Journal of Machine Learning Research 14 (2013) 2583-2615 Submitted 12/12; Revised 5/13; Published 9/13

Efficient Active Learning of Halfspaces: An Aggressive Approach

Alon Gonen ALONGNN@CS.HUJI.AC.IL
The Rachel and Selim Benin School of Computer Science and Engineering
The Hebrew University
Givat Ram, Jerusalem 91904, Israel

Sivan Sabato SIVAN.SABATO@MICROSOFT.COM
Microsoft Research New England
1 Memorial Drive
Cambridge, MA, 02142

Shai Shalev-Shwartz SHAIS@CS.HUJI.AC.IL
The Rachel and Selim Benin School of Computer Science and Engineering
The Hebrew University
Givat Ram, Jerusalem 91904, Israel

Editor: John Shawe-Taylor

Abstract

We study pool-based active learning of half-spaces. We revisit the aggressive approach for active learning in the realizable case, and show that it can be made efficient and practical, while also having theoretical guarantees under reasonable assumptions. We further show, both theoretically and experimentally, that it can be preferable to mellow approaches. Our efficient aggressive active learner of half-spaces has formal approximation guarantees that hold when the pool is separable with a margin. While our analysis is focused on the realizable setting, we show that a simple heuristic allows using the same algorithm successfully for pools with low error as well. We further compare the aggressive approach to the mellow approach, and prove that there are cases in which the aggressive approach results in significantly better label complexity compared to the mellow approach. We demonstrate experimentally that substantial improvements in label complexity can be achieved using the aggressive approach, for both realizable and low-error settings.

Keywords: active learning, linear classifiers, margin, adaptive sub-modularity

1. Introduction

We consider pool-based active learning (McCallum and Nigam, 1998), in which a learner receives a pool of unlabeled examples, and can iteratively query a teacher for the labels of examples from the pool. The goal of the learner is to return a low-error prediction rule for the labels of the examples, using a small number of queries. The number of queries used by the learner is termed its *label complexity*. This setting is most useful when unlabeled data is abundant but labeling is expensive, a common case in many data-laden applications. A pool-based algorithm can be used to learn a classifier in the standard PAC model, while querying fewer labels. This can be done by first drawing a random unlabeled sample to be used as the pool, then using pool-based active learning to identify its labels with few queries, and then using the resulting labeled sample as input to a regular “passive” PAC-learner.

Most active learning approaches can be loosely described as more ‘aggressive’ or more ‘mellow’. A more aggressive approach is one in which only highly informative queries are requested (where the meaning of ‘highly informative’ depends on the particular algorithm) (Tong and Koller, 2002; Balcan et al., 2007; Dasgupta et al., 2005), while the mellow approach, first proposed in the CAL algorithm (Cohn et al., 1994), is one in which the learner essentially queries all the labels it has not inferred yet.

In recent years a significant advancement has been made for active learning in the PAC model. In particular, it has been shown that when the data is realizable (relative to some assumed hypothesis class), the mellow approach can guarantee an exponential improvement in label complexity, compared to passive learning (Balcan et al., 2006a). This exponential improvement depends on the properties of the distribution, as quantified by the *Disagreement Coefficient* proposed in Hanneke (2007). Specifically, when learning half-spaces in Euclidean space, the disagreement coefficient implies a low label complexity when the data distribution is uniform or close to uniform. Guarantees have also been shown for the case where the data distribution is a finite mixture of Gaussians (El-Yaniv and Wiener, 2012).

An advantage of the mellow approach is its ability to obtain label complexity improvements in the agnostic setting, which allows an arbitrary and large labeling error (Balcan et al., 2006a; Dasgupta et al., 2007). Nonetheless, in the realizable case the mellow approach is not always optimal, even for the uniform distribution (Balcan et al., 2007). In this work we revisit the aggressive approach for the realizable case, and in particular for active learning of half-spaces in Euclidean space. We show that it can be made efficient and practical, while also having theoretical guarantees under reasonable assumptions. We further show, both theoretically and experimentally, that it can sometimes be preferable to mellow approaches.

In the first part of this work we construct an efficient aggressive active learner for half-spaces in Euclidean space, which is approximately optimal, that is, achieves near-optimal label complexity, if the pool is separable with a margin. While our analysis is focused on the realizable setting, we show that a simple heuristic allows using the same algorithm successfully for pools with low error as well. Our algorithm for halfspaces is based on a greedy query selection approach as proposed in Tong and Koller (2002) and Dasgupta (2005). We obtain improved target-dependent approximation guarantees for greedy selection in a general active learning setting. These guarantees allow us to prove meaningful approximation guarantees for halfspaces based on a margin assumption.

In the second part of this work we compare the greedy approach to the mellow approach. We prove that there are cases in which this highly aggressive greedy approach results in significantly better label complexity compared to the mellow approach. We further demonstrate experimentally that substantial improvements in label complexity can be achieved compared to mellow approaches, for both realizable and low-error settings.

The first greedy query selection algorithm for learning halfspaces in Euclidean space was proposed by Tong and Koller (2002). The greedy algorithm is based on the notion of a *version space*: the set of all hypotheses in the hypothesis class that are consistent with the labels currently known to the learner. In the case of halfspaces, each version space is a convex body in Euclidean space. Each possible query thus splits the current version space into two parts: the version space that would result if the query received a positive label, and the one resulting from a negative label. Tong and Koller proposed to query the example from the pool that splits the version space as evenly as possible. To implement this policy, one would need to calculate the volume of a convex body in Euclidean space, a problem which is known to be computationally intractable (Brightwell and Winkler, 1991). Tong and Koller thus implemented several heuristics that attempt to follow their proposed selection principle using an efficient algorithm. For instance, they suggest to choose the example which is closest to the max-margin solution of the data labeled so far. However, none of their heuristics provably follow this greedy selection policy.

The label complexity of greedy pool-based active learning algorithms can be analyzed by comparing it to the best possible label complexity of any pool-based active learner on the same pool. The *worst-case label complexity* of an active learner is the maximal number of queries it would make on the given pool, where the maximum is over all the possible classification rules that can be consistent with the pool according to the given hypothesis class. The *average-case label complexity* of an active learner is the average number of queries it would make on the given pool, where the average is taken with respect to some fixed probability distribution P over the possible classifiers in the hypothesis class. For each of these definitions, the optimal label complexity is the lowest label complexity that can be achieved by an active learner on the given pool. Since implementing the optimal label complexity is usually computationally intractable, an alternative is to implement an efficient algorithm, and to guarantee a bounded factor of approximation on its label complexity, compared to the optimal label complexity.

