Abstract

The problem of nearest-neighbor condensation deals with finding a subset $R$ from a set of labeled points $P$ such that for every point $p \in P$ the nearest-neighbor of $p$ in $R$ has the same label as $p$. This is motivated by applications in classification, where the nearest-neighbor rule assigns to an unlabeled query point the label of its nearest-neighbor in the point set. In this context, condensation aims to reduce the size of the set needed to classify new points. However, finding such subsets of minimum cardinality is NP-hard, and most research has focused on practical heuristics without performance guarantees. Additionally, the use of exact nearest-neighbors is always assumed, ignoring the effect of condensation in the classification accuracy when nearest-neighbors are computed approximately.

In this paper, we address these shortcomings by proposing new approximation-sensitive criteria for the nearest-neighbor condensation problem, along with practical algorithms with provable performance guarantees. We characterize sufficient conditions to guarantee correct classification of unlabeled points using approximate nearest-neighbor queries on these subsets, which introduces the notion of coresets for classification with the nearest-neighbor rule. Moreover, we prove that it is NP-hard to compute subsets with these characteristics, whose cardinality approximates that of the minimum cardinality subset. Additionally, we propose new algorithms for computing such subsets, with tight approximation factors in general metrics, and improved factors for doubling metrics and $\ell_p$ metrics with $p \geq 2$. Finally, we show an alternative implementation scheme that reduces the worst-case time complexity of one of these algorithms, becoming the first truly subquadratic approximation algorithm for the nearest-neighbor condensation problem.

1 Introduction

In the context of non-parametric classification, a training set $P$ consists of $n$ points in a metric space $(X, d)$, such that $P \subseteq X$ and metric $d : X^2 \to \mathbb{R}^+$ defines the distance between any two points in $X$. Additionally, $P$ is partitioned into a finite set of classes, such that each point $p \in P$ has a label $l(p)$, indicating the class to which it belongs. Given an unlabeled query point $q \in X$, the goal of a classifier is to predict $q$’s label using the training set $P$.

The nearest-neighbor rule is among the best-known classification techniques, classifying a query point $q \in X$ with the label of its closest point in $P$ according to metric $d$. Despite its simplicity, the nearest-neighbor rule exhibits good classification accuracy both experimentally and theoretically [12]. However, it is often criticized for its high space and time complexities, as clearly, $P$ must be stored to answer nearest-neighbor queries, and the time required for such queries depends to a large degree on the size and dimensionality of the data. These drawbacks raise the question of whether is possible to replace $P$ with a significantly smaller subset,
without reducing the classification accuracy under the nearest-neighbor rule. This problem is called nearest-neighbor condensation.

While many practical and widely-used heuristics for nearest-neighbor condensation have been proposed in the machine-learning literature, only a handful of theoretical results are known. In this paper, we present the first provable results on the performance of practical algorithms for this problem, for both the standard notion of condensation and in the context of approximate nearest-neighbor searching. This helps to reconcile the observed performance of state-of-the-art condensation algorithms, with theoretical guarantees on their selection size. Moreover, we prove that these algorithms select subsets whose cardinality approximates the one of the optimum solution. More importantly, we present the first approximation algorithm with subquadratic worst-case time complexity for condensation.

**Preliminaries.** Given a point \( p \in P \), define an enemy of \( p \) to be any point in \( P \) of different class than \( p \). The nearest-enemy of \( p \), denoted \( ne(p) \), is the closest such point according to metric \( d \). Finally, define the nearest-enemy distance as \( d_{ne}(p) = d(p, ne(p)) \). Similarly, denote the nearest-neighbor of \( p \) as \( mn(p) \), and the nearest-neighbor distance as \( d_{mn}(p) = d(p, mn(p)) \).

Through a suitable uniform scaling, we may assume that the diameter of \( P \) (that is, the maximum distance between any two points in the training set) is 1. The spread of \( P \), denoted as \( \Delta \), is defined to be the ratio between the largest and smallest distances in \( P \). Define the margin of \( P \), denoted \( \gamma \), to be the smallest nearest-enemy distance in \( P \). Clearly, \( 1/\gamma \leq \Delta \).

A metric space \((X, d)\) is said to be doubling if there exist some bounded value \( \lambda \) such that any metric ball of radius \( r \) can be covered with at most \( \lambda \) metric balls of radius \( r/2 \). Its doubling dimension is the base-2 logarithm of \( \lambda \), denoted as \( \operatorname{ddim}(X) = \log \lambda \). Throughout the paper, we consider \( \operatorname{ddim}(X) \) to be constant. Moreover, for any subset \( R \subseteq X \) with spread \( \Delta_R \), the size of \( R \) is bounded by \(|R| \leq \lfloor \Delta_R \operatorname{ddim}(X) \rfloor + 1 \). Many metrics spaces of interest are doubling, like the \( d \)-dimensional Euclidean space whose doubling dimension is \( O(d) \).

**Related Work.** A subset \( R \subseteq P \) is said to be consistent if and only if for every \( p \in P \) its nearest-neighbor in \( R \) is of the same class as \( p \). Intuitively, \( R \) is consistent if and only if all points of \( P \) are correctly classified using the nearest-neighbor rule over \( R \). Formally, the problem of nearest-neighbor condensation consists of finding a consistent subset of \( P \). Yet another criterion used for condensation is known as selectiveness. A subset \( R \subseteq P \) is said to be selective if and only if for all \( p \in P \) its nearest-neighbor in \( R \) is closer to \( p \) than its nearest-enemy in \( P \). Clearly selectiveness implies consistency, as the nearest-enemy distance in \( R \) of any point of \( P \) is at least its nearest-enemy distance in \( P \), and neither consistency or selectiveness imply that every query point of \( X \) is correctly classified, but only those in \( P \).

It is known that the problems of computing consistent and selective subsets of minimum cardinality are both NP-hard. An approximation algorithm called NET was proposed for the problem of finding minimum cardinality consistent subsets, along with almost matching hardness lower-bounds. The algorithm simply computes a \( \gamma \)-net of \( P \), where \( \gamma \) is the minimum nearest-enemy distance in \( P \), which clearly results in a consistent subset of \( P \) (also selective). In practice, \( \gamma \) tends to be small, which results in subsets of much higher cardinality than needed. To overcome this issue, the authors propose a post-processing pruning technique to further reduce the selected subset. Unfortunately, even after the extra pruning, NET is often outperformed by more practical algorithms, with respect to their runtime and selection size. More recently, a subexponential-time algorithm was proposed for finding minimum

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1 The same problem is also referred to as the Instance Selection or Prototype Selection problems.
cardinality consistent subsets of point sets $P \subseteq \mathbb{R}^2$ in the plane, along with other case-specific algorithms for specific instances of the problem in the plane. On the other hand, less is known about computing minimum cardinality selective subsets: there is only a worst-case exponential time algorithm called SNN \cite{Deng2014} for computing such optimal subsets.

Most research has focused on proposing practical heuristics to find either consistent or selective subsets of $P$ (for comprehensive surveys see \cite{Kirkland2015, Kriegel2014}). CNN (Condensed Nearest-Neighbor) \cite{Kirkland2012} was the first algorithm proposed to compute consistent subsets. Even though it has been widely used in the literature, CNN suffers from several drawbacks: its running time is cubic in the worst-case, and the resulting subset is order-dependent, meaning that the result is determined by the order in which points are considered by the algorithm. Alternatives include FCNN (Fast CNN) \cite{Deng2014} and MSS (Modified Selective Subset) \cite{Hathaway1996}, which compute consistent and selective subsets respectively. Both algorithms run in $O(n^2)$ worst-case time, and are order-independent. While such heuristics have been extensively studied experimentally \cite{Kriegel2010}, theoretical results are scarce. Recently, it has been shown \cite{Kriegel2018} that the size of the subsets selected by MSS cannot be bounded, while for FCNN it is still unknown whether is possible to establish any bound. The same paper proposes two algorithms, namely RSS (Relaxed Selective Subset) and VSS (Voronoi Selective Subset), to find selective subsets of $P$ in $O(n^2)$ worst-case time. Moreover, both algorithms provide guarantees on its selection size (only for Euclidean space), and are considered the state-of-the-art for the problem of condensation.

**Drawbacks of Condensation.** In general, state-of-the-art condensation algorithms tend to select points near the boundaries between clusters of points of the same class (see Figures \cite{Kriegel2010} and \cite{Kriegel2014}). These points characterize the decision boundaries of the nearest-neighbor rule, and thus are key in maintaining its classification accuracy after condensation.

However, in practice, nearest-neighbors are not computed exactly, but rather approximately. Given $\varepsilon > 0$, an $\varepsilon$-ANN query returns any point whose distance from the query point is within a factor of $(1 + \varepsilon)$ times the true nearest-neighbor distance. When the condensation is performed without consideration of the approximation error in nearest-neighbor queries,
Coresets for the Nearest-Neighbor Rule

Figure 2 Heatmap of chromatic density values of points in \( \mathbb{R}^2 \) with respect to the subsets computed by different condensation algorithms (FCNN, RSS, and \( \alpha \)-RSS). Yellow • corresponds to chromatic density values \( \geq 0.5 \), while blue • corresponds to 0. Evidently, \( \alpha \)-RSS helps maintaining high chromatic density values when compared to state-of-the-art condensation algorithms.

