a leaf in the depth-first traversal, we have both the corresponding parameter interval \( I \subset [0, 1] \), as well as the cluster tree \( T \) such that \( A_{merge}^*(S) = T \) for all \( \alpha \in I \). We then evaluate the loss \( l(T, Y) \) to get one piece of the piecewise constant loss function. Detailed pseudocode for this approach is given in Algorithm 4 in Appendix B.

**Theorem 2.** Let \( S = \{x_1, \ldots, x_n\} \) be a clustering instance and \( D_0 \) and \( D_1 \) be any two merge functions. Suppose that the execution tree of \( A_{merge}(D_0, D_1) \) on \( S \) has \( E \) edges. Then the total running time of Algorithm 2 is \( O(En^2K) \), where \( K \) is the cost of evaluating \( D_0 \) and \( D_1 \) once.

In many cases the merge functions can be evaluated in constant time, at the cost of maintaining an \( O(n^2) \)-memory data structure storing the merge distances between clusters. For example, when using single linkage we can maintain an \( n \times n \) matrix of merge distances between pairs of clusters (i.e., the distance between each pair of cluster’s closest pair of points). Whenever we merge a pair of clusters, we can update this matrix in \( O(n) \) time, since we only need to compute single-linkage distances between each cluster and
the newly merged cluster, and those distances are the minimum of two entries in the previous matrix. Given that the \( O(n) \) cost of updating the distance matrix is smaller than the \( O(n^2) \) cost of finding the best pair of clusters to merge, maintaining the distance matrix does not significantly increase the overall running time of the algorithm.

We can express the running time of Algorithm 4 in terms of the number of discontinuities of the function \( \alpha \mapsto A_{\alpha}^{\text{merge}}(S) \). There is one leaf of the execution tree for each constant interval of this function, and the path from the root of the execution tree to that leaf is of length \( n - 1 \). Therefore, the cost associated with that path is at most \( O(Kn^3) \) and enumerating the execution tree to obtain the piecewise constant loss function for a given instance \( S \) spends \( O(Kn^3) \) time for each constant interval of \( \alpha \mapsto A_{\alpha}^{\text{merge}}(S) \). In contrast, the combinatorial approach of Balcan et al. \[4\] requires that we run \( \alpha \)-linkage once for every interval in their partition of \([0, 1]\), which always contains \( O(n^5) \) intervals (i.e., it is a refinement of the piecewise constant partition). Since each run of \( \alpha \)-Linkage costs \( O(Kn^2 \log n) \) time, this leads to a running time of \( O(Kn^{10} \log n) \). The key advantage of our approach stems from the fact that the number of discontinuities of the function \( \alpha \mapsto A_{\alpha}^{\text{merge}}(S) \) is often several orders of magnitude smaller than \( O(n^8) \).

**Optimizing the Metric.** Next, we show that a similar algorithmic approach can be used for finding the piecewise constant loss function for the family \( A_{\text{metric}}(d_0, d_1) \) on a clustering instance \( S \). We prove that the execution tree is well defined, and provide an efficient algorithm for finding the children of each node in the execution tree, allowing us to use a depth-first traversal to find the piecewise constant loss function for any clustering instance \( S \).

**Lemma 6.** For any metrics \( d_0 \) and \( d_1 \) and any clustering instance \( S \), the execution tree for the family \( A_{\text{metric}}(d_0, d_1) \) when run on \( S \) is well defined. That is, there exists a partition tree s.t. for any node \( v \) at depth \( t \), the same sequence of first \( t \) merges is performed by \( A_{\beta}^{\text{metric}} \) for all \( \beta \) in \( v \)'s interval.