Dasgupta (2005) showed that if a greedy algorithm splits the probability mass of the version space as evenly as possible, as defined by the fixed probability distribution P over the hypothesis class, then the approximation factor for its average label complexity, with respect to the same distribution, is bounded by

$O(\log(1/p_{\min}))$, where $p_{\min}$ is the minimal probability of any possible labeling of the pool, if the classifier is drawn according to the fixed distribution. Golovin and Krause (2010) extended Dasgupta's result and showed that a similar bound holds for an approximate greedy rule. They also showed that the approximation factor for the worst-case label complexity of an approximate greedy rule is also bounded by $O(\log(1/p_{\min}))$, thus extending a result of Arkin et al. (1993). Note that in the worst-case analysis, the fixed distribution is only an analysis tool, and does not represent any assumption on the true probability of the possible labelings.

Returning to greedy selection of halfspaces in Euclidean space, we can see that the fixed distribution over hypotheses that matches the volume-splitting strategy is the distribution that draws a halfspace uniformly from the unit ball.[1] The analysis presented above thus can result in poor approximation factors, since if there are instances in the pool that are very close to each other, then $p_{\min}$ might be very small.

We first show that mild conditions suffice to guarantee that $p_{\min}$ is bounded from below. By proving a variant of a result due to Muroga et al. (1961), we show that if the examples in the pool are stored using number of a finite accuracy $1/c$, then $p_{\min} \geq (c/d)^{d^2}$, where d is the dimensionality of the space. It follows that the approximation factor for the worst-case label complexity of our algorithm is at most $O(d^2 \log(d/c))$.

While this result provides us with a uniform lower bound on $p_{\min}$, in many real-world situations the probability of the target hypothesis (i.e., one that is consistent with the true labeling) could be much larger than $p_{\min}$. A noteworthy example is when the target hypothesis separates the pool with a margin of γ. In this case, it can be shown that the probability of the target hypothesis is at least γ^d, which can be significantly larger than $p_{\min}$. An immediate question is therefore: can we obtain a *target-dependent* label complexity approximation factor that would depend on the probability of the target hypothesis, $P(h)$, instead of the minimal probability of any labeling?

We prove that such a target dependent bound *does not* hold for a general approximate-greedy algorithm. To overcome this, we introduce an algorithmic change to the approximate greedy policy, which allows us to obtain a label complexity approximation factor of $\log(1/P(h))$. This can be achieved by running the approximate-greedy procedure, but stopping the procedure early, before reaching a pure version space that exactly matches the labeling of the pool. Then, an approximate majority vote over the version space, that is, a random rule which approximates the majority vote with high probability, can be used to determine the labels of the pool. This result is general and holds for any hypothesis class and distribution. For halfspaces, it implies an approximation-factor guarantee of $O(d \log(1/\gamma))$.

We use this result to provide an efficient approximately-optimal active learner for half-spaces, called *ALuMA*, which relies on randomized approximation of the volume of the version space (Kannan et al., 1997). This allows us to prove a margin-dependent approximation factor guarantee for ALuMA. We further show an additional, more practical implementation of the algorithm, which has similar guarantees under mild conditions which often hold in practice. The assumption of separation with a margin can be relaxed if a lower bound on the total hinge-loss of the best separator for the pool can be assumed. We show that under such an assumption a simple transformation on the data allows running ALuMA as if the data was separable with a margin. This results in approximately optimal label complexity with respect to the new representation.

We also derive lower bounds, showing that the dependence of our label-complexity guarantee on the accuracy c, or the margin parameter γ, is indeed necessary and is not an artifact of our analysis. We do not know if the dependence of our bounds on d is tight. It should be noted that some of the most popular learning algorithms (e.g., SVM, Perceptron, and AdaBoost) rely on a large-margin assumption to derive dimension-independent sample complexity guarantees. In contrast, here we use the margin for computational reasons. Our approximation guarantee depends logarithmically on the margin parameter, while the sample complexities of SVM, Perceptron, and AdaBoost depend polynomially on the margin. Hence, we require a much smaller margin than these algorithms do. In a related work, Balcan et al. (2007) proposed an active learning algorithm with dimension-independent guarantees under a margin assumption. These guarantees hold for a restricted class of data distributions.

In the second part of this work, we compare the greedy approach to the mellow approach of CAL in the realizable case, both theoretically and experimentally. Our theoretical results show the following:

1. We discuss the challenges presented by other natural choices of a distribution in Section 2.

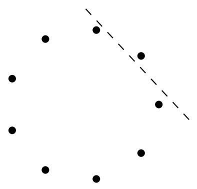
1. In the simple learning setting of thresholds on the line, our margin-based approach is preferable to the mellow approach when the true margin of the target hypothesis is large.
2. There exists a distribution in Euclidean space such that the mellow approach cannot achieve a significant improvement in label complexity over passive learning for halfspaces, while the greedy approach achieves such an improvement using more unlabeled examples.
3. There exists a pool in Euclidean space such that the mellow approach requires exponentially more labels than the greedy approach.

We further compare the two approaches experimentally, both on separable data and on data with small error. The empirical evaluation indicates that our algorithm, which can be implemented in practice, achieves state-of-the-art results. It further suggests that aggressive approaches can be significantly better than mellow approaches in some practical settings.

2. On the Challenges in Active Learning for Halfspaces

The approach we employ for active learning does not provide absolute guarantees for the label complexity of learning, but a relative guarantee instead, in comparison with the optimal label complexity. One might hope that an absolute guarantee could be achieved using a different algorithm, for instance in the case of half-spaces. However, the following example from Dasgupta (2005) indicates that no meaningful guarantee can be provided that holds for all possible pools.

Example 1 *Consider a distribution in $\mathbb{R}^d$ for any $d \geq 3$. Suppose that the support of the distribution is a set of evenly-distributed points on a two-dimensional sphere that does not circumscribe the origin, as illustrated in the following figure. As can be seen, each point can be separated from the rest of the points with a halfspace.*



In this example, to distinguish between the case in which all points have a negative label and the case in which one of the points has a positive label while the rest have a negative label, any active learning algorithm will have to query every point at least once. It follows that for any $\varepsilon > 0$, if the number of points is $1/\varepsilon$, then the label complexity to achieve an error of at most ε is $1/\varepsilon$. On the other hand, the sample complexity of passive learning in this case is order of $\frac{1}{\varepsilon}\log\frac{1}{\varepsilon}$, hence no active learner can be significantly better than a passive learner on this distribution.

Since we provide margin-dependent guarantees, one may wonder if a margin assumption alone can guarantee that few queries suffice to learn the half-space. This is not the case, as evident by the following variation of Example 1.