2 Approximation-Sensitive Condensation

Given a subset \( R \subseteq P \) and an approximation parameter \( \alpha \geq 0 \), we say a query point \( q \in \mathcal{X} \) with respect to a set \( P \subseteq \mathcal{X} \), defined as

\[
\delta(q, P) = \frac{d_{\text{nn}}(q, P)}{d_{\text{nn}}(q, P)} - 1.
\]

Therefore, if \( \delta(q, P) > \varepsilon \) then \( q \) will be correctly classified\(^2\) by \( \varepsilon \)-ANN queries over \( P \), as all possible candidates for the approximate nearest-neighbor belong to the same class as \( q \)'s true nearest-neighbor. Therefore, it is essential to maintain high chromatic density values after condensation if we hope to correctly classify query points using ANN queries. We introduce new approximation-sensitive criteria for nearest-neighbor condensation, along with practical algorithms for computing subset with higher chromatic density values (see Figures 2c and 2d).

By correct classification, we mean that the classification is the same as the classification that results from applying the nearest-neighbor rule exactly on the entire training set \( P \).
2.1 Guarantees on Classification Accuracy

Having a lower-bound on the chromatic density of points of $P$ does not immediately imply the same for any query point $q \in \mathcal{X}$. In this section, we provide useful lower-bounds along with guarantees on the classification accuracy of the nearest-neighbor rule over $\alpha$-consistent subsets.

**Lemma 1.** Let $q \in \mathcal{X}$ be a query point, and $R$ an $\alpha$-consistent subset of $P$. Then

$$\delta(q, R) > \frac{\alpha \delta(q, P) - 2}{\delta(q, P) + \alpha + 3}.$$  

**Proof.** First let’s consider the nearest-enemy distance of the query point $q$ in $R$. Clearly, any condensation of $P$ can only increase the nearest-enemy distance, that is $d_{\text{ne}}(q, R) \geq d_{\text{ne}}(q, P)$. This gives us an initial lower-bound on the chromatic density of $q$ with respect to $R$ as $\delta(q, R) \geq d_{\text{ne}}(q, P)/d_{\text{nn}}(q, R) - 1$. Consider now the nearest-neighbor distance of $q$ in $R$. Let $p \in P$ be the nearest-neighbor of $q$ in the initial training set $P$, there are two possible cases:

(a) If $p \in R$, clearly $d_{\text{nn}}(q, R) = d_{\text{nn}}(q, P)$. Then, $\delta(q, R) \geq \delta(q, P)$.

(b) If $p \notin R$, we can upper-bound the nearest-neighbor distance of $q$ in $R$ as follows:

By definition of $\alpha$-consistency we know that $\delta(p, R) > \alpha$, meaning there exists a point $r \in R$ such that $(1 + \alpha) d(p, r) \leq d_{\text{ne}}(p)$. Furthermore, by triangle inequality we get $d_{\text{ne}}(p) \leq d_{\text{ne}}(q) + d_{\text{nn}}(q)$. Additionally, the definition of chromatic density implies that $d_{\text{ne}}(q) = (1 + \delta(q, P)) d_{\text{nn}}(q)$. All together, we have $(1 + \alpha) d(p, r) \leq (2 + \delta(q, P)) d_{\text{nn}}(q)$. Now:

$$d_{\text{nn}}(q, R) \leq d(q, r) \leq d(q, p) + d(p, r) = d_{\text{nn}}(q) \left(1 + \frac{2 + \delta(q, P)}{1 + \alpha}\right).$$

Finally, from our initial bound on $\delta(q, R)$, we have that:

$$\delta(q, R) \geq \frac{(1 + \delta(q, P)) d_{\text{nn}}(q)}{d_{\text{nn}}(q) \left(1 + \frac{2 + \delta(q, P)}{1 + \alpha}\right)} - 1 = \frac{1}{1 + \alpha} \frac{(1 + \delta(q, P))}{\delta(q, P) + \alpha + 3} - 1 = \frac{\alpha \delta(q, P) - 2}{\delta(q, P) + \alpha + 3}. \quad \Box$$

By simple algebraic manipulation of the bound derived in Lemma 1 we have that if $\delta(q, P) \geq (\alpha \varepsilon + 3 \varepsilon + 2)/(\alpha - \varepsilon)$ then $\delta(q, R) > \varepsilon$. As $\alpha$ and $\varepsilon$ are both upper-bounded by some constant, we obtain the following bound on the chromatic density.

**Theorem 2.** Consider two parameters $\alpha > \varepsilon > 0$ upper-bounded by some constant, and let $R$ be an $\alpha$-consistent subset of $P$. Any query point $q \in \mathcal{X}$ with chromatic density in $P$ to be $\delta(q, P) = \Omega(1/(\alpha - \varepsilon))$, its chromatic density in $R$ is $\delta(q, R) > \varepsilon$. That is, $q$ is correctly classified using $\varepsilon$-ANN queries on $R$.

So far, we have assumed that classification over $P$ is performed exactly, but the above result can be applied when approximation is used on both $P$ and $R$. The following theorem indicates how to set the value of $\alpha$, so that an $\varepsilon_2$-ANN query on $R$ correctly classifies a given query point, assuming that an $\varepsilon_1$-ANN query on $P$ correctly classifies the same point.

**Theorem 3.** Consider two parameters $\varepsilon_1 \geq \varepsilon_2 > 0$ upper-bounded by some constant, and let $R$ be an $\alpha$-consistent subset of $P$ with $\alpha = \Omega(1/(\varepsilon_1 - \varepsilon_2))$. Any query point $q \in \mathcal{X}$ with chromatic density in $P$ to be $\delta(q, P) > \varepsilon_1$, its chromatic density in $R$ is $\delta(q, R) > \varepsilon_2$. That is, $q$ is correctly classified using $\varepsilon_2$-ANN queries on $R$.

This also follows from the bound derived in Lemma 1. As $\varepsilon_1$ and $\delta(q, P)$ are both positive values, $\alpha$ is non-negative, and knowing that $\delta(q, P) > \varepsilon_1$, the following inequality holds:

$$\delta(q, R) > \frac{\alpha \delta(q, P) - 2}{\delta(q, P) + \alpha + 3} > \frac{\alpha \varepsilon_1 - 2}{\varepsilon_1 + \alpha + 3}.$$
For this expression to be lower-bounded by $\varepsilon_2$, it is easy to see that the condition on $\alpha$ must be $\alpha \geq (\varepsilon_1 \varepsilon_2 + 3\varepsilon_2 + 2)/(\varepsilon_1 - \varepsilon_2)$. Therefore, as both $\varepsilon_1$ and $\varepsilon_2$ are upper-bounded by some constant, setting $\alpha$ to be $\Omega(1/(\varepsilon_1 - \varepsilon_2))$ implies that $\delta(q, R) > \varepsilon_2$.

Another way to view the above result is to restrict a set of query points of interest based on their chromatic density, and then ask how high must the value of $\alpha$ be in order to guarantee correct classification when queries are answered exactly with respect to $R$. Such a subset bears a resemblance to the concept of a coreset in computational geometry [1], in the sense that an exact result on the coreset corresponds to an approximate result on the original set. In a slight abuse of terminology, we say that a set $R \subseteq P$ is an $\varepsilon$-coreset with respect to chromatic nearest-neighbor if for a query point $q \in X$, the class of its exact nearest-neighbor in $R$ is the same as the class of any $\varepsilon$-ANN with respect to $P$. A coreset is said to be weak if the approximation guarantee is only valid for a subset of all possible queries. By setting $\varepsilon_2 = 0$ in the preceding lower-bound for $\alpha$, it follows that $\alpha \geq 2/\varepsilon_1$, implying the following.

**Theorem 4.** Any $(2/\varepsilon)$-consistent subset of $P$ is a weak $\varepsilon$-coreset for the chromatic nearest-neighbor of $P$ for any query point $q \in X$ with chromatic density $\delta(q, P) > \varepsilon$.

### 3 Computation

#### 3.1 $\alpha$-Consistent Subsets

Let Min-$\alpha$-CS be the problem of finding an $\alpha$-consistent subset of $P$ of minimum cardinality. Evidently, this problem is NP-hard following a simple reduction from the standard version of the problem where $\alpha$ is zero [19,26,27]. This section presents results related to the hardness of approximation of the problem, as well as algorithmic approaches for finding $\alpha$-consistent subsets of $P$ whose cardinality approximates the cardinality of the optimal solution.

**Theorem 5.** The Min-$\alpha$-CS problem is NP-hard to approximate in polynomial time within a factor of $2^{(d\dim(X))\log((1+\alpha)/\gamma)^{1-\varepsilon}(\alpha)}$.