Next, we provide an efficient procedure for determining the children of a node \( v \) in the execution tree of \( A_{\text{metric}}(d_0, d_1) \). Given the node’s parameter interval \( I = [\beta_{lo}, \beta_{hi}] \) and the set of clusters \( C_1, \ldots, C_m \) resulting from that node’s sequence of merges, we again use a sweep-line procedure to find the possible next merges and the corresponding parameter intervals. First, we determine the pair of clusters that will be merged by \( A_{\beta}^{\text{metric}} \) for \( \beta = \beta_{lo} \) by enumerating all pairs of clusters. Suppose the winning pair is \( C_i \) and \( C_j \) and let \( x \in C_i \) and \( x' \in C_j \) be the farthest pair of points between the two clusters. Next, we find the largest value of \( \beta' \) for which we will still merge the clusters \( C_i \) and \( C_j \). To do this, we enumerate all other pairs of clusters \( C_k \) and \( C_l \) and all pairs of points \( y \in C_k \) and \( y' \in C_l \), and solve the linear equation \( d_\beta(x, x') = d_\beta(y, y') \), keeping track of the minimal solution larger than \( \beta \). Denote the minimal solution larger than \( \beta \) by \( c \). We are guaranteed that for all \( \beta' \in [\beta, c) \), the pair of clusters merged will be \( C_i \) and \( C_j \). Then we repeat the process with \( \beta = c \) to find the next merge and corresponding interval, and so on, until \( \beta \geq \beta_{hi} \). Pseudocode for this procedure is given in Algorithm 5. The following Lemma bounds the running time:

**Lemma 7.** Let \( C_1, \ldots, C_m \) be a collection of clusters, \( d_0 \) and \( d_1 \) be any pair of metrics, and \( [\beta_{lo}, \beta_{hi}] \) be a subset of the parameter space. If there are \( M \) distinct cluster pairs \( C_i, C_j \) that complete linkage would merge when using the metric \( d_\beta \) for \( \beta \in [\beta_{lo}, \beta_{hi}] \), the running time of Algorithm 5 is \( O(Mn^2) \).

Our algorithm for computing the piecewise constant loss function for an instance \( S \) is almost identical for the case of the merge function: it performs a depth-first traversal of the leaves of the execution tree for \( A_{\text{metric}}(d_0, d_1) \), using Algorithm 5 to determine the children of each node. Detailed pseudocode for this approach is given in Algorithm 6 in Appendix B. The following Theorem characterizes the overall running time of the algorithm.

**Theorem 3.** Let \( S = \{x_1, \ldots, x_n\} \) be a clustering instance and \( d_0 \) and \( d_1 \) be any two merge functions. Suppose that the execution tree of \( A_{\text{metric}}(d_0, d_1) \) on \( S \) has \( E \) edges. Then the total running time of Algorithm 6 is \( O(En^2) \).

**General Algorithm Families.** The key idea in our efficient selection procedures is to define an execution tree that describes all possible execution paths for the algorithm family when run on a fixed instance \( S \) with varying parameters. Next, we perform a depth-first traversal of the leaves of the execution tree to find a
Our first distribution over clustering tasks corresponds to clustering subsets of the MNIST dataset [12], which contains 80,000 hand-written examples of the digits 0 through 9. We generate a random clustering instance from the MNIST data as follows: first, we select $k = 5$ digits from $\{0, \ldots, 9\}$ at random, then we randomly select 200 examples belonging to each of the selected digits, giving a total of $n = 1000$ images. The target clustering for this instance is given by the ground-truth digit labels. We measure distances between any pair of digits in terms of the Euclidean distance between their images represented as vectors of pixel intensities.

CIFAR-10 Subsets. We also consider a distribution over clustering tasks that corresponds to clustering subsets of the CIFAR-10 dataset [12]. This dataset contains 6000 images of each of the following classes: airplane,
automobile, bird, cat, deer, dog, frog, horse, ship, and truck. Each example is a 32 × 32 color image with 3 color channels. We pre-process the data to obtain neural-network feature representations for each example. We include 50 randomly rotated and cropped versions of each example and obtain feature representations from layer ‘in4d’ of a pre-trained Google inception network. This gives a 144-dimensional feature representation for each of the 3000000 examples (50 randomly rotated copies of the 600000 examples for each of the 10 classes).

We generate clustering tasks from CIFAR-10 as follows: first, select \( k = 5 \) classes at random, then choose 50 examples belonging to each of the selected classes, giving a total of \( n = 250 \) images. The target clustering for this instance is given by the ground-truth class labels. We measure distance between any pair of images as the distance between their feature embeddings.