Example 2 *Let $\gamma \in (0, \frac{1}{2})$ be a margin parameter. Consider a pool of m points in $\mathbb{R}^d$, such that all the points are on the unit sphere, and for each pair of points x_1 and x_2, $\langle x_1, x_2 \rangle \leq 1 - 2\gamma$. It was shown in Shannon (1959) that for any $m \leq O(1/\gamma^d)$, there exists a set of points that satisfy the conditions above. For any point x in such a pool, there exists a (biased) halfspace that separates x from the rest of the points with a margin of γ. This can be seen by letting $w = x$ and $b = 1 - \gamma$. Then $\langle w, x \rangle - b = \gamma$ while for any $z \neq x$ in the set, $\langle w, z \rangle - b = \langle x, z \rangle - 1 + \gamma \leq -\gamma$. By adding a single dimension, this example can be transformed to one with homogeneous (unbiased) halfspaces. Each point in this pool can be separated from the rest of the points by a halfspace. Thus, if the correct labeling is all-positive, then all m examples need to be queried to label the pool correctly.*

These examples show that there are “difficult” pools, where no active learner can do well. The advantage of the greedy approach is that the optimal label complexity is used as a natural measure of the difficulty of the pool.

At first glance it might seem that there are simpler ways to implement an efficient greedy strategy for halfspaces, by using a different distribution over the hypotheses. For instance, if there are m examples in d dimensions, Sauer’s lemma states that the effective size of the hypothesis class of halfspaces will be at most m^d. One can thus use the uniform distribution over this finite class, and greedily reduce the number of possible hypotheses in the version space, obtaining a $d\log(m)$ factor relative to the optimal label complexity. However, a direct implementation of this method will be exponential in d, and it is not clear whether this approach has a polynomial implementation.

Another approach is to discretize the version space, by considering only halfspaces that can be represented as vectors on a d-dimensional grid $\{-1,-1+c,\ldots,1-c,1\}^d$. This results in a finite hypothesis class of size $(2/c+1)^d$, and we get an approximation factor of $O(d\log(1/c))$ for the greedy algorithm, compared to an optimal algorithm on the same finite class. However, it is unknown whether a greedy algorithm for reducing the number of such vectors in a version space can be implemented efficiently, since even determining whether a single grid point exists in a given version space is NP-hard (see, e.g., Matoušek, 2002, Section 2.2). In particular, the volume of the version space cannot be used to estimate this quantity, since the volume of a body and the number of grid points in this body are not correlated. For example, consider a line in $\mathbb{R}^2$, whose volume is 0. It can contain zero grid points or many grid points, depending on its alignment with respect to the grid. Therefore, the discretization approach is not straightforward as one might first assume. In fact, if this approach is at all computationally feasible, it would probably require the use of some approximation scheme, similarly to the volume-estimation approach that we describe below.

Yet another possible direction for pool-based active learning is to greedily select a query whose answer would determine the labels of the largest amount of pool examples. The main challenge in this direction is how to analyze the label complexity of such an algorithm: it is unclear whether competitiveness with the optimal label complexity can be guaranteed in this case. Investigating this idea, both theoretically and experimentally, is an important topic for future work. Note that the CAL algorithm (Cohn et al., 1994), which we discuss in Section 6, can be seen as implementing a mellow version of this approach, since it decreases the so-called “disagreement region” in each iteration.

3. Definitions and Preliminaries

In pool-based active learning, the learner receives as input a set of instances, denoted $X=\{x_1,\ldots,x_m\}$. Each instance x_i is associated with a label $L(i)\in\{\pm1\}$, which is initially unknown to the learner. The learner has access to a teacher, represented by the oracle $L:[m]\to\{-1,1\}$. An active learning algorithm $\mathcal{A}$ obtains (X,L,T) as input, where T is an integer which represents the label budget of $\mathcal{A}$. The goal of the learner is to find the values $L(1),\ldots,L(m)$ using as few calls to L as possible. We assume that L is determined by a function h taken from a predefined hypothesis class $\mathcal{H}$. Formally, for an oracle L and a hypothesis $h\in\mathcal{H}$, we write $L \Leftarrow h$ to state that for all i, $L(i)=h(x_i)$.

Given $S\subseteq X$ and $h\in\mathcal{H}$, we denote the partial realization of h on S by

$$h|_S=\{(x,h(x)) : x\in S\}\ .$$

We denote by $V(h|_S)$ the version space consisting of the hypotheses which are consistent with $h|_S$. Formally,

$$V(h|_S)=\{h'\in\mathcal{H} : \forall x\in S,\ \ h'(x)=h(x)\ \}.$$

Given X and $\mathcal{H}$, we define, for each $h\in\mathcal{H}$, the equivalence class of h over $\mathcal{H}$, $[h]=\{h'\in\mathcal{H}\mid \forall x\in X, h(x)=h'(x)\}$. We consider a probability distribution P over $\mathcal{H}$ such that $P([h])$ is defined for all $h\in\mathcal{H}$. For brevity, we denote $P(h)=P([h])$. Similarly, for a set $V\subseteq\mathcal{H}$, $P(V)=P(\cup_{h\in V}[h])$. Let $p_{\min}=\min_{h\in\mathcal{H}}P(h)$.

We specifically consider the hypothesis class of homogeneous halfspaces in $\mathbb{R}^d$. In this case, $X\subseteq\mathbb{R}^d$. The hypothesis class $\mathcal{H}$ is defined by $\mathcal{W}=\{x\mapsto \operatorname{sgn}(\langle w,x\rangle)\mid w\in\mathbb{R}^d\}$, where $\langle w,x\rangle$ is the inner product between the vectors w and x.

For a given active learning algorithm $\mathcal{A}$, we denote by $N(\mathcal{A},h)$ the number of calls to L that $\mathcal{A}$ makes before outputting $(L(x_1),\dots,L(x_m))$, under the assumption that $L \Lleftarrow h$. The worst-case label complexity of $\mathcal{A}$ is defined to be

$$c_{\mathrm{wc}}(\mathcal{A}) \stackrel{\mathrm{def}}{=} \max_{h\in\mathcal{H}} N(\mathcal{A},h).$$

We denote the optimal worst-case label complexity for the given pool by $\mathrm{OPT}_{\max}$. Formally, we define $\mathrm{OPT}_{\max} = \min_{\mathcal{A}} c_{\mathrm{wc}}(\mathcal{A})$, where the minimum is taken over all possible active learners for the given pool.

Given a probability distribution P over $\mathcal{H}$, the average-case label complexity of $\mathcal{A}$ is defined to be

$$c_{\mathrm{avg}}(\mathcal{A}) \stackrel{\mathrm{def}}{=} \mathbb{E}_{h\sim P} N(\mathcal{A},h).$$

The optimal average label complexity for the given pool X and probability distribution P is defined as $\mathrm{OPT}_{\mathrm{avg}} = \min_{\mathcal{A}} c_{\mathrm{avg}}(\mathcal{A})$.