The full proof is omitted, but it follows from a modification of the hardness bounds proof for the Min-0-CS problem described in [16], which is based on a reduction from the Label Cover problem. Proving Theorem 5 involves a careful adjustment of the distances in this reduction, making all points in such construction to have chromatic density of at least $\alpha$. Consequently, this implies that the minimum nearest-enemy distance is reduced by a factor of $1/(1+\alpha)$, explaining the resulting bound for Min-$\alpha$-CS. From the same paper, the NET algorithm can be generalized to compute $\alpha$-consistent subsets of $P$ as follows. We call $\alpha$-NET the algorithm that computes a $\gamma/(1+\alpha)$-net of $P$, where $\gamma$ is the smallest nearest-enemy distance in $P$. The covering property of $\varepsilon$-nets implies that the resulting subset is $\alpha$-consistent, while the packing property suggests that its cardinality is $O\left(\left(\left(1+\alpha/\gamma\right)^{d\dim(X)+1}\right)\right)$, making it a tight approximation to the optimum solution of the Min-$\alpha$-CS problem.

However, the NET algorithm is not practical, and even after using the post-processing technique described in the original paper to further reduce the subset, the final cardinality of its selected subset is much higher when compared to other state-of-the-art algorithms. The same applies for $\alpha$-NET (see Section A for the experimental results).

There is, however, an efficient and practical algorithm to find consistent subsets, called FCNN [3]. This is an iterative algorithm that incrementally builds a consistent subset of $P$. First, it begins by selecting the set of centroids of each class, and then continues with the iterative process until the subset is consistent. On each iteration, the algorithm identifies all points of $P$ that are misclassified with the current subset (that is, whose nearest-neighbor...
is of different class), and adds some of these points to the subset. In particular, for every point \( p \) already in the subset, FCNN selects one representative among all the points not yet selected, whose nearest-neighbor is \( p \), and that belong to a different class than \( p \). That is, the representative is selected from the set \( \text{voren}(p, R, P) = \{ q \in P \mid \text{nn}(q, R) = p \land l(q) \neq l(p) \} \). Usually, the representative chosen is the one closest to \( p \), although different approaches can be used. Finally, during each iteration, one representative per every point in the current subset is added (all in a batch), until no misclassified points are left. See Algorithm 1 in the appendix for a formal description. While not immediately evident, FCNN can be implemented to run in \( O(nm) \) worst-case time, where \( m \) is the final size of the selected subset.

Unfortunately, no upper-bounds for the selection of FCNN are possible. By adding points in a batch on every iteration, these new points can be arbitrarily close to each other; a behavior that can be exploited to create a training set where the selected subset is unbounded in terms of either \( \kappa \) or the optimum solution (see Theorem 15 in the appendix). However, this design choice is not necessary for any of the key features of the algorithm. Therefore, we propose a simple modification of the algorithm where only one single representative of some already selected point, is added on each iteration. We call this modified algorithm SFCNN or \( \alpha \)-SFCNN. We can further extend this algorithm to compute \( \alpha \)-consistent subsets, calling it the \( \alpha \)-SFCNN algorithm, by redefining the set \( \text{voren}(p, R, P) \) of misclassified points that can be selected as representatives of a point \( p \) in the current selected subset \( R \) as follows \( \{ q \in P \mid \text{nn}(q, R) = p \land (l(q) = l(p) \Rightarrow \delta(q, R) < \alpha) \} \). That is, all points closer to \( p \) than any other point in \( R \), who are enemies of \( p \) or whose chromatic density with respect to \( R \) is less than \( \alpha \). Now, it is possible to successfully analyze the selection size of the algorithm.

\textbf{Theorem 6.} \( \alpha \)-SFCNN computes a tight approximation for the Min-\( \alpha \)-CS problem.

\textbf{Proof.} This follows from a direct comparison to the resulting subset of the \( \alpha \)-NET algorithm. For any point \( p \in \alpha \)-NET, let \( B_{p,\alpha} \) be the set of points of \( P \) “covered” by \( p \), that is, whose distance to \( p \) is at most \( \gamma/(1+\alpha) \). By the covering property of \( \epsilon \)-nets, this defines a partition on \( P \) when considering every point \( p \) selected by \( \alpha \)-NET.

Lets analyze the size of \( B_{p,\alpha} \cap \alpha \)-SFCNN, that is, for any given \( B_{p,\alpha} \) how many points could have been selected by the \( \alpha \)-SFCNN algorithm. Let \( a, b \in B_{p,\alpha} \cap \alpha \)-SFCNN be two such points, where without loss of generality, point \( a \) was selected in an iteration before \( b \). Both \( a \) and \( b \) must belong to the same class as \( p \), as their distance to \( p \) is at most \( \gamma/(1+\alpha) \) where \( \gamma \) is the smallest nearest-enemy distance in \( P \). Moreover, by the definition of the \text{voren} function, it is easy to show that \( d(a, b) \geq \gamma/(1+\alpha) \). By a simple packing argument in doubling metrics, the size of any \( B_{p,\alpha} \cap \alpha \)-SFCNN is at most \( 2^{\dim(X)+1} \). All together, we have that the size of the subset selected by \( \alpha \)-SFCNN is \( 2^{\dim(X)+1} \mid \alpha \)-NET\( ] = \mathcal{O}
( (1+\alpha)/\gamma)^{\dim(X)+1} \).

With this, we close the open problem \cite{14} of whether it is possible to reconcile the practical performance of the FCNN algorithm with theoretical guarantees regarding its selection size. Additionally, we establishing bounds in more absolute terms with respect to \( \kappa \), as these nearest-enemy points characterize the boundaries between points of different classes in \( P \).

\textbf{Theorem 7.} \( \alpha \)-SFCNN selects \( \mathcal{O} \left( \kappa \log \frac{1}{\gamma} (2+\alpha)^{\dim(X)+1} \right) \) points.

\subsection{\( \alpha \)-Selective Subsets}

Let Min-\( \alpha \)-SS be the problem of finding an \( \alpha \)-selective subset of \( P \) of minimum cardinality. It goes without saying that this problem is NP-hard, following the hardness of the special case where \( \alpha \) is zero \cite{26,27}. This section presents results related to the hardness of approximation.
of the problem, as well as algorithmic approaches for finding \( \alpha \)-selective subsets of \( P \) whose cardinality approximates the cardinality of the optimal solution.

There is a clear connection between this problem and covering problems, in particular that of finding a minimum hitting set. Given a set of elements \( U \) and a family \( C \) of subsets of \( U \), a hitting set of \( (U, C) \) is a subset \( H \subseteq U \) such that every set in \( C \) contains at least one element of \( H \). Therefore, let \( S_{p,\alpha} \) be the set of points of \( P \) whose distance to \( p \) is less than \( d_{\text{ne}}(p)/(1+\alpha) \), any hitting set of \( (P, \{ S_{p,\alpha} \mid p \in P \}) \) is an \( \alpha \)-selective subset of \( P \), and vice versa. This simple reduction implies a \( O(n^3) \) worst-case time \( O(\log n) \)-approximation algorithm for \( \text{MIN-}\alpha-\text{SS} \), based on the classic greedy algorithm for computing hitting sets \([11,24]\). Call this approach \( \alpha\text{-HSS} \) or \( \alpha\text{-Hitting Selective Subset} \). The following theorem suggests that for general metrics, this is the best approximation possible under standard complexity assumptions.

\[ \textbf{Theorem 8.} \] The \( \text{MIN-}\alpha-\text{SS} \) problem is \( \text{NP-hard} \) to approximate in polynomial time within a factor of \( (1 - o(1)) \log n \) unless \( \text{NP} \subseteq \text{DTIME}(n^{\log\log n}) \).

This result follows from the hardness of another related covering problem: the minimum dominating set \([13,20,22]\). The full proof is left in the appendix, and involves a simple L-reduction from any instance of this problem to an instance of \( \text{MIN-}\alpha-\text{SS} \), which preserves the approximation ratio. The general idea is as follows: given a graph \( G \), create an edge-weighted graph with two copies of \( G \), such that every node and its corresponding copy are connected by an edge of length \( 1+\alpha \), and the original edges have length 1. Thus, solving the \( \text{MIN-}\alpha-\text{SS} \) on this graph, using the shortest-path metric, and labeling the nodes of one copy of \( G \) as blue and the others red, essentially solves the minimum dominating set problem on \( G \).

Therefore, \( \alpha\text{-HSS} \) computes a tight approximation of the optimum solution in general metric spaces, a behavior that is confirmed by the experimental results of Section \([4]\). However, its runtime is clearly outperformed by other algorithms, given its cubic time complexity.

Consider RSS \([14]\), a state-of-the-art algorithm for finding selective subsets. Its selection process can be described as follows: beginning with an empty set, points of \( P \) are examined in increasing order with respect to their nearest-enemy distance in \( P \). For every point \( p \in P \), if the distance from \( p \) to any previously selected point is less than \( d_{\text{ne}}(p) \), point \( p \) is added to the subset. This algorithm clearly computes a selective subset, and a simple implementation yields quadratic worst-case time complexity. We now define \( \alpha\text{-RSS} \) as a parameterized version of the algorithm that computes \( \alpha \)-selective subsets, such that whenever deciding if a point \( p \in P \) should be added to the subset, it checks if any previously selected point is closer to \( p \) than \( d_{\text{ne}}(p)/(1+\alpha) \). See Algorithm \([2]\) in the appendix for a formal description. It is easy to see that this modification implies \( \alpha \)-selectiveness, while retaining the order independence and quadratic worst-case time complexity of the original algorithm.