**Omniglot Subsets.** Next, we consider a distribution over clustering tasks corresponding to clustering subsets of the Omniglot dataset \([13]\). The Omniglot dataset consists of written characters from 50 different alphabets with a total of 1623 different characters. The dataset includes 20 examples of each character, leading to a total of 32,460 examples. We generate a random clustering instance from the Omniglot data as follows: first, we choose one of the alphabets at random. Next, we choose \( k \) uniformly in \( \{5, \ldots, 10\} \) and choose \( k \) random characters from that alphabet. The clustering instance includes 20\( k \) examples and the target clustering is given by the ground-truth character labels.

We use two different distance metrics on the Omniglot dataset. First, we use the cosine distance between neural network feature embeddings. The neural network was trained to perform digit classification on MNIST. Second, each example has both an image of the written character, as well as the stroke trajectory (i.e., a time series of \((x, y)\) coordinates of the tip of the pen when the character was written). We also use the following distance defined in terms of the strokes: Given two trajectories \( s = (x_t, y_t)_{t=1}^T \) and \( s' = (x'_t, y'_t)_{t=1}^T \), we define the distance between them by:

\[
d(s, s') = \frac{1}{T+\epsilon} \left( \sum_{t=1}^T d((x_t, y_t), s') + \sum_{t=1}^T d((x'_t, y'_t), s) \right),
\]

where \( d((x_t, y_t), s') \) denotes the Euclidean distance from the point \((x_t, y_t)\) to the closest point in \( s' \). This is the average distance from any point from either trajectory to the nearest point on the other trajectory. This hand-designed metric provides a complementary notion of distance to the neural network feature embeddings.

**Synthetic Rings and Disks.** We consider a two dimensional synthetic distribution where each clustering instance has 4 clusters, where two are ring-shaped and two are disk-shaped. To generate each instance we sample 100 points uniformly at random from each ring or disk. The two rings have radiiuses 0.4 and 0.8, respectively, and are both centered at the origin. The two disks have radius 0.4 and are centered at \((1.5, 0.4)\) and \((1.5, -0.4)\), respectively. For this data, we measure distances between points in terms of the Euclidean distance between them.

**Results.**

**Learning the Merge Function.** Figure 2 shows the average loss when interpolating between single and complete linkage as well as between average and complete linkage for each of the clustering instance distributions described above. For each value of the parameter \( \alpha \in [0, 1] \), we report the average loss over \( N = 1000 \) i.i.d. instances drawn from the corresponding distribution. We see that the optimal parameters vary across different clustering instances. For example, when interpolating between single and complete linkage, the optimal parameters are \( \alpha = 0.874 \) for MNIST, \( \alpha = 0.98 \) for CIFAR-10, \( \alpha = 0.179 \) for Rings and Disks, and \( \alpha = 0.931 \) for Omniglot. Moreover, using the parameter that is optimal for one distribution on another would lead to significantly worse clustering performance. Next, we also see that for different distributions, it is possible to achieve non-trivial improvements over single, complete, and average linkage by interpolating between them. For example, on the Rings and Disks distribution we see an improvement of almost 0.2 error, meaning that an additional 20% of the data is correctly clustered.

**Learning the metric for Omniglot.** Next we consider learning the best metric for the Omniglot clustering distribution. In this case, we interpolate between the two distance metrics described above: the cosine distance between neural network embeddings of each example image, and a hand-designed stroke distance. Figure 3 shows the empirical loss for each parameter \( \beta \) averaged over \( N = 4000 \) samples from the Omniglot distribution. The best “base” metric is the neural network feature embedding, which results in an average
Figure 3: Empirical loss for interpolating between single and complete linkage as well as between average and complete linkage over 1000 sampled clustering instances from the MNIST Subsets, CIFAR-10 Subsets, Rings and Disks, and Omniglot distributions.

loss of 0.421. The optimal parameter value occurs at $\beta = 0.514$ with an average loss of 0.330, giving an improvement of 0.091. In other words, running complete linkage with the mixed metric correctly clusters almost an extra 10% of the data correctly.

Figure 4: Empirical loss for interpolating between the two distance metrics on the Omniglot data. $\beta = 0$ is the stroke distance, while $\beta = 1$ is the neural network embedding.

5 Conclusion

In this work we study both the sample and algorithmic complexity of learning linkage-based clustering algorithms with low loss for specific application domains. We give strong bounds on the number of sample instances required from an application domain in order to find an approximately optimal algorithm from a rich family of algorithms that allows us to vary both the metric and merge function used by the algorithm. We complement our sample complexity results with efficient algorithms for finding empirically optimal algorithms.
for a sample of instances. Finally, we carry out experiments on both real-world and synthetic clustering domains demonstrating that our procedures can often find algorithms that significantly outperform standard linkage-based clustering algorithms.