For a given active learner, we denote by $V_t \subseteq \mathcal{H}$ the version space of an active learner after t queries. Formally, suppose that the active learning queried instances $i_1,\dots,i_t$ in the first t iterations. Then

$$V_t = \{h \in \mathcal{H} \mid \forall j \in [t], h(x_{i_j}) = L(i_j)\}.$$

For a given pool example $x \in X$, denote by $V^j_{t,x}$ the version spaces that would result if the algorithm now queried x and received label j. Formally,

$$V^j_{t,x} = V_t \cap \{h \in \mathcal{H} \mid h(x) = j\}.$$

A greedy algorithm (with respect to a probability distribution P) is an algorithm $\mathcal{A}$ that at each iteration $t = 1,\dots,T$, the pool example x that $\mathcal{A}$ decides to query is one that splits the version space as evenly as possible. Formally, at every iteration t $\mathcal{A}$ queries some example in $\mathrm{argmin}_{x\in X} \max_{j\in\{\pm1\}} P(V^j_{t,x})$. Equivalently, a greedy algorithm is an algorithm $\mathcal{A}$ that at every iteration t queries an example in

$$\operatorname*{argmax}_{x\in X} P(V^{-1}_{t,x}) \cdot P(V^{+1}_{t,x}).$$

To see the equivalence, note that $P(V^{-1}_{t,x}) = P(V_t) - P(V^{+1}_{t,x})$. Therefore,

$$P(V^{-1}_{t,x}) \cdot P(V^{+1}_{t,x}) = (P(V_t) - P(V^{+1}_{t,x}))P(V^{+1}_{t,x}) = (P(V_t)/2)^2 - (P(V_t)/2 - P(V^{+1}_{t,x}))^2.$$

It follows that the expression is monotonic decreasing in $|P(V_t)/2 - P(V^{+1}_{t,x})|$.

This equivalent formulation motivates the following definition of an approximately greedy algorithm, following Golovin and Krause (2010).

Definition 3 *An algorithm $\mathcal{A}$ is called* α-approximately greedy *with respect to P, for $\alpha \geq 1$, if at each iteration $t = 1,\dots,T$, the pool example x that $\mathcal{A}$ decides to query satisfies*

$$P(V^1_{t,x})P(V^{-1}_{t,x}) \geq \frac{1}{\alpha} \max_{\tilde{x}\in X} P(V^1_{t,\tilde{x}})P(V^{-1}_{t,\tilde{x}}),$$

and the output of the algorithm is $(h(x_1),\dots,h(x_m))$ for some $h \in V_T$.

It is easy to see that by this definition, an algorithm is exactly greedy if it is approximately greedy with $\alpha = 1$.

By Dasgupta (2005) we have the following guarantee: For any exactly greedy algorithm $\mathcal{A}$ with respect to distribution P,

$$c_{\mathrm{avg}}(\mathcal{A}) = O(\log(1/p_{\min}) \cdot \mathrm{OPT}_{\mathrm{avg}}).$$

Golovin and Krause (2010) show that for an α approximately greedy algorithm,

$$c_{\mathrm{avg}}(\mathcal{A}) = O(\alpha \cdot \log(1/p_{\min}) \cdot \mathrm{OPT}_{\mathrm{avg}}).$$

In addition, they show a similar bound for the worst-case label complexity. Formally,

$$c_{\mathrm{wc}}(\mathcal{A}) = O(\alpha \cdot \log(1/p_{\min}) \cdot \mathrm{OPT}_{\max}). \tag{1}$$

4. Results for Greedy Active Learning

The approximation factor guarantees cited above all inversely depend on $p_{\min}$, the smallest probability of any hypothesis in the given hypothesis class, according to the given distribution. Thus, if $p_{\min}$ is very small, the approximation factor is large, regardless of the true target hypothesis. We show that by slightly changing the policy of an approximately-greedy algorithm, we can achieve a better approximation factor whenever the true target hypothesis has a larger probability than $p_{\min}$. This can be done by allowing the algorithm to stop before it reaches a pure version space, that is before it can be certain of the correct labeling of the pool, and requiring that in this case, it would output the labeling which is most likely based on the current version space and the fixed probability distribution P. We say that $\mathcal{A}$ *outputs an approximate majority vote* if whenever V_T is pure enough, the algorithm outputs the majority vote on V_T. Formally, we define this as follows.

Definition 4 *An algorithm $\mathcal{A}$ outputs a β-approximate majority vote for $\beta \in (\frac{1}{2}, 1)$ if whenever there exists a labeling $Z : X \to \{\pm 1\}$ such that $\mathbb{P}_{h \sim P}[Z \Leftarrow h \mid h \in V_T] \geq \beta$, $\mathcal{A}$ outputs Z.*

In the following theorem we provide the target-dependent label complexity bound, which holds for any approximate greedy algorithm that outputs an approximate majority vote. We give here a sketch of the proof idea, the complete proof can be found in Appendix A.

Theorem 5 *Let $X = \{x_1, \ldots, x_m\}$. Let $\mathcal{H}$ be a hypothesis class, and let P be a distribution over $\mathcal{H}$. Suppose that $\mathcal{A}$ is α-approximately greedy with respect to P. Further suppose that it outputs a β-approximate majority vote. If $\mathcal{A}$ is executed with input (X, L, T) where $L \Leftarrow h \in \mathcal{H}$, then for all*

$$T \geq \alpha(2\ln(1/P(h)) + \ln(\frac{\beta}{1-\beta})) \cdot \mathrm{OPT}_{\max},$$

$\mathcal{A}$ outputs $L(1), \ldots, L(m)$.