Naturally, we would like to analyze the selection size of this seemingly heuristic algorithm. The remaining of this section establishes upper-bounds and approximation guarantees of the \( \alpha \)-RSS on any doubling metric space, with improved results in the Euclidean space. This solves the open problem of whether RSS approximates the \( \text{MIN-}\alpha-\text{CS} \) and \( \text{MIN-}\alpha-\text{SS} \) problems.

\[ \textbf{Size in Doubling spaces.} \] Going beyond the scope of general metrics, we consider the case when the underlying metric space \( (X, d) \) of \( P \) is doubling. The following results depend on the doubling dimension \( \text{ddim}(X) \) of the metric space, and the margin \( \gamma \) of set \( P \).

\[ \textbf{Theorem 9.} \] \( \alpha\text{-RSS} \) computes an \( O\left(\log \left( \min \left( \frac{\gamma\alpha}{1+\alpha}, \frac{1}{\alpha} \right) \right) \right) \)-approximation of the \( \text{MIN-}\alpha-\text{SS} \) problem, which is an \( O(1) \)-approximation for \( \alpha = \Omega(1) \).

\[ \textbf{Proof.} \] Let \( \text{OPT}_\alpha \) be the optimum solution to the \( \text{MIN-}\alpha-\text{SS} \) problem, i.e., the minimum cardinality \( \alpha \)-selective subset of \( P \). For every point \( p \in \text{OPT}_\alpha \) in such solution, define \( S_{p,\alpha} \) to
be the set of points in $P$ “covered” by $p$, or simply $S_{p, \alpha} = \{ r \in P \mid \text{d}(r, p) < d_{\text{ne}}(r)/(1 + \alpha) \}$. Additionally, for any value $\sigma \in [\gamma, 1]$, define $\alpha$-RSS$_{p, \sigma}$ to be the subset of points selected by $\alpha$-RSS which also belong to $S_{p, \alpha}$ and whose nearest-enemy distance is between $\sigma$ and $2\sigma$. That is, $\alpha$-RSS$_{p, \sigma} = \{ r \in \alpha$-RSS $\cap S_{p, \alpha} \mid d_{\text{ne}}(r) \in [\sigma, 2\sigma) \}$. Clearly, these subsets define a partitioning of $\alpha$-RSS for all $p \in \text{OPT}_\alpha$ and values of $\sigma = \gamma 2^i$ for $i = \{0, 1, 2, \ldots, \lceil \log \frac{2 + \alpha}{\alpha} \rceil \}$. 

However, depending on $\alpha$, some values of $\sigma$ would yield empty $\alpha$-RSS$_{p, \sigma}$ sets. Consider some point $q \in S_{p, \alpha}$, we can bound its nearest-enemy distance with respect to the nearest-enemy distance of point $p$. In particular, by leveraging simple triangle inequality arguments, we can prove that $d_{\text{ne}}(p) \frac{2 + \alpha}{2 \gamma} \leq d_{\text{ne}}(q) \leq d_{\text{ne}}(p) \frac{2 + \alpha}{2 \gamma}$. Therefore, the values of $\sigma$ that yield non-empty $\alpha$-RSS$_{p, \sigma}$ sets are $\sigma = d_{\text{ne}}(p) \frac{2 + \alpha}{2 \gamma} 2^j$ for $j = \{0, \ldots, \lceil \log \frac{2 + \alpha}{\alpha} \rceil \}$.

The proof now follows by bounding the size of $\alpha$-RSS$_{p, \sigma}$ which can be achieved by bounding its spread. Thus, let’s consider the smallest and largest pairwise distances among points in $\alpha$-RSS$_{p, \sigma}$. Take any two points $a, b \in \alpha$-RSS$_{p, \sigma}$ where without loss of generality, $d_{\text{ne}}(a) \leq d_{\text{ne}}(b)$. One of the key features of $\alpha$-RSS is that the points selected cannot be “too close” to each other; that is, as $a$ and $b$ were selected by the algorithm, we know that $(1 + \alpha) \cdot d(a, b) \geq d_{\text{ne}}(b) \geq \sigma$. Therefore, the smallest pairwise distance in $\alpha$-RSS$_{p, \sigma}$ is at least $\sigma/(1 + \alpha)$. Additionally, by triangle inequality, we can bound the maximum pairwise distance using their distance to $p$ as $d(a, b) \leq d(a, p) + d(p, b) \leq 4\sigma/(1 + \alpha)$. Then, by the packing properties of doubling spaces, the size of $\alpha$-RSS$_{p, \sigma}$ is at most $4^{d\text{dim}(X)+1}$.

All together, for each point $p \in \text{OPT}_\alpha$ there are $\lceil \log \left( \min \left( \frac{2 + \alpha}{\alpha}, \frac{1}{\gamma} \right) \right) \rceil$ non-empty $\alpha$-RSS$_{p, \sigma}$ subsets with at most $4^{d\text{dim}(X)+1}$ points each. Thus, in doubling spaces with constant doubling dimension $d\text{dim}(X)$, $\alpha$-RSS computes an $O(\log \left( \min \left( \frac{2 + \alpha}{\alpha}, \frac{1}{\gamma} \right) \right))$-approximation of the minimum cardinality $\alpha$-selective subset of $P$.

Additionally, using similar packing arguments to the ones in the proof of Theorem 9, we can show that for any training set $P$, the size of the subset selected by $\alpha$-RSS is at most $O(2^{d\text{dim}(X)+1})$ times the size of the subset selected by $\alpha$-NET. This implies that $\alpha$-RSS also computes a tight approximation of the minimum cardinality $\alpha$-consistent subset of $P$, up to constant factors, for training sets with constant doubling dimension.

While these results are meaningful from a theoretical perspective, it is also important to establish the selection size of $\alpha$-RSS in terms of the geometry of the learning space, which is characterized by the boundaries between points of different classes. Thus, using similar packing arguments as above, we bound the selection size of the algorithm with respect to $\kappa$.

**Theorem 10.** $\alpha$-RSS selects $\mathcal{O} \left( \kappa \log \frac{1}{\gamma} \left( 2 + \alpha \right)^{d\text{dim}(X)+1} \right)$ points.

**Size in Euclidean space.** In the case where $P \subset \mathbb{R}^d$ lies in $d$-dimensional Euclidean space, the analysis of $\alpha$-RSS can be further improved, leading to a constant-factor approximation of $\text{Min-\alpha-SS}$ for any value of $\alpha \geq 0$, and reduced dependency on the dimensionality of $P$.

**Theorem 11.** In Euclidean space $\mathbb{R}^d$, $\alpha$-RSS computes an $O(1)$-approximation of the $\text{Min-\alpha-SS}$ problem.

**Proof.** Similar to the proof of Theorem 9, define $\alpha$-RSS$_p = S_{p, \alpha} \cap \alpha$-RSS as the points selected by $\alpha$-RSS that are “covered” by $p$ in the optimum solution $\text{OPT}_\alpha$. Consider two such points $a, b \in \alpha$-RSS$_p$ where without loss of generality, $d_{\text{ne}}(a) \leq d_{\text{ne}}(b)$. By the definition of $S_{p, \alpha}$ we know that $d(a, p) < d_{\text{ne}}(a)/(1 + \alpha)$, and similarly with $b$. Additionally, from the selection of the algorithm we know that $d(a, b) \geq d_{\text{ne}}(b)/(1 + \alpha)$. Overall, these inequalities imply that the angle $\angle p_{\alpha} p_{\pi} \geq \pi/3$. By a simple packing argument, the size of $\alpha$-RSS$_p$
is bounded by the kissing number in \(d\)-dimensional Euclidean space, or just \(O((3/\pi)^{d-1})\). Therefore, we have that \(|\alpha\text{-RSS}| = \sum_{p \in \text{OPT}} |\alpha\text{-RSS}_p| = |\text{OPT}_\alpha| \cdot O((3/\pi)^{d-1}).\)

This analysis is tight up to constant factors. In Figure 3 we illustrate a training set \(P\) consisting of red and blue points in \(\mathbb{R}^d\), where \(\alpha\text{-RSS}\) selects \(\Theta(c^{d-2} |\text{OPT}_\alpha|)\) points. Consider two helper points (which do not belong to \(P\)) \(c_r = 0\bar{u}_d\) and \(c_b = (1+\alpha)\bar{u}_d\), where \(\bar{u}_d\) is the unit vector parallel to the \(d\)-th coordinate. Add to \(P\) as red points, the points \(r_i\) on the surface of the \(d-1\) unit ball centered at \(c_r\) and perpendicular to \(\bar{u}_d\). Similarly with blue points \(b_i\) around \(c_b\). Finally, add two points \(r_\ast = -\xi\bar{u}_d\) and \(b_\ast = (1+\alpha + \xi)\bar{u}_d\), for a suitable value \(\xi\) such that \(|r_\ast r_i| < 1\). Clearly, the nearest-enemy distance of every \(r_i\) and \(b_i\) point is \(1 + \alpha\), while it is greater than \(1 + \alpha\) for \(r_\ast\) and \(b_\ast\). Thus, \(\text{OPT}_\alpha = \{r_\ast, b_\ast\}\) while \(\alpha\text{-RSS}\) selects \(\Theta(c^{d-2})\) points \(r_i\) and \(b_i\) at distance greater than \(1\) from each other.