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Lemma 1. Let \( T \) be the number of regions in the sign-pattern partition of \( \mathbb{R}^p \) induced by \( f_1, \ldots, f_M : \mathbb{R}^p \to \mathbb{R} \).
1. If the functions are linear, i.e., $f_i(\zeta) = w_i^T \zeta + r_i$ for $w_i \in \mathbb{R}^p$ and $r_i \in \mathbb{R}$, then $T \leq (3M)^p$.
2. If the functions are quadratic, i.e., $f_i(\zeta) = \zeta^T Q_i \zeta + w_i^T \zeta + r_i$ for $Q_i \in \mathbb{R}^{p \times p}$, $w_i \in \mathbb{R}^p$, and $r_i \in \mathbb{R}$, then $T \leq (3M)^{p^2 + p}$.

Proof. The proof of the first statement follows from the work of Buck [9], which shows that if $\mathcal{H}$ is a collection of $M$ hyperplanes in $\mathbb{R}^p$, then the number of connected components of $\mathbb{R}^p \setminus \mathcal{H}$ is at most $(3M)^p$. To connect this to the sign-pattern partitioning induced by the collection of linear functions $f_1, \ldots, f_M$, let $\mathcal{H}$ be the set of $M$ hyperplanes defined by $\{\zeta \in \mathbb{R}^p \mid f_i(\zeta) = 0\}$ for $i \in [M]$. The connected components of $\mathbb{R}^p \setminus \mathcal{H}$ correspond exactly to the sign-pattern partition of the functions $f_1, \ldots, f_M$, and by the result of Buck [9], it follows that the number of regions in the partition is at most $(3M)^p$. Equivalently, we know that $|\{F(\zeta) \mid \zeta \in \mathbb{R}^p\}| \leq (3M)^p$, where $F(\zeta) = (\text{sign}(f_1(\zeta)), \ldots, \text{sign}(f_M(\zeta)))$ is the sign-pattern function. That is, $F$ takes at most $(3M)^p$ distinct values.

Next we use the first statement to prove the second statement. Let $\varphi : \mathbb{R}^p \to \mathbb{R}^{p^2 + p}$ be the function that maps a vector $\zeta$ to the vector containing all products of elements from $\zeta$ and all elements of $\zeta$:

$$\varphi(\zeta) = (\zeta_1 \zeta_1, \ldots, \zeta_1 \zeta_d, \ldots, \zeta_d \zeta_1, \ldots, \zeta_d \zeta_d, \zeta_1, \ldots, \zeta_d).$$

Let $q(\zeta) = \zeta^T Q \zeta + w^T \zeta + r$ be a quadratic function where $Q \in \mathbb{R}^{p \times p}$, $w \in \mathbb{R}^p$, and $r \in \mathbb{R}$. Now let

$$v = (q_{11}, \ldots, q_{1d}, \ldots, q_{d1}, \ldots, q_{dd}, w_1, \ldots, w_d).$$

Then we have that $q(\zeta) = v^T \varphi(\zeta)$. In other words, $q$ is a linear function of $\zeta$. This guarantees that we can find $M$ linear functions $h_1, \ldots, h_M : \mathbb{R}^{p^2 + p} \to \mathbb{R}$ such that $f_i(\zeta) = h_i(\varphi(\zeta))$ for all $i \in [M]$. Let $H : \mathbb{R}^{p^2 + p} \to \{\pm 1\}^M$ be the sign-pattern function for $h_1, \ldots, h_M$. Then we have

$$|\{F(\zeta) \mid \zeta \in \mathbb{R}^p\}| = |\{H(\varphi(\zeta)) \mid \zeta \in \mathbb{R}^p\}| \leq |\{H(\phi) \mid \phi \in \mathbb{R}^{p^2 + p}\}| \leq (3M)^{p^2 + p},$$

where the last inequality follows from the first statement for linear functions. It follows that the number of regions in the sign-pattern partition induced by $M$ quadratic functions is at most $(3M)^{p^2 + p}$. \hfill \qed

