Nearest Neighbor Condensation with Guarantees

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Abstract

The problem of nearest-neighbor (NN) condensation deals with reducing the training-set P for the NN-rule classifier. We propose a new NN condensation algorithm called RSS, and prove that selects a subset of size at most $\mathcal{O}(k \log \Delta)$, where k is the number of points in the decision borders of P, and Δ its spread. Similarly, we show that a state-of-the-art algorithm called MSS, selects a subset of size at most $\mathcal{O}(k)$. To the best of our knowledge, these are the first bounds on the sizes of point sets generated by NN condensation algorithms. Additionally, we proof the probability of correctly classifying a query point with ϵ-ANN using RSS, grows exponentially with respect to the size of the RSS set.

1 Introduction

Consider a training-set $P \subset \mathbb{R}^d$ of n points, where each point $p \in P$ belongs to one of a set of discrete classes, denoted $l(p)$. The goal of nonparametric classification techniques, is to accurately predict the class of new points. Among the most well-known techniques is the *nearest-neighbor* (NN) *rule*, which given a query point $q \in \mathbb{R}^d$, assigns it the class of its nearest neighbor in P, denoted $\mathrm{NN}(q)$.

Despite its simplicity, the NN rule exhibits good classification accuracy. Theoretical results show that its probability of error is bounded by twice the Bayes probability of error (the minimum of any decision rule). However, the NN rule is often criticized on the basis of its memory requirements, as P must be stored to answer queries. For this reason, we consider the problem of *Nearest Neighbor Condensation*: selecting a subset of P that maintains its classification performance.

2 Related work

Consider the *Delaunay triangulation* of P. Points with at least one neighbor of a different class are called *border points*, while others are called *internal points*. One approach for NN condensation is to select the set of *border points* of P. This is called *Voronoi condensation* [7]. Unfortunately, a straightforward algorithm is impractical in high-dimensional spaces. For the planar case, an output-sensitive algorithm was proposed [3], which runs in $\mathcal{O}(n \log k)$ time when k is the number of *border points* in P. Yet, it remains an open problem whether this is possible for higher dimensions.

There are other properties that can be used to condense P. First, let's introduce the concept of *enemy*; an enemy of a point $p \in P$ is any point in P of different class, and the *nearest enemy* of p is denoted as $\mathrm{NE}(p)$. Now, let $R \subseteq P$ we say that:

- R is a *consistent* subset of P *iff* for every point $p \in P$, its NN in R is of the same class as p (i.e., p is correctly classified by R).
- R is a *selective* subset of P *iff* for every point $p \in P$, its NN in R is closer to p than is NE in P. Clearly, selectiveness implies consistency.

It has been shown that both problems of finding minimum-size *consistent* and *selective* subsets are NP-complete [8]. Therefore, many heuristics have been proposed to find subsets with such properties (for a comprehensive survey see [6]). Among them, CNN [4] was the first algorithm proposed for computing *consistent* subsets. It has been widely used, despite its worst-case cubic running time, and being order-dependent[1]. Recent efforts resulted in FCNN [1] and MSS [2], which produce *consistent* and *selective* subsets respectively. Both algorithms run in $\mathcal{O}(n^2)$ time, and are order-independent. Unfortunately, to the best of our knowledge, no bounds are known for the size of the subsets generated by any of these algorithms.

Moreover, condensation can introduce problems during classification. In general, these algorithms focus on selecting border points, as they are key in maintaining the classification accuracy on exact NN queries. However, we argue that keeping internal points can be beneficial when performing *approximate* NN queries, increasing the chances of correct classification, and reducing the query time [5].

3 Relaxed Selective Subset

We propose an algorithm for NN condensation called RSS, or *Relaxed Selective Subset* (See Algorithm 1). First let's introduce some extra notation. Let $d(p, q)$

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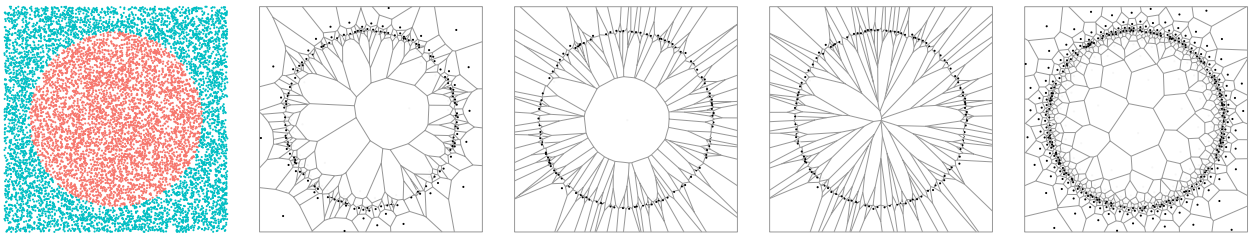
[1] Order-dependence means the resulting subset is determined by the order in which points are considered by the algorithm.



(a) Dataset (10^4 pts) (b) CNN (281 pts) (c) FCNN (222 pts) (d) MSS (233 pts) (e) RSS (627 pts)

Figure 1: An illustrative example of the subsets selected by CNN, FCNN, MSS, and RSS.

be the distance between any two points $p, q \in \mathbb{R}^d$, and $d_{\text{NE}}(p)$ be the *nearest enemy* distance of any point $p \in P$, defined as $d_{\text{NE}}(p) = d(p, \text{NE}(p))$.

Algorithm 1: Relaxed Selective Subset

Input: Initial point set P
Output: Condensed point set RSS $\subseteq P$

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Let {p_i}_{i=1}^n be the points of P sorted in increasing
  order of NE distance d_NE(p_i)
RSS ← φ
foreach p_i ∈ P, where i = 1...n do
    if ¬∃ r ∈ RSS such that d(p_i, r) < d_NE(r) then
        RSS ← RSS ∪ {p_i}
return RSS
```

RSS runs in $\mathcal{O}(n^2)$ time, and it is order-independent as points are sorted before being considered. Moreover:

Theorem 1 RSS *is a selective subset of* P.

This places RSS among state-of-the-art algorithms for NN condensation. However, how do these algorithms compare in terms of the size of their selected subsets? While other algorithms tend to select border points (or points close to the decision borders), the idea behind RSS is to also select internal points following a particular strategy. Figure 1 illustrates the way RSS selects points in comparison with other NN condensation algorithms. In the following theorems, we formalize the bounds on the size of RSS and MSS.

Theorem 2 *Let k be the number of border points of P, and Δ the spread of P. Then,* $|\text{RSS}| \leq \mathcal{O}(k \log \Delta)$.

Theorem 3 *Let k be the number of border points of P. Then,* $|\text{MSS}| \leq \mathcal{O}(k)$.

While RSS can select more points than MSS, we argue that these extra points are beneficial during classification. These internal points will increase the probability of correct classification when using ϵ-approximate NN queries. This intuition is formalized as follows:

Theorem 4 *Let point $q \in \mathbb{R}^d$ be drawn uniformly at random from the minimum enclosing ball of P, where P has k border points and spread Δ. Then, the probability of equally classifying q with* RSS*, using both exact and ϵ-approximate* NN *queries (for $\epsilon \leq 2$), is bounded by:*

$$Pr\left[l(\text{NN}_{\text{RSS}}(q)) = l(\text{ANN}_{\text{RSS}}(\epsilon, q)) \right] \geq \frac{k 2^{\Omega(\frac{j\text{RSS}j}{k})}}{\Delta^d}$$

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