Proof [Sketch] Fix a pool X. For any algorithm alg, denote by $V_t(\mathrm{alg}, h)$ the version space induced by the first n labels it queries if the true labeling of the pool is consistent with h. Denote the average version space reduction of alg after t queries by

$$f_{\mathrm{avg}}(\mathrm{alg}, t) = 1 - \mathbb{E}_{h \sim P}[P(V_t(\mathrm{alg}, h))].$$

Golovin and Krause (2010) prove that since $\mathcal{A}$ is α-approximately greedy, for any pool-based algorithm alg, and for every $k, t \in \mathbb{N}$,

$$f_{\mathrm{avg}}(\mathcal{A}, t) \geq f_{\mathrm{avg}}(\mathrm{alg}, k)(1 - \exp(-t/\alpha k)). \tag{2}$$

Let opt be an algorithm that achieves $\mathrm{OPT}_{\max}$. We show (see Appendix A) that for any hypothesis $h \in \mathcal{H}$ and any active learner alg,

$$f_{\mathrm{avg}}(\mathrm{opt}, \mathrm{OPT}_{\max}) - f_{\mathrm{avg}}(\mathrm{alg}, t) \geq P(h)(P(V_t(\mathrm{alg}, h)) - P(h)).$$

Combining this with Equation (2) we conclude that if $\mathcal{A}$ is α-approximately greedy then

$$\frac{P(h)}{P(V_t(\mathcal{A}, h))} \geq \frac{P(h)^2}{\exp(-\frac{t}{\alpha \mathrm{OPT}_{\max}}) + P(h)^2}.$$

This means that if $P(h)$ is large enough and we run an approximate greedy algorithm, then after a sufficient number of iterations, most of the remaining version space induces the correct labeling of the sample. Specifically, if $t \geq \alpha(2\ln(1/P(h)) + \ln(\frac{\beta}{1-\beta})) \cdot \mathrm{OPT}_{\max}$, then $P(h)/P(V_t(\mathcal{A}, h)) \geq \beta$. Since $\mathcal{A}$ outputs a β-approximate majority labeling from $V_t(\mathcal{A}, h)$, $\mathcal{A}$ returns the correct labeling. ■

When $P(h) \gg p_{\min}$, the bound in Theorem 5 is stronger than the guarantee in Equation (1), obtained by Golovin and Krause (2010). Note, however, that this bound depends on the probability of the target hypothesis and thus is not known a-priori, unless additional assumptions are made. The margin assumption, which we discuss below, is an example for such a plausible assumption. Moreover, our experimental results indicate that even when such an apriori bound is not known, using a majority vote is preferable to selecting an arbitrary random hypothesis from an impure version space (see Figure 1 in Section 6.2).

Importantly, such an improved approximation factor *cannot be obtained* for a general approximate-greedy algorithm, even in a very simple setting. Thus, we can conclude that some algorithmic change is necessary. To show this, consider the setting of *thresholds on the line*. In this setting, the domain of examples is $[0,1]$, and the hypothesis class includes all the hypotheses defined by a threshold on $[0,1]$. Formally,

$$\mathcal{H}_{\text{line}} = \{h_c \mid c \in [0,1], h_c(x) = 1 \Leftrightarrow x \geq c\}.$$

Note that this setting is isomorphic to the case of homogeneous halfspaces with examples on a line in any Euclidean space of two or more dimensions.

Theorem 6 *Consider pool-based active learning on $\mathcal{H}_{\text{line}}$, and assume that P on $\mathcal{H}_{\text{line}}$ selects h_c by drawing the value c uniformly from $[0,1]$. For any $\alpha > 1$ there exists an α-approximately greedy algorithm $\mathcal{A}$ such that for any $m > 0$ there exists a pool $X \subseteq [0,1]$ of size m, and a threshold c such that $P(h_c) = 1/2$, while the label-complexity of $\mathcal{A}$ for $L \Leftarrow h_c$ is $\frac{m}{\lceil \log(m) \rceil} \cdot \mathrm{OPT}_{\max}$.*

Proof For the hypothesis class $\mathcal{H}_{\text{line}}$, the possible version spaces after a partial run of an active learner are all of the form $[a,b] \subseteq [0,1]$.

First, it is easy to see that binary search on the pool can identify any hypothesis in $[0,1]$ using $\lceil \log(m) \rceil$ example, thus $\mathrm{OPT}_{\max} = \lceil \log(m) \rceil$. Now, Consider an active learning algorithm that satisfies the following properties:

- If the current version space is $[a,b]$, it queries the smallest x that would still make the algorithm α-approximately greedy. Formally, it selects
$$x = \min\{x \in X \mid (x-a)(b-x) \geq \frac{1}{\alpha} \max_{\tilde{x} \in X \cap [a,b]} (\tilde{x}-a)(b-\tilde{x})\}.$$
- When the budget of queries is exhausted, if the version space is $[a,b]$, then the algorithm labels the points above a as positive and the rest as negative.

It is easy to see that this algorithm is α-approximately greedy, since in this problem $V_{t,x}^{1} \cdot V_{t,x}^{-1} = (x-a)(b-x)$ for all $x \in [a,b] = V_t$. Now for a given pool size $m \geq 2$, consider a pool of examples defined as follows. First, let $x_1 = 1$, $x_2 = 1/2$ and $x_3 = 0$. Second, for each $i \geq 3$, define x_{i+1} recursively as the solution to $(x_{i+1} - x_i)(1 - x_{i+1}) = \frac{1}{\alpha}(x_2 - x_i)(x_1 - x_2)$. Since $\alpha > 1$, it is easy to see by induction that for all $i \geq 3$, $x_{i+1} \in (x_i, x_2)$. Furthermore, suppose the true labeling is induced by $h_{3/4}$; Thus the only pool example with a positive label is x_1, and $P(h_{3/4}) = 1/2$. In this case, the algorithm we just defined will query all the pool examples $x_4, x_5, \ldots, x_m$ in order, and only then will it query x_2 and finally x_1. If stopped at any time $t \leq m-1$, it will label all the points that it has not queried yet as positive, thus if $t < m-1$ the output will be an erroneous labeling. Finally, note that the same holds for the pool $x_1, x_2, x_4, \ldots, x_m$ that does not include x_3, so the algorithm must query this entire pool to identify the correct labeling. ■

Interestingly, this theorem does not hold for $\alpha = 1$, that is for the exact greedy algorithm. This follows from Theorem 18, which we state and prove in Section 6.

So far we have considered a general hypothesis class. We now discuss the class of halfspaces in $\mathbb{R}^d$, denoted by $\mathcal{W}$ above. For simplicity, we will slightly overload notation and sometimes use w to denote the halfspace it determines. Every hypothesis in $\mathcal{W}$ can be described by a vector $w \in \mathbb{B}_1^d$, where $\mathbb{B}_1^d$ is the Euclidean unit ball, $\mathbb{B}_1^d = \{w \in \mathbb{R}^d \mid \|w\| \leq 1\}$. We fix the distribution P to be the one that selects a vector w uniformly from $\mathbb{B}_1^d$. Our active learning algorithm for halfspaces, which is called ALuMA, is presented in Section 5. ALuMA receives as input an extra parameter $\delta \in (0,1)$, which serves as a measure of the desired confidence level. The following lemma, which we prove in Section 5, shows that ALuMA has the desired properties described above with high probability.

Lemma 7 *If ALuMA is executed with confidence δ, then with probability $1-\delta$ over its internal randomization, ALuMA is 4-approximately greedy and outputs a $2/3$-approximate majority vote. Furthermore, ALuMA is polynomial in the pool size, the dimension, and* $\log(1/\delta)$.