## B Appendix for Efficient Algorithm Selection

### B.1 Learning the Merge Function

#### Algorithm 4

**Depth-first Enumeration of α-linkage Execution Tree**

**Input:** Point set $x_1, \ldots, x_n$, cluster distance functions $a_1$ and $d_2$.

1. Let $r$ be the root node of the execution tree with $r.\mathcal{N} = \{(x_1), \ldots, (x_n)\}$ and $r.I = [0, 1]$.
2. Let $s$ be a stack of execution tree nodes, initially containing the root $r$.
3. Let $\mathcal{T} = \emptyset$ be the initially empty set of possible cluster trees.
4. Let $\mathcal{I} = \emptyset$ be the initially empty set of intervals.
5. While the stack $s$ is not empty:
   a. Pop execution tree node $e$ off stack $s$.
   b. If $e.\mathcal{N}$ has a single cluster, add $e.\mathcal{N}$ to $\mathcal{T}$ and $e.I$ to $\mathcal{I}$.
   c. Otherwise, for each merge $(C_i, C_j)$ and interval $I_e$ returned by Algorithm [2] run on $e.\mathcal{N}$ and $e.I$:
      i. Let $e$ be a new node with state given by $e.\mathcal{N}$ after merging $C_i$ and $C_j$ and $e.I = I_e$.
      ii. Push $e$ onto the stack $s$.
6. Return $\mathcal{T}$ and $\mathcal{I}$.

#### Lemma 4

For any merge functions $D_0$ and $D_1$ and any clustering instance $S$, the execution tree for $A_{\text{merge}}(D_0, D_1)$ when run on $S$ is well defined. That is, there exists a partition tree $s.t.$ for any node $v$ at depth $t$, the same sequence of $t$ merges is performed by $A_{\alpha}^{\text{merge}}$ for all $\alpha$ in node $v$’s interval.
**Proof.** The proof is by induction on the depth $t$. The base case is for depth $t = 0$, in which case we can use a single node whose interval is $[0, 1]$. Since all algorithms in the family start with an empty-sequence of merges, this satisfies the execution tree property.

Now suppose that there is a tree of depth $t$ with the execution tree property. If $t = |S| - 1$ then we are finished, since the algorithms in $A_{\text{merge}}(D_0, D_1)$ make exactly $|S| - 1$ merges. Otherwise, consider any leaf node $v$ of the depth $t$ tree with parameter interval $I_v$. It is sufficient to show that we can partition $I_v$ into subintervals such that for $\alpha$ in each subinterval the next merge performed is constant. By the inductive hypothesis, we know that the first $t$ merges made by $A_{\text{merge}}^\alpha$ are the same for all $\alpha \in I_v$. After performing these merges, the algorithm will have arrived at some set of clusters $C_1, \ldots, C_m$ with $m = |S| - t$. For each pair of clusters $C_i$ and $C_j$, the distance $D_{\alpha}(C_i, C_j) = (1 - \alpha) D_0(C_i, C_j) + \alpha D_1(C_i, C_j)$ is a linear function of the parameter $\alpha$. Therefore, for any clusters $C_i, C_j, C_k$, and $C_l$, the algorithm will prefer to merge $C_i$ and $C_j$ over $C_j$ and $C_k$ for a (possibly empty) sub-interval of $I_v$, corresponding to the values of $\alpha \in I_v$ where $D_{\alpha}(C_i, C_j) < D_{\alpha}(C_k, C_l)$. For any fixed pair of clusters $C_i$ and $C_j$, taking the intersection of these intervals over all other pairs $C_j$ and $C_k$ guarantees that clusters $C_i$ and $C_j$ will be merged exactly for parameter values in some subinterval of $I_v$. For each merge with a non-empty parameter interval, we can introduce a child node of $v$ labeled by that parameter interval. These children partition $I_v$ into intervals where the next merge is constant, as required.

**Lemma 5.** Let $C_1, \ldots, C_m$ be a collection of clusters, $D_0$ and $D_1$ be any pair of merge functions, and $[\alpha_{lo}, \alpha_{hi})$ be a subset of the parameter space. If there are $M$ distinct cluster pairs $C_i, C_j$ that minimize $D_{\alpha}(C_i, C_j)$ for values of $\alpha \in [\alpha_{lo}, \alpha_{hi})$, then the running time of Algorithm $[2]$ is $O(Mm^2K)$, where $K$ is the cost of evaluating the merge functions $D_0$ and $D_1$.