Furthermore, a similar constant-factor approximation can be achieved for any training set \(P\) in \(\ell_p\) space for \(p \geq 3\). This follows analogously to the proof of Theorem 11 exploiting the bounds between \(\ell_p\) and \(\ell_2\) metrics, where \(1/\sqrt{d} \leq \|v\|_p \leq \|v\|_2 \leq \sqrt{d} \|v\|_p\). This would imply that the angle between any two points in \(\alpha\text{-RSS}_p\) is \(\Omega(1/d)\). Therefore, it shows that \(\alpha\text{-RSS}\) achieves an approximation factor of \(O(d^{d-1})\), or simply \(O(1)\) for constant dimension.

Similarly to the case of doubling spaces, we also establish upper-bounds in terms of \(\kappa\) for the selection size of the algorithm in Euclidean space. The following result improves the exponential dependence on the dimensionality of \(P\) (from \(d \text{dim}(\mathbb{R}^d) = O(d)\) to \(d-1\)), while keeping the dependency on the margin \(\gamma\), which contrast with the approximation factor results. Moreover, it is possible to prove that these upper-bounds are tight up to constant factors.

**Theorem 12.** In Euclidean space \(\mathbb{R}^d\), \(\alpha\text{-RSS}\) selects \(O\left(\kappa \log \frac{1}{\gamma} \left(1 + \alpha\right)^{d-1}\right)\) points.

### 3.3 A Subquadratic Implementation Scheme

In standard nearest-neighbor condensation, when \(\alpha\) is zero, the algorithm with lowest worst-case time complexity is FCNN which runs in \(O(nm)\) time, where \(m\) is the size of its selected subset. In the remaining of this section, we describe an implementation scheme for \(\alpha\text{-RSS}\) that allows to reduce the worst-case time complexity of the algorithm to be truly subquadratic.

The \(\alpha\text{-RSS}\) algorithm consists of two main stages: computing the nearest-enemy distances of all points in \(P\) (and sorting the points based on these), and the selection process itself. The first stage requires a total of \(n\) nearest-enemy queries, plus additional \(O(n \log n)\) time for sorting. The second stage performs \(n\) nearest-enemy queries on the current selected subset, which needs to be updated \(m\) times (\(m\) is the final size of the selected subset). In both cases, using exact nearest-neighbor search techniques would degenerate into linear search due to the curse of dimensionality. Thus, the first and second stage of the algorithm would need \(O(n^2)\) and \(O(nm)\) worst-case time respectively.

These bottlenecks can be overcome by leveraging approximate nearest-neighbor techniques. Clearly, the first stage of the algorithm can be improved by computing nearest-enemy distances.
approximately, using as many $\varepsilon$-ANN structures as classes there are in $P$, which is considered to be a small constant. Therefore, by also applying a simple brute-force search for nearest-neighbors in the second stage, result (i) of the next theorem follows immediately. Moreover, by combining this with standard techniques for static-to-dynamic conversions \[9\], we have result (ii) below. Denote this variant of the $\alpha$-RSS algorithm as $(\alpha, \varepsilon)$-RSS.

**Theorem 13.** Given a data structure for $\varepsilon$-ANN searching with construction time $t_c$ and query time $t_q$ (which potentially depend on $n$ and $\varepsilon$), the $(\alpha, \varepsilon)$-RSS variant can be implemented with the following worst-case time complexities, where $m$ is the size of the selected subset.

1. $O(t_c + n(t_q + m + \log n))$
2. $O((t_c + n t_q)(\log n))$

More generally, if we are given an additional data structure for dynamic $\varepsilon$-ANN searching with construction time $t'_c$, query time $t'_q$, and insertion time $t'_i$, the overall running time will be $O(t_c + t'_c + n(t_q + t'_q + \log n) + m t'_i)$. Indeed, this can be used to obtain (ii) from the static-to-dynamic conversions \[9\], which propose an approach to convert static search structures into dynamic ones. These results directly imply implementations of $(\alpha, \varepsilon)$-RSS with subquadratic worst-case time complexities, based on $\varepsilon$-ANN techniques \[3, 5\] for low-dimensional Euclidean space, and using techniques like LSH \[2\] that are suitable for $\varepsilon$-ANN in high-dimensional Hamming and Euclidean spaces.

**Lemma 14.** There exist a data structure for dynamic $\varepsilon$-ANN queries in sets $P$ in $d$-dimensional Euclidean space, that can be constructed in $t'_c = O(n \log n)$ time, queried in $t'_q = O(\log n + 1/\varepsilon^{d-1})$ time, and where points of $P$ can be inserted in $t'_i = O(\log n)$ time.

Together with the dynamic-structure scheme described above, this lemma implies that there is a variant of $\alpha$-RSS for Euclidean space that runs in $O(n \log n + n/\varepsilon^{d-1})$ time. Such a data structure can be built from a standard BBD tree \[6\] as follows. First, construct the tree from the entire set $P$, thus taking $t'_c = O(n \log n)$ time. However, each node of the tree has some additional data: a boolean flag indicating if the subtree rooted at such node contains a point of the “active” subset $R$. Initially, all flags are set to false, making the initial active subset being empty. To add a point $p \in P$ to the active subset $R$, all the flags from the root of the tree to the leaf node containing $p$ must be set to true, thus making the insertion time $t'_i = O(\log n)$. Finally, an $\varepsilon$-ANN query on such tree would perform as usual, only avoiding to visit nodes whose flag is set to false, yielding a query time of $t'_q = O(\log n + 1/\varepsilon^{d-1})$.

**Dealing with uncertainty.** Such implementation schemes for $\alpha$-RSS would incur into some approximation error (of up to $1 + \varepsilon$) on the computed distances: either only during the first stage if (i) is implemented, or during both stages if (ii) or the dynamic-structure scheme are implemented. The uncertainty introduced by these approximate queries, imply that in order to guarantee finding $\alpha$-selective subsets, we must modify the condition for adding point during the second stage of the algorithm. Denote $d_{ne}(p, \varepsilon)$ to be the $\varepsilon$-approximate nearest-enemy distance of $p$ computed in the first stage, and $d_{an}(p, \alpha$-RSS, $\varepsilon$) to be the $\varepsilon$-approximate nearest-neighbor distance of $p$ over points of the current subset (computed in the second stage). Then, $(\alpha, \varepsilon)$-RSS adds a point $p$ into the subset if $(1 + \alpha) d_{an}(p, \alpha$-RSS, $\varepsilon) \geq d_{ne}(p, \varepsilon)/(1 + \varepsilon)$.

By similar arguments to the ones described in Section 3.2 size guarantees can be extended to $(\alpha, \varepsilon)$-RSS. First, the size of the subset selected by $(\alpha, \varepsilon)$-RSS, in terms of the number of nearest-enemy points in the set, would be bounded by the size of the subset selected by $\alpha$-RSS with $\tilde{\alpha} = (1 + \alpha)(1 + \varepsilon)^2 - 1$. Additionally, the approximation factor of $(\alpha, \varepsilon)$-RSS in both doubling and Euclidean metric spaces would increase by a factor of $O(((1 + \varepsilon)^2)^{d \dim(X)} + 1)$. 

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A Experimental Evaluation

In order to get a clearer impression of the relevance of these results in practice, we performed experimental trials on several training sets, both synthetically generated and widely used benchmarks. First, we consider 21 training sets from the UCI Machine Learning Repository\(^3\) which are commonly used in the literature to evaluate condensation algorithms [15]. These consist of a number of points ranging from 150 to 58000, in \(d\)-dimensional Euclidean space with \(d\) between 2 and 64, and 2 to 26 classes. We also generated some synthetic training sets, containing \(10^5\) uniformly distributed points, in 2 to 3 dimensions, and 3 classes. All training sets used in these experimental trials are summarized in Table 1. The implementation of the algorithms, training sets used, and raw results, are publicly available\(^4\).