Combining the above lemma with Theorem 5 we immediately obtain that ALuMA's label complexity is $O(\log(1/P(h)) \cdot \mathrm{OPT}_{\max})$. We can upper-bound $\log(1/P(h))$ using the familiar notion of *margin*: For any hypothesis $h \in \mathcal{W}$ defined by some $w \in \mathbb{B}_1^d$, let $\gamma(h)$ be the maximal margin of the labeling of X by h, namely $\gamma(h) = \max_{v:\|v\|=1} \min_{i\in[m]} h(x_i)\langle v, x_i\rangle / \|x_i\|$. We have the following lemma, which we prove in Appendix D:

Lemma 8 *For all $h \in \mathcal{W}$, $P(h) \geq \left(\frac{\gamma(h)}{2}\right)^d$.*

From Lemma 8 and Lemma 7, we obtain the following corollary, which provides a guarantee for ALuMA that depends on the margin of the target hypothesis.

Corollary 9 *Let $X = \{x_1, \ldots, x_m\} \subseteq \mathbb{B}_1^d$, where $\mathbb{B}_1^d$ is the unit Euclidean ball of $\mathbb{R}^d$. Let $\delta \in (0,1)$ be a confidence parameter. Suppose that ALuMA is executed with input (X, L, T, δ), where $L \Leftarrow h \in \mathcal{W}$ and $T \geq 4(2d\ln(2/\gamma(h)) + \ln(2)) \cdot \mathrm{OPT}_{\max}$. Then, with probability of at least $1-\delta$ over ALuMA's own randomization, it outputs $L(1), \ldots, L(m)$.*

Note that ALuMA is allowed to use randomization, and it can fail to output the correct label with probability δ. In contrast, in the definition of $\mathrm{OPT}_{\max}$ we required that the optimal algorithm always succeeds, in effect making it deterministic. One may suggest that the approximation factor we achieve for ALuMA in Lemma 7 is due to this seeming advantage for ALuMA. We now show that this is not the case—the same approximation factor can be achieved when ALuMA and the optimal algorithm are allowed the same probability of failure. Let m be the size of the pool and let d be the dimension of the examples, and set $\delta_0 = \frac{1}{2m^d}$. Denote by $N_\delta(\mathcal{A}, h)$ the number of calls to L that $\mathcal{A}$ makes before outputting $(L(x_1), \ldots, L(x_m))$ with probability at least $1-\delta$, for $L \Leftarrow h$. Define $\mathrm{OPT}_{\delta_0} = \min_A \max_h N_{\delta_0}(A, h)$.

First, note that by setting $\delta = \delta_0$ in ALuMA, we get that $N_\delta(\mathrm{ALuMA}, h) \leq O(\log(1/P(h)) \cdot \mathrm{OPT}_{\max})$. Moreover, ALuMA with $\delta = \delta_0$ is polynomial in m and d (since it is polynomial in $\ln(1/\delta)$). Second, by Sauer's lemma there are at most m^d different possible labelings for the given pool. Thus by the union bound, there exists a fixed choice of the random bits used by an algorithm that achieves OPT_{δ_0}, that leads to the correct identification of the labeling for *all* possible labelings $L(1), \ldots, L(m)$. It follows that $\mathrm{OPT}_{\delta_0} = \mathrm{OPT}_{\max}$. Therefore the same factor of approximation can be achieved for ALuMA with $\delta = \delta_0$, compared to OPT_{δ_0}.

Our result for ALuMA provides a target-dependent approximation factor guarantee, depending on the margin of the target hypothesis. We can also consider the minimal possible margin, $\gamma = \min_{h\in\mathcal{W}} \gamma(h)$, and deduce from Corollary 9, or from the results of Golovin and Krause (2010), a uniform approximation factor of $O(d\log(1/\gamma))$. How small can γ be? The following result bounds this minimal margin from below under the reasonable assumption that the examples are represented by numbers of a finite accuracy.

Lemma 10 *Let $c > 0$ be such that $1/c$ is an integer and suppose that $X \subset \{-1, -1+c, \ldots, 1-c, 1\}^d$. Then, $\min_{h\in\mathcal{W}} \gamma(h) \geq (c/\sqrt{d})^{d+2}$.*

The proof, given in Appendix D, is an adaptation of a classic result due to Muroga et al. (1961). We conclude that under this assumption for halfspaces, $p_{\min} = \Omega((c/d)^{d^2})$, and deduce an approximation factor of $d^2\log(d/c)$ for the worst-case label complexity of ALuMA. The exponential dependence of the minimal margin on d here is necessary; as shown in Håstad (1994), the minimal margin can indeed be exponentially small, even if the points are taken only from $\{\pm 1\}^d$.

We also derive a lower bound, showing that the dependence of our bounds on γ or on c is necessary. Whether the dependence on d is also necessary is an open question for future work.

Theorem 11 *For any $\gamma \in (0, 1/8)$, there exists a pool $X \subseteq \mathbb{B}_1^2 \cap \{-1, 1+c, \ldots, 1-c, 1\}^2$ for $c = \Theta(\gamma)$, and a target hypothesis $h^* \in \mathcal{W}$ for which $\gamma(h^*) = \Omega(\gamma)$, such that there exists an exact greedy algorithm that requires $\Omega(\ln(1/\gamma)) = \Omega(\ln(1/c))$ labels in order to output a correct majority vote, while the optimal algorithm requires only $O(\log(\log(1/\gamma)))$ queries.*

The proof of Theorem 11 is provided in Appendix D. In the next section we describe the ALuMA algorithm in detail.

5. The ALuMA Algorithm

We now describe our algorithm, listed below as Alg. 1, and explain why Lemma 7 holds. We name the algorithm *Active Learning under a Margin Assumption* or ALuMA. Its inputs are the unlabeled sample X, the labeling oracle L, the maximal allowed number of label queries T, and the desired confidence $\delta \in (0,1)$. It returns the labels of all the examples in X.

As we discussed earlier, in each iteration, we wish to choose among the instances in the pool, the instance whose label would lead to the maximal (expected) reduction in the version space. Denote by I_t the set of indices corresponding to the elements in the pool whose label was not queried yet ($I_0 = [m]$). Then, in round t, we wish to find

$$k = \operatorname*{argmax}_{i \in I_t} P(V^1_{t,x_i}) \cdot P(V^{-1}_{t,x_i}). \tag{3}$$

Recall we take P to be uniform over $\mathcal{W}$, the class of homogenous half-spaces in $\mathbb{R}^d$. In this case, the probability of a version space is equivalent to its volume, up to constant factors. Therefore, in order to be able to solve Equation (3), we need to calculate the volumes of the sets $V^1_{t,x}$ and $V^{-1}_{t,x}$ for every element x in the pool. Both of these sets are convex sets obtained by intersecting the unit ball with halfspaces. The problem of calculating the volume of such convex sets in $\mathbb{R}^d$ is #P-hard if d is not fixed (Brightwell and Winkler, 1991). In many learning applications d is large, therefore, indeed d should not be taken as fixed. Moreover, deterministically approximating the volume is NP-hard in the general case (Matoušek, 2002). Luckily, it is possible to approximate this volume using randomization. Specifically, in Kannan et al. (1997) a randomized algorithm with the following guarantees is provided, where $\mathrm{Vol}(K)$ denotes the volume of the set K.