**Proof.** The loop in step 4 of Algorithm $[2]$ runs once for each possible merge, giving a total of $M$ iterations. Each iteration finds the closest pair of clusters according to $D_{\alpha}$ using $O(m^2)$ evaluations of the merge functions $D_0$ and $D_1$. Calculating the critical parameter value $c$ involves solving $O(m^2)$ linear equations whose coefficients are determined by four evaluations of $D_0$ and $D_1$. It follows that the cost of each iteration is $O(m^2K)$, where $K$ is the cost of evaluating $D_0$ and $D_1$, and the overall running time is $O(Mm^2K)$.

**Theorem 2.** Let $S = \{x_1, \ldots, x_n\}$ be a clustering instance and $D_0$ and $D_1$ be any two merge functions. Suppose that the execution tree of $A_{\text{merge}}(D_0, D_1)$ on $S$ has $E$ edges. Then the total running time of Algorithm $[3]$ is $O(Em^2K)$, where $K$ is the cost of evaluating $D_0$ and $D_1$ once.

**Proof.** Fix any node $v$ in the execution tree with $m$ clusters $C_1, \ldots, C_m$ and $M$ outgoing edges (i.e., $M$ possible merges from the state represented by $v$). We run Algorithm $[2]$ to determine the children of $v$, which by Lemma $[5]$ costs $O(Mm^2K)$, since $m \leq n$. Summing over all non-leaves of the execution tree, the total cost is $O(Em^2K)$. In addition to computing the children of a given node, we need to construct the children nodes, but this takes constant time per child.

**B.2 Learning the Metric**

**Lemma 6.** For any metrics $d_0$ and $d_1$ and any clustering instance $S$, the execution tree for the family $A_{\text{metric}}(d_0, d_1)$ when run on $S$ is well defined. That is, there exists a partition tree s.t. for any node $v$ at depth $t$, the same sequence of first merges is performed by $A_{\beta}^{\text{metric}}$ for all $\beta$ in node $v$’s interval.

**Proof.** The proof is by induction on the depth $t$. The base case is for depth $t = 0$, in which case we can use a single node whose interval is $[0, 1]$. Since all algorithms in the family start with an empty-sequence of merges, this satisfies the execution tree property.

Now suppose that there is a tree of depth $t$ with the execution tree property. If $t = |S| - 1$ then we are finished, since the algorithms in $A_{\text{metric}}(d_0, d_1)$ make exactly $|S| - 1$ merges. Otherwise, consider any leaf node $v$ of the depth $t$ tree with parameter interval $I_v$. It is sufficient to show that we can partition $I_v$ into subintervals such that for $\beta$ in each subinterval the next merge performed is constant. By the inductive hypothesis, we know that the first $t$ merges made by $A_{\beta}^{\text{metric}}$ are the same for all $\beta \in I_v$. After performing these merges, the algorithm will have arrived at some set of clusters $C_1, \ldots, C_m$ with $m = |S| - t$. For each pair of clusters $C_i$ and $C_j$, the distance $D_{\alpha}(C_i, C_j)$ is a linear function of the parameter $\alpha$. Therefore, by the inductive hypothesis, the algorithm will prefer to merge $C_i$ and $C_j$ over $C_j$ and $C_k$ for a (possibly empty) sub-interval of $I_v$, corresponding to the values of $\alpha \in I_v$ where $D_{\alpha}(C_i, C_j) < D_{\alpha}(C_k, C_l)$. For any fixed pair of clusters $C_i$ and $C_j$, taking the intersection of these intervals over all other pairs $C_j$ and $C_k$ guarantees that clusters $C_i$ and $C_j$ will be merged exactly for parameter values in some subinterval of $I_v$. For each merge with a non-empty parameter interval, we can introduce a child node of $v$ labeled by that parameter interval. These children partition $I_v$ into intervals where the next merge is constant, as required.
Theorem 3. Let $S = \{x_1, \ldots, x_n\}$ be a clustering instance and $d_0$ and $d_1$ be any two merge functions. Suppose that the execution tree of $A_{\text{metric}}(d_0, d_1)$ on $S$ has $E$ edges. Then the total running time of Algorithm 5 is $O(En^2)$.