| Training set | \(n\) | \(d\) | \(c\) | \(\kappa\) (\%) |
|--------------|------|------|------|--------------|
| banana       | 5300 | 2    | 2    | 811 (15.30%) |
| cleveland    | 297  | 13   | 5    | 125 (42.09%) |
| glass        | 214  | 9    | 6    | 87 (40.65%)  |
| iris         | 150  | 4    | 3    | 20 (13.33%)  |
| iris2d       | 150  | 2    | 3    | 13 (8.67%)   |
| letter       | 20000| 16   | 26   | 6100 (30.50%)|
| magic        | 19020| 10   | 2    | 5191 (27.29%)|
| monk         | 432  | 6    | 2    | 300 (69.44%) |
| optdigits    | 5620 | 64   | 10   | 1245 (22.15%)|
| pageblocks   | 5472 | 10   | 5    | 429 (7.84%)  |
| penbased     | 10992| 16   | 10   | 1352 (12.30%)|
| pima         | 768  | 8    | 2    | 293 (38.15%) |
| ring         | 7400 | 20   | 2    | 2369 (32.01%)|
| satimage     | 6435 | 36   | 6    | 1167 (18.14%)|
| segmentation | 2100 | 19   | 7    | 398 (18.95%) |
| shuttle      | 58000| 9    | 7    | 920 (1.50%)  |
| thyroid      | 7200 | 21   | 3    | 779 (10.82%) |
| twonorm      | 7400 | 20   | 2    | 1298 (17.54%)|
| wdbc         | 569  | 30   | 2    | 123 (21.62%) |
| wine         | 178  | 13   | 3    | 37 (20.79%)  |
| wisconsin    | 683  | 9    | 2    | 35 (5.12%)   |
| v-100000-2-3-15 | 100000 | 2   | 3    | 1909 (1.90%) |
| v-100000-2-3-5  | 100000 | 2   | 3    | 788 (0.78%)  |
| v-100000-3-3-15 | 100000 | 3   | 3    | 7043 (7.04%) |
| v-100000-3-3-5  | 100000 | 3   | 3    | 3738 (3.73%) |
| v-100000-4-3-15 | 100000 | 4   | 3    | 13027 (13.02%)|
| v-100000-4-3-5  | 100000 | 4   | 3    | 10826 (10.82%)|
| v-100000-5-3-15 | 100000 | 5   | 3    | 22255 (22.25%)|
| v-100000-5-3-5  | 100000 | 5   | 3    | 17705 (17.70%)|

Table 1 Training sets used to evaluate the performance of condensation algorithms. Indicates the number of points \(n\), dimensions \(d\), classes \(c\), nearest-enemy points \(\kappa\) (also in percentage w.r.t. \(n\)).

These experimental trials compare the performance of different condensation algorithms when applied to vastly different training sets. We use two measures of comparison on these algorithms: their runtime in the different training sets, and the size of the subset selected. Clearly, these values might differ greatly on training sets whose size are too distinct. Therefore, before comparing the raw results, these are normalized. The runtime of an algorithm for a given training set is normalized by dividing it by \(n\), the size of the training set. The size of the selected subset is normalized by dividing it by \(\kappa\), the number of nearest-enemy points in the training set, which characterizes the complexity of the boundaries between classes.

\(^3\)https://archive.ics.uci.edu/ml/index.php
\(^4\)https://github.com/afloresv/nnc/
Algorithm Comparison. The first experiment evaluates the performance of five algorithms, namely $\alpha$-RSS, $\alpha$-FCNN, $\alpha$-SFCNN, $\alpha$-NET, and $\alpha$-HSS, while varying the value of $\alpha$ from 0 to 1. By $\alpha$-FCNN we refer to the generalization of the FCNN algorithm using the extended definition of the $voren$ function. It differs from $\alpha$-SFCNN by adding points in a batch on every iteration, for which $\alpha$-SFCNN only adds one point at a time. We decided to include both generalizations of FCNN to compare the impact of the SFCNN modification. Additionally, the $\alpha$-NET algorithm was implemented with the post-processing pruning technique that further reduces the selected subset after computing the $\varepsilon$-net. The results show that $\alpha$-RSS outperforms the other algorithms in terms of running time by a big margin, and irrespective of the value of $\alpha$ (see Figure 4a). Additionally, the number of points selected by $\alpha$-RSS, $\alpha$-FCNN, and $\alpha$-SFCNN are comparable to $\alpha$-HSS, which guarantees the best possible approximation factor in general metrics, while $\alpha$-NET is significantly outperformed.

Subquadratic Approach. Using the same experiment framework, we evaluate performance of the subquadratic implementation $(\alpha, \varepsilon)$-RSS described in Section 3.3. Thus, we change the value of $\varepsilon$ to assess its effect on the running time and selection size over the algorithm, for two values of $\alpha$ (see Figure 5). The results show an expected increase of the number of selected points, while significantly improving its running time.
B Proofs and Missing Details

B.1 On $\alpha$-Consistent Subsets

Just as stated in Section 3, FCNN is a state-of-the-art algorithm to compute consistent subsets (see Algorithm 1). It is an iterative algorithm that incrementally builds a consistent subset of $P$ as follows. First, it selects the centroids of each class, and then continues adding points iteratively until the subset is consistent. On each iteration and for every $p \in P$, one representative from the set $voren(p, FCNN, P) = \{ q \in P | nn(q, FCNN) = p \land l(q) \neq l(p) \}$ is selected. The representative is chosen using the $rep$ function, which is usually defined as the closest to $p$ (although different approaches can be used). As evidenced in the algorithm, all the representatives chosen in one iteration are added to the subset in a batch (set $S$). We show that such batch addition prevents FCNN from having any upper-bound on its selection size.

\begin{algorithm}[
\topskip \baselineskip \parskip \small
\centering
\textbf{Fast Condensed Nearest-Neighbor}\vspace{0.5em}
\textbf{Input:} Initial training set $P$
\textbf{Output:} Condensed training set $FCNN \subseteq P$
\begin{algorithmic}[1]
\State $FCNN \leftarrow \emptyset$
\State $S \leftarrow \text{centroids}(P)$
\While {$S \neq \emptyset$}
\State $FCNN \leftarrow FCNN \cup S$
\State $S \leftarrow \emptyset$
\ForAll {$p \in FCNN$}
\State $S \leftarrow S \cup \{rep(p, voren(p, FCNN, P))\}$
\EndFor
\EndWhile
\State \textbf{return} FCNN
\end{algorithmic}
\caption{Algorithm 1: Fast Condensed Nearest-Neighbor}
\end{algorithm}

\begin{thm}
There exists a training set $P \subset \mathbb{R}^d$, with constant number of classes and $\kappa$ number of nearest-enemy points, such that FCNN selects $\Omega(\kappa/\xi)$ points, for any $0 < \xi < 1$.
\end{thm}

\textbf{Proof.} Without loss of generality, let $\xi = 1/2^t$ for some value $t > 3$, we construct a training set $P \subset \mathbb{R}^3$ with constant number of classes, and number of nearest-enemy points $\kappa$ equal to $O(1/\xi)$, for which FCNN is forced to select $O(1/\xi^2)$ points. The key downside of the algorithm occurs when points are added to FCNN in the same iteration. In general, during any given iteration, the representatives of two neighboring points in FCNN can be arbitrarily close to each other. This flaw can be exploited to force FCNN to add $O(1/\xi)$ such points.

Intuitively, our constructed training set $P$ consists of several layers of points arranged parallel to the $xy$-plane, and stacked on top of each other around the $z$-axis (see Figure 6). Each layer is a disk-like arrangement, formed by a center point and points at distance 1 from this center. Thus, define the backbone points of $P$ as the center points $c_i = 2i \vec{v}_z$ for $i \geq 0$. We now describe the different arrangements of points as follows (see Figure 6):

$B = c_0 \cup \{y_j = c_0 + \vec{v}_x R_z(j\pi/4) \mid j \in [0, \ldots, 8]\}$

$\mathcal{M}_i = \{c_{2i}, c_{2i+1}, m_i = (c_{2i} + c_{2i+1})/2\}$

$\cup \{r_{ij} = c_{2i} + \vec{v}_x R_z(j\pi/2^{1+i}) \mid j \in [0, \ldots, 2^{2+i}]\}$

$\cup \{b_{ij} = c_{2i+1} + \vec{v}_x R_z(j\pi/2^{1+i}) \mid j \in [0, \ldots, 2^{2+i}]\}$

$\cup \{w_{ij} = c_{2i+1} + \vec{v}_x R_z((2j+1)\pi/2^{2+i} - \xi^2) \mid j \in [0, \ldots, 2^{2+i}]\}$
\[ \mathcal{R}_i = \{c_{2i}, c_{2i+1}\} \]

\[ \cup \{r_{ij} = c_{2i} + v_{s+1}^j R_z(j2\pi/\xi) \mid j \in [0, \ldots, \xi]\} \]

\[ \cup \{b_{ij} = c_{2i+1} + v_{s+1}^j R_z(j2\pi/\xi) \mid j \in [0, \ldots, \xi]\} \]

These points belong to one of 11 classes named \( \{1, \ldots, 8, \text{red, blue, white}\} \). Then define the labeling function \( l \) as follows: \( l(c_i) \) is red when \( i \) is even and blue when \( i \) is odd, \( l(m_i) \) is white, \( l(y_{ij}) \) is the \( j \)-th class, \( l(r_{ij}) \) is red, \( l(b_{ij}) \) is blue, and \( l(w_{ij}) \) is white.

- **Base arrangement \( \mathcal{B} \):** Consists of one single layer of points, with one red center point \( c_0 \) and 8 points \( y_j \) in the circumference of the unit disk (parallel to the \( xy \)-plane), each labeled with a unique class \( j \) (see Figure 6a). The goal of this arrangement is that each of these points is the centroid of its corresponding class. The centroids of the blue and white classes can be fixed to be far enough, so we won’t consider them for now. Hence, the first iteration of FCNN will add all the points of \( \mathcal{B} \). In the next iteration, each of these points will select a representative in the arrangement above. Clearly, the size of \( \mathcal{B} \) is 9, and it contributes with 8 nearest-enemy points in total.