Lemma 12 *Let $K \subseteq \mathbb{R}^d$ be a convex body with an efficient separation oracle. There exists a randomized algorithm, such that given $\epsilon, \delta > 0$, with probability at least $1-\delta$ the algorithm returns a non-negative number Γ such that $(1-\epsilon)\Gamma < \mathrm{Vol}(K) < (1+\epsilon)\Gamma$. The running time of the algorithm is polynomial in $d, 1/\epsilon, \ln(1/\delta)$.*

We denote an execution of this algorithm on a convex body K by $\Gamma \leftarrow \mathrm{VolEst}(K,\epsilon,\delta)$. The algorithm is polynomial in $d, 1/\epsilon, \ln(1/\delta)$. ALuMA uses this algorithm to estimate $P(V^1_{t,x})$ and $P(V^{-1}_{t,x})$ with sufficient accuracy. We denote these approximations by $\hat{v}_{x,1}$ and $\hat{v}_{x,-1}$ respectively. Using the constants in ALuMA, we can show the following.

Lemma 13 *With probability at least $1-\delta/2$, Alg. 1 is 4-approximately greedy.*

Proof Fix some $t \in [T]$. Let $k \in I_t$ be the index chosen by ALuMA. Let k^* be the index corresponding to the value of Equation (3). Since ALuMA performs at most $2m$ approximations in each round, we obtain by Lemma 12 and the union bound that with probability at least $1-\frac{\delta}{2T}$, for each $i \in I_t$ and each $j \in \{-1,1\}$,

$$\hat{v}_{x_i,j} \in \left(\frac{2}{3}\mathrm{Vol}(V^j_{t,x_i}), \frac{4}{3}\mathrm{Vol}(V^j_{t,x_i})\right).$$

In addition, $\hat{v}_{x_k,1} \cdot \hat{v}_{x_k,-1} \geq \hat{v}_{x_{k^*},1} \cdot \hat{v}_{x_{k^*},-1}$. Hence, with probability at least $1-\frac{\delta}{2T}$,

$$\frac{16}{9}\mathrm{Vol}(V^{-1}_{t,x_k}) \cdot \mathrm{Vol}(V^1_{t,x_k}) \geq \frac{4}{9}\mathrm{Vol}(V^{-1}_{t,x_{k^*}}) \cdot \mathrm{Vol}(V^1_{t,x_{k^*}}).$$

Applying the union bound over T iteration completes our proof. ■

After T iterations, ALuMA needs to output the majority vote of a version space that has a high enough purity level. To output an approximate majority vote from the final version space V, we would like to uniformly draw several hypotheses from V and label X according to a majority vote over these hypotheses. The

Algorithm 1 The **ALuMA** algorithm

```
1: **Input:** $X = \{x_1, \dots, x_m\}$, $L : [m] \to \{-1, 1\}$, $T$, $\delta$
2: $I_1 \leftarrow [m]$, $V_1 \leftarrow \mathbb{B}_1^d$
3: **for** $t = 1$ to $T$ **do**
4:     $\forall i \in I_t, j \in \{\pm 1\}$, do $\hat{v}_{x_i,j} \leftarrow \mathrm{VolEst}(V^j_{t,x_i}, \frac{1}{3}, \frac{\delta}{4mT})$
5:     Select $i_t \in \mathrm{argmax}_{i \in I_t} (\hat{v}_{x_i,1} \cdot \hat{v}_{x_i,-1})$
6:     $I_{t+1} \leftarrow I_t \setminus \{i_t\}$
7:     Request $y = L(i_t)$
8:     $V_{t+1} \leftarrow V_t \cap \{w : y\langle w, x_{i_t}\rangle > 0\}$
9: **end for**
10: $M \leftarrow \lceil 72 \ln(2/\delta) \rceil$.
11: Draw $w_1, \dots, w_M$ $\frac{1}{12}$-uniformly from $V_{T+1}$.
12: For each $x_i$ return the label $y_i = \mathrm{sgn}\left(\sum_{j=1}^M \mathrm{sgn}(\langle w_j, x_i \rangle)\right)$.
```

task of uniformly drawing hyphteses from V can be approximated using the hit-and-run algorithm (Lovász, 1999). The hit-and-run algorithm efficiently draws a random sample from a convex body K according to a distribution which is close in total variation distance to the uniform distribution over K. Formally, The following definition parametrizes the closeness of a distribution to the uniform distribution:

Definition 14 *Let $K \subseteq \mathbb{R}^d$ be a convex body with an efficient separation oracle, and let τ be a distribution over K. τ is λ-*uniform *if* $\sup_A |\tau(A) - P(A)/P(K)| \leq \lambda$, *where the supremum is over all measurable subsets of K.*

The hit-and-run algorithm draws a sample from a λ-uniform distribution in time $\tilde{O}(d^3/\lambda^2)$. The next lemma shows that using the hit-and-run as suggested above indeed produces a majority vote classification.

Lemma 15 *ALuMA outputs a* $2/3$*-approximate majority vote with probability at least* $1 - \delta/2$*.*

Proof Assume that there exists a labeling $Z : X \to \{\pm 1\}$ such that $\mathbb{P}_{h \sim P}[Z \Leftarrow h \mid h \in V_{T+1}] \geq 2/3$. In step 11 of ALuMA, $M \geq 72 \ln(2/\delta)$ hypotheses are drawn $\frac{1}{12}$-uniformly at random from V_t. Therefore each hypothesis $h_i \in V_{T+1}$ is consistent with Z with probability at least $\frac{7}{12}$. By Hoeffding's inequality,

$$\mathbb{P}\left[\frac{1}{M}\sum_{i=1}^{M} I[h_i \in V(h|_X)] \leq \frac{1}{2}\right] \leq \exp(-M/72) = \frac{\delta}{2}.$$

Therefore, with probability at least $1 - \delta/2$, ALuMA outputs a $2/3$-approximate majority vote. ■

We can now prove Lemma 7.