Proof. Fix any node $v$ in the execution tree with $m$ clusters $C_1, \ldots, C_m$ and $M$ outgoing edges (i.e., $M$ possible merges from the state represented by $v$). We run Algorithm 3 to determine the children of $v$, which by Lemma 7 costs $O(Mn^2)$. Summing over all non-leaves of the execution tree, the total cost is $O(En^2)$. \qed

Recall that algorithms in the family $A_{\text{metric}}(d_0, d_1)$ run complete linkage using the metric $d_\beta$. Complete linkage can be implemented in such a way that it only makes comparisons between pairwise point distances (i.e., is $d_\beta(x, x')$ larger or smaller than $d_\beta(y, y')$?). To see this, for any pair of clusters, we can find the farthest pair of points between them using only distance comparisons. And, once we have the farthest pair of points between all pairs of clusters, we can find the pair of clusters to merge by again making only pairwise comparisons. It follows that if two parameters $\beta$ and $\beta'$ have the same outcome for all pairwise distance comparisons, then the next merge to be performed must be the same. We use this observation to partition the interval $I_0$ into subintervals where the next merge is constant. For any pair of points $x, x' \in S$, the distance $d_\beta(x, x') = (1 - \beta)d_0(x, x') + \beta d_1(x, x')$ is a linear function of the parameter $\beta$. Therefore, for any points $x, x', y, y' \in S$, there is at most one critical parameter value where the relative order of $d_\beta(x, x')$ and $d_\beta(y, y')$ changes. Between these $O(|S|^4)$ critical parameter values, the ordering on all pairwise merges is constant, and the next merge performed by the algorithm will also be constant. Therefore, there must exist a partitioning of $I_0$ into at most $O(|S|^4)$ sub-intervals such that the next merge is constant on each interval.

We let the children of $v$ correspond to the coarsest such partition. \qed

Lemma 7. Let $C_1, \ldots, C_m$ be a collection of clusters, $d_0$ and $d_1$ be any pair of metrics, and $[\beta_{lo}, \beta_{hi})$ be a subset of the parameter space. If there are $M$ distinct cluster pairs $C_i, C_j$ that complete linkage would merge when using the metric $d_\beta$ for $\beta \in [\beta_{lo}, \beta_{hi})$, the running time of Algorithm 3 is $O(Mn^2)$.

Proof. The loop in step 4 of Algorithm 3 runs once for each possible merge, giving a total of $M$ iterations. Each iteration finds the merge performed by complete linkage using the $d_\beta$ metric, which takes $O(n^2)$ time, and then solves $O(n^2)$ linear equations to determine the largest value of $\beta'$ such that the same merge is performed. It follows that the cost of each iteration is $O(n^2)$, leading to an overall running time of $O(Mn^2)$. Note, we assume that the pairwise distances $d_\beta(x, x')$ can be evaluated in constant time. This can always be achieved by precomputing two $n \times n$ distance matrices for the base metrics $d_0$ and $d_1$, respectively. \qed

Algorithm 5 Depth-first Enumeration of $\beta$-linkage Execution Tree

Input: Point set $x_1, \ldots, x_n$, cluster distance functions $d_1$ and $d_2$.
1. Let $r$ be the root node of the execution tree with $r.N = \{(x_1), \ldots, (x_n)\}$ and $r.I = [0, 1]$.
2. Let $s$ be a stack of execution tree nodes, initially containing the root $r$.
3. Let $T = \emptyset$ be the initially empty set of possible cluster trees.
4. Let $I = \emptyset$ be the initially empty set of intervals.
5. While the stack $s$ is not empty:
   (a) Pop execution tree node $e$ off stack $s$.
   (b) If $e.N$ has a single cluster, add $e.N$ to $T$ and $e.I$ to $I$.
   (c) Otherwise, for each merge $(C_i, C_j)$ and interval $I_i$ returned by Algorithm 3 run on $e.N$ and $e.I$:
      i. Let $c$ be a new node with state given by $e.N$ after merging $C_i$ and $C_j$ and $e.I = I_c$.
      ii. Push $c$ onto the stack $s$.
6. Return $T$ and $I$. 

s