- **Multiplier arrangement \( \mathcal{M}_i \):** Our final goal is to have \( O(1/\xi) \) arbitrarily close points selecting representatives on a single iteration; currently, we only have 9 (the base arrangement). While this could be simply achieved with \( O(1/\xi) \) points in \( \mathcal{B} \) each with a unique class, we want to use a constant number of classes. Instead, we use each multiplier arrangement to double the number of representatives selected. \( \mathcal{M}_i \) consists of (1) a layer with a blue center \( c_{2i} \) and \( 2^{2+i} \) red points \( r_{ij} \) around the unit disk’s circumference, (2) a layer with a red center \( c_{2i+1} \) and \( 2^{2+i} \) blue points \( b_{ij} \) and white \( w_{ij} \) points around the unit disk’s circumference, and (3) a middle white center point \( m_i \) between the red and blue center points (see Figure 6b). Suppose at iteration \( 3i - 1 \) all the points \( r_{ij} \) and \( c_{2i} \) of the first layer are added as representatives of the previous arrangement, which is given for \( \mathcal{M}_1 \) from the selection of \( \mathcal{B} \). Then, during iteration \( 3i \) each \( r_{ij} \) adds the point \( b_{ij} \) right above, while \( c_{2i} \) adds point \( m_i \) (the red arrows in Figure 6a). Finally, during iteration \( 3i + 1 \), \( m_i \) adds \( c_{2i+1} \), and each \( b_{ij} \) adds point \( w_{ij} \) as its the closest point inside the voronoi cell of \( b_{ij} \) (see the blue arrows in Figure 6a). Now, with all the points of this layer added, each continues to select points in the following arrangement (either \( \mathcal{M}_{i+1} \) or \( \mathcal{R}_{i+1} \)). The size of each \( \mathcal{M}_i \) is \( 3(1 + 2^{2+i}) = O(2^{2+i}) \), and contributes with \( 3 + 2(2^{2+i}) = O(2^{2+i}) \) to the total number of nearest-enemy points. In order to select \( 1/\xi = 2^t \) points in a single iteration, we need to stack \( \mathcal{M}_i \)’s for \( i \in [1, \ldots, t-3] \).

- **Repetitive arrangement \( \mathcal{R}_i \):** Once the algorithm reaches the last multiplier layer \( \mathcal{M}_{t-3} \), it will select \( 1/\xi \) points during the following iteration. The repetitive arrangement allows us to continue adding these many points on every iteration, while only increasing the number of nearest-enemy points by a constant. This arrangement consists of (1) a first layer with a blue center \( c_{2i} \), surrounded by \( 1/\xi \) red points \( r_{ij} \) around the unit disk circumference, and (2) a second layer with red center \( c_{2i+1} \) and blue points \( b_{ij} \) in the circumference (see Figure 6b). Once the first layer is added all in a single iteration, during the following iteration \( c_{2i} \) adds \( c_{2i+1} \), and each \( r_{ij} \) adds \( b_{ij} \). The size of each \( \mathcal{R}_i \) is \( 2(1+1/\xi) = O(1/\xi) \), and it contributes with 4 points to the total number of nearest-enemy points. Now, we stack \( O(1/\xi) \) such arrangements \( \mathcal{R}_i \) for \( i \in [t-2, \ldots, 1/\xi] \), such that we obtain the desired ratio between selected points and number of nearest-enemy points of the training set.

The training set is then defined as \( P = \mathcal{B} \cup_{i=1}^{t-3} \mathcal{M}_i \cup_{i=t-2}^{1/\xi} \mathcal{R}_i \cup \mathcal{F} \), where \( \mathcal{F} \) is a set of points designed to fix the centroids of \( P \). These extra points are located far enough from the remaining points of \( P \), and are carefully placed such that the centroids of \( P \) are all the points of \( \mathcal{B} \), plus a blue and white point from \( \mathcal{F} \). Additionally, all the points of \( \mathcal{F} \) should be closer
(a) Entire arrangement of points, by stacking the different arrangements along the z-axis. The arrows illustrate the selection process by FCNN on a multiplicative arrangement $M_i$.

(b) Base arrangement $B$. Each point in the circumference belongs to a unique class (here colored in yellow and numbered 1 to 8 for clarity).

(c) A multiplier arrangement $M_i$. This forces FCNN to duplicate the number of representatives around the circumference selected on an iteration.

(d) A repetitive arrangement $R_i$. This maintains the number of representatives selected by FCNN on each iteration of the algorithm.

Figure 6 Example of a training set $P \subset \mathbb{R}^3$ for which FCNN selects $\Omega(\kappa/\xi)$ points.

to its corresponding class centroid than to any enemy centroid, and they should increase the number of nearest-enemy points by a constant. This can be done with $O(n)$ extra points.

All together, by adding up the corresponding terms, the ratio between the size of FCNN and $\kappa$ (the number of nearest-enemy points of $P$) is $O(1/\xi)$. Therefore, there exists a training set in 3-dimensional Euclidean space for which FCNN selects $O(\kappa/\xi)$ for any $\xi < 1/8$. ▶

B.2 On $\alpha$-Selective Subsets

Similarly, many details related to the computation of $\alpha$-selective subsets where omitted throughout the paper due to space constraints. This section provides a formal proof for the hardness of approximation of the MIN-$\alpha$-SS problem. Additionally, we present a formal description of the $\alpha$-RSS algorithm (which is an extension of RSS [14]) along with the proofs of some of the guarantees related to this algorithm.
The following is the proof of Theorem 8:

**Proof.** The result follows from the hardness of another related covering problem: the minimum dominating set \[13,20,22\]. We describe a simple L-reduction from any instance of this problem to an instance of MIN-\(\alpha\)-SS, which preserves the approximation ratio.

1. Consider any instance of minimum dominating set, consisting of the graph \(G = (V, E)\).

2. Generate a new edge-weighted graph \(G'\) as follows:
   
   Create two copies of \(G\), namely \(G_r = (V_r, E_r)\) and \(G_b = (V_b, E_b)\), of red and blue nodes respectively. Set all edge-weights of \(G_r\) and \(G_b\) to be 1. Finally, connect each red node \(v_r\) to its corresponding blue node \(v_b\) by an edge \(\{v_r, v_b\}\) of weight \(1 + \alpha + \xi\) for a sufficiently small constant \(\xi > 0\). Formally, \(G'\) is defined as the edge-weighted graph \(G' = (V', E')\) where the set of nodes is \(V' = V_r \cup V_b\), the set of edges is \(E' = E_r \cup E_r \cup \{\{v_r, v_b\} | v \in V\}\), and an edge-weight function \(w : E' \rightarrow \mathbb{R}^+\) where \(w(e) = 1\) iff \(e \in E_r \cup E_b\), and \(w(e) = 1 + \alpha + \xi\) otherwise.

3. A labeling function \(l\) where \(l(v) = \text{red}\) iff \(v \in V_r\), and \(l(v) = \text{blue}\) iff \(v \in V_b\).

4. Compute the shortest-path metric of \(G'\), denoted as \(d_{G'}\).

5. Solve the MIN-\(\alpha\)-SS problem for the set \(V'\), on metric \(d_{G'}\), and the labels defined by \(l\).

A dominating set of \(G\) consists of a subset of nodes \(D \subseteq V\), such that every node \(v \in V \setminus D\) is adjacent to a node in \(D\). Given any dominating set \(D \subseteq V\) of \(G\), it is easy to see that the subset \(R = \{v_r, v_b | v \in D\}\) is an \(\alpha\)-selective subset of \(V'\), where \(|R| = 2|D|\). Similarly, given an \(\alpha\)-selective subset \(R' \subseteq V'\), there is a corresponding dominating set \(D\) of \(G\), where \(|D| \leq |R'|/2\), as \(D\) can be either \(R \cap V_r\) or \(R \cap V_b\). Therefore, MIN-\(\alpha\)-SS is as hard to approximate as the minimum dominating set problem. □

**Algorithm 2: \(\alpha\)-Relaxed Selective Subset**

\[\text{Input:}\] Initial training set \(P\) and parameter \(\alpha \geq 0\)

\[\text{Output:}\] Condensed training set \(\alpha\text{-RSS} \subseteq P\)

1. \(\alpha\text{-RSS} \leftarrow \phi\)

2. Let \(\{p_i\}_{i=1}^n\) be the points of \(P\) sorted in increasing order of nearest-enemy distance

3. \textbf{foreach} \(p_i \in P\), where \(i = 1 \ldots n\) \textbf{do}

4. \hspace{1cm} if \((1 + \alpha) d_{\text{nn}}(p_i, \alpha\text{-RSS}) \geq d_{\text{ne}}(p_i)\) then

5. \hspace{2cm} \(\alpha\text{-RSS} \leftarrow \alpha\text{-RSS} \cup \{p_i\}\)

6. return \(\alpha\text{-RSS}\)

**On the \(\alpha\text{-RSS}\) algorithm.** The following results deal with the characteristics and guarantees of the \(\alpha\text{-RSS}\) algorithm (see Algorithm 2). While it was already described in Section 3.2, some details were left aside. Clearly, its order independence follows from the initial sorting step of the algorithm. It is less obvious why the resulting subset is \(\alpha\)-selective. Consider a point \(p \in P\). If \(p \in \alpha\text{-RSS}\), its nearest neighbor in \(\alpha\text{-RSS}\) is itself, making \(\delta(p, \alpha\text{-RSS}) = \infty\). Otherwise, if \(p \notin \alpha\text{-RSS}\), by the selection process of the algorithm, \(d_{\text{nn}}(p, \alpha\text{-RSS}) < d_{\text{ne}}(p)/(1+\alpha) \leq d_{\text{ne}}(p)\). This, on its own, implies that \(\alpha\text{-RSS}\) is selective. Additionally, clearly \(d_{\text{ne}}(p) \leq d_{\text{ne}}(p, \alpha\text{-RSS})\).

All together, the chromatic density of \(p\) with respect to \(\alpha\text{-RSS}\) is at least \(\alpha\):

\[
\delta(p, \alpha\text{-RSS}) = \frac{d_{\text{nn}}(p, \alpha\text{-RSS})}{d_{\text{nn}}(p, \alpha\text{-RSS})} - 1 > \frac{d_{\text{ne}}(p)}{d_{\text{ne}}(p)/(1+\alpha)} - 1 = \alpha
\]
Additionally, we should analyze the worst-case time complexity of the algorithm. The initial step requires $\mathcal{O}(n^2)$ time for computing the nearest-enemy distances of each point in $P$ and $\mathcal{O}(n \log n)$ time for sorting the points according to such distance. The main loop iterates through each point in $P$, and searches their nearest neighbor in the current subset, incurring into additional $\mathcal{O}(n^2)$ time. Therefore, its worst-case time complexity is $\mathcal{O}(n^2)$.

The following is the proof of Theorem 10.

Proof. The proof follows from a charging argument on each nearest-enemy point of $P$. First, consider one such nearest-enemy point $p \in P$ and a value $\alpha \in [\gamma, 1)$, then define $\alpha$-RSS$^\prime_{p, \sigma}$ to be the subset of points from $\alpha$-RSS such that their nearest-enemy is $p$ and their nearest-enemy distance is between $\sigma$ and $b\sigma$, for some $b > 1$. Throughout this proof, we use $b = \frac{\gamma + \alpha}{1 + \alpha}$.

Clearly, such subsets define a partition of $\alpha$-RSS when considering all nearest-enemy points of $P$, and values of $\sigma = \gamma b^i$ for $i = \{0, 1, 2, \ldots, \lceil \log_\gamma \frac{1}{\gamma} \rceil \}$.

We now analyze the size of each subset $\alpha$-RSS$^\prime_{p, \sigma}$ by bounding its spread. Consider any two points $p_i, p_j \in \alpha$-RSS$^\prime_{p, \sigma}$, where without loss of generality $d_{ne}(p_i) \leq d_{ne}(p_j)$. One of the key features of $\alpha$-RSS is that the points selected cannot be “too close” to each other; that is, as $p_i$ and $p_j$ where selected by the algorithm, we know that $(1 + \alpha) d(p_i, p_j) \geq d_{ne}(p_j) \geq \sigma$.

Therefore, the smallest pairwise distance in $\alpha$-RSS$^\prime_{p, \sigma}$ is at least $\sigma/(1 + \alpha)$. Additionally, by a simple use of the triangle inequality, we can use the common nearest-enemy point $p$ as follows $d(p_i, p_j) \leq d(p_i, p) + d(p, p_j) = d_{ne}(p_i) + d_{ne}(p_j) \leq 2\sigma$. Hence, the diameter of $\alpha$-RSS$^\prime_{p, \sigma}$ (i.e., its largest pairwise distance) is at most $2\sigma$. Finally, using the aforementioned property of doubling spaces, we obtain the following upper-bound for the size of $\alpha$-RSS$^\prime_{p, \sigma}$:

$$|\alpha\text{-RSS}^\prime_{p, \sigma}| \leq \left[ \frac{2\sigma}{\frac{\gamma + \alpha}{1 + \alpha}} \right]^{d\dim(X)+1} = \lceil 4 + 2\alpha \rceil^{d\dim(X)+1}$$

All together, we have that:

$$|\alpha\text{-RSS}| \leq \sum_{p} \sum_{i=0}^{\log_\gamma \frac{1}{\gamma}} |\alpha\text{-RSS}^\prime_{p, b^i}| \leq \kappa \left[ \log_\gamma \frac{1}{\gamma} \right] \lceil 4 + 2\alpha \rceil^{d\dim(X)+1}$$

For constant $\alpha$ and doubling dimension $d\dim(X)$, the size of $\alpha$-RSS is $\mathcal{O}(\kappa \log \frac{1}{\gamma})$. □

The following is the proof of Theorem 12.

Proof. Let $p$ be any nearest-enemy point of $P$ and $\sigma \in [\gamma, 1)$, similarly define $\alpha$-RSS$^\prime_{p, \sigma}$ to be the set of points selected by $\alpha$-RSS whose nearest-enemy is $p$ and their nearest-enemy distance is between $\sigma$ and $b\sigma$, for $b = \frac{(1+\alpha)^2}{\alpha(2+\alpha)}$. Equivalently, these subsets define a partitioning of $\alpha$-RSS for all nearest-enemy points $p$ and values of $\sigma = \gamma b^i$ for $i = \{0, 1, 2, \ldots, \lceil \log_\gamma \frac{1}{\gamma} \rceil \}$. Thus, the proof follows from bounding the minimum angle between points in these subsets. For any two such points $p_i, p_j$, we lower bound the angle $\angle p_i pp_j$. Assume without loss of generality that $d_{ne}(p_i) \leq d_{ne}(p_j)$. By definition of the partitioning, we also know that $d_{ne}(p_j) \leq b\sigma \leq b d_{ne}(p_i)$. Therefore, altogether we have that $d_{ne}(p_i) \leq d_{ne}(p_j) \leq b d_{ne}(p_i)$.

First, consider the set of points whose distance to $p_i$ is $(1+\alpha)$ times their distance to $p$, which defines a multiplicative weighted bisector between points $p$ and $p_i$, with weights equal to 1 and $1/(1+\alpha)$ respectively. This is characterized as a $d$-dimensional ball (see Figure 7a) with center $c_i = (p_i - p) b + p$ and radius $d_{ne}(p_i) b/(1+\alpha)$. Thus, $p$, $p_i$ and $c_i$ are collinear, and the distance between $p$ and $c_i$ is $d(p, c_i) = b d_{ne}(p_i)$. In particular, let’s
consider the relation between \( p_j \) and such bisector. As \( p_j \) was selected by the algorithm after \( p_i \), we know that \((1 + \alpha) d(p_j, p_i) \geq d_{ae}(p_j)\) where \( d_{ae}(p_j) = d(p_j, p) \). Therefore, clearly \( p_j \) lies either outside or in the surface of the weighted bisector between \( p \) and \( p_i \) (see Figure 7b).

For angle \( \angle p_i p p_j \), we can frame the analysis to the plane defined by \( p, p_i \) and \( p_j \). Let \( x \) and \( y \) be two points in this plane, such that they are the intersection points between the weighted bisector and the balls centered at \( p \) of radii \( d_{ae}(p_i) \) and \( b d_{ae}(p_i) \) respectively (see Figure 7c). By the convexity of the weighted bisector between \( p \) and \( p_i \), we can say that \( \angle p_i p p_j \geq \min(\angle xpp_i, \angle ypc_i) \). Now, consider the triangles \( \triangle xp p_i \) and \( \triangle py c_i \). By the careful selection of \( b \), these triangles are both isosceles and similar. In particular, for \( \triangle xp p_i \) the two sides incident to \( p \) have length equal to \( d_{ae}(p_i) \), and the side opposite to \( p \) has length equal to \( d_{ae}(p_i)/(1 + \alpha) \). For \( \triangle py c_i \), the side lengths are \( b d_{ae}(p_i) \) and \( d_{ae}(p_i) b/(1 + \alpha) \). Therefore, the angle \( \angle p_i p p_j \geq \angle xpp_i \geq 1/(1 + \alpha) \).

By a simple packing argument based on this minimum angle, we have that the size of \( \alpha\text{-RSS}_{p,\sigma}^\prime \) is \( O((1 + \alpha)^{d-1}) \). All together, following the defined partitioning, we have that:

\[
|\alpha\text{-RSS}| = \sum_p \sum_{i=0}^{\lceil \log_b \frac{1}{\gamma} \rceil} |\alpha\text{-RSS}_{p,b}^\prime| \leq \kappa \left\lceil \log_b \frac{1}{\gamma} \right\rceil O \left((1 + \alpha)^{d-1}\right)
\]

For constant \( \alpha \) and \( d \), the size of \( \alpha\text{-RSS} \) is \( O(\kappa \log \frac{1}{\gamma}) \). Moreover, when \( \alpha \) is zero we get \( |0\text{-RSS}| = O(\kappa \ c^{d-1}) \), matching the previously known bound for RSS in Euclidean space. \( \blacksquare \)