Proof (Of Lemma 7) Lemma 13 and Lemma 15 above prove the first two parts of the lemma. We only have left to analyze the time complexity of ALuMA. In each iteration, the cost of ALuMA is dominated by the cost of performing at most $2m$ volume approximation, each of which costs $O(d^5 \ln(1/\delta))$. As we discussed above, implementing the majority vote costs polynomial time in d and $\ln(1/\delta)$. Overall, the runtime of ALuMA is polynomial in m (which upper bounds T), d and $\log(1/\delta)$. ■

5.1 A Simpler Implementation of ALuMA

The ALuMA algorithm described in Alg. 1 uses $O(Tm)$ volume estimations as a black-box procedure, where T is the budget of labels and m is the pool size. The complexity of each application of the volume estimation procedure is $\tilde{O}(d^5)$ where d is the dimension. Thus the overall complexity of the algorithm is $\tilde{O}(Tmd^5)$. This complexity can be somewhat improved under some "luckiness" conditions.

The volume estimation procedure uses λ-uniform sampling based on hit-and-run as its core procedure. Instead, we can use hit-and-run directly as follows: At each iteration of ALuMA, instead of step 4, perform the following procedure:

Algorithm 2 Estimation Procedure

```
1: Input: $\lambda \in (0, \frac{1}{24}), V_t, I_t$
2: $k \leftarrow \frac{\ln(2Nm/\delta)}{2\lambda^2}$
3: Sample $h_1, \dots, h_k \in V_t$ $\lambda$-uniformly.
4: $\forall i \in I_t, j \in \{-1, +1\}$, $\hat{v}_{x_i,j} \leftarrow \frac{1}{k}|\{i \mid h_i(x_i) = j\}|$.
```

The complexity of ALuMA when using this procedure is $\tilde{O}(T(d^3/\lambda^4 + m/\lambda^2))$, which is better than the complexity of the full Alg. 1 for a constant λ. An additional practical benefit of this alternative estimation procedure is that when implementing, it is easy to limit the actual computation time used in the implementation by running the procedure with a smaller number k and a smaller number of hit-and-run mixing iterations.[2] This provides a natural trade-off between computation time and labeling costs.

The following theorem shows that under mild conditions, using the estimation procedure listed in Alg. 2 also results in an approximately greedy algorithm, as does the original implementation of ALuMA.

Theorem 16 *If for each iteration t of the algorithm, the greedy choice x^* satisfies*

$$\forall j \in \{-1, +1\}, \quad \mathbb{P}[h(x^*) = j \mid h \in V_t] \geq 4\sqrt{\lambda}$$

then ALuMA with the estimation procedure is a 2-approximate greedy algorithm. Moreover, it is possible to efficiently verify that this condition holds while running the algorithm.

Proof Fix the iteration t, and denote $p_{x,1} = P(V_{t,x}^1)/P(V_t)$ and $p_{x,-1} = P(V_{t,x}^1)/P(V_t)$. Note that $p_{x,1} + p_{x,-1} = 1$. Since $h_1, \dots, h_k$ are sampled λ-uniformly from the version space, we have

$$\forall i \in [k], |\mathbb{P}[h_i \in V_{t,x}^j] - p_{x,j}| \leq \lambda. \tag{4}$$

In addition, by Hoeffding's inequality and a union bound over the examples in the pool and the iterations of the algorithm,

$$\mathbb{P}[\exists x, |\hat{v}_{x_i,j} - \mathbb{P}[h_i \in V_{t,x}^j]| \geq \lambda] \leq 2m\exp(-2k\lambda^2). \tag{5}$$

From Alg. 2 we have $k = \frac{\ln(2m/\delta)}{2\lambda^2}$. Combining this with Equation (4) and Equation (5) we get that

$$\mathbb{P}[\exists x, |\hat{v}_{x_i,j} - p_{x_i,j}]| \geq 2\lambda] \leq \delta.$$

The greedy choice for this iteration is

$$x^* \in \operatorname*{argmax}_{x \in X} \Delta(h|_X, x) = \operatorname*{argmax}_{x \in X}(p_{x,1}p_{x,-1}).$$

By the assumption in the theorem, $p_{x^*,j} \geq 4\sqrt{\lambda}$ for $j \in \{-1, +1\}$. Since $\lambda \in (0, \frac{1}{64})$, we have $\lambda \leq \sqrt{\lambda}/8$. Therefore $p_{x^*,j} - 2\lambda \geq 4\sqrt{\lambda} - \sqrt{\lambda}/4 \geq \sqrt{10\lambda}$. Therefore

$$\hat{v}_{x^*,1}\hat{v}_{x^*,-1} \geq (p_{x^*,1} - 2\lambda)(p_{x^*,-1} - 2\lambda) \geq 10\lambda. \tag{6}$$

2. Gilad-Bachrach et al. (2005) report that the actual mixing time of hit-and-run is much faster than the one guaranteed by the theoretical bounds, and we have observed a similar phenomenon in our experiments.

Let $\tilde{x} = \operatorname{argmax}(\hat{v}_{x,-1}\hat{v}_{x,+1})$ be the query selected by ALuMA using Alg. 2. Then

$$\hat{v}_{x^*,-1}\hat{v}_{x^*,+1} \leq \hat{v}_{\tilde{x},-1}\hat{v}_{\tilde{x},+1} \leq (p_{\tilde{x},1}+2\lambda)(p_{\tilde{x},-1}+2\lambda) \leq p_{\tilde{x},1}p_{\tilde{x},-1}+4\lambda.$$

Where in the last inequality we used the facts that $p_{\tilde{x},1}+p_{\tilde{x},-1}=1$ and $4\lambda^2 \leq 2\lambda$. On the other hand, by Equation (6)

$$\hat{v}_{x^*,-1}\hat{v}_{x^*,+1} \geq 5\lambda + \frac{1}{2}\hat{v}_{x^*,-1}\hat{v}_{x^*,+1} \geq 5\lambda + \frac{1}{2}(p_{x^*,-1}-2\lambda)(p_{x^*,-1}-2\lambda) \geq 4\lambda + \frac{1}{2}p_{x^*,-1}p_{x^*,-1}.$$

Combining the two inequalities for $\hat{v}_{x^*,-1}\hat{v}_{x^*,+1}$ it follows that $p_{\tilde{x},1}p_{\tilde{x},-1} \geq \frac{1}{2}p_{x^*,-1}p_{x^*,-1}$, thus this is a 2-approximately greedy algorithm.

To verify that the assumption holds at each iteration of the algorithm, note that for all $x = x_i$ such that $i \in I_t$

$$p_{x,-1}p_{x,+1} \geq (\hat{v}_{x,-1}-2\lambda)(\hat{v}_{x,+1}-2\lambda) \geq \hat{v}_{x,-1}\hat{v}_{x,+1}-2\lambda.$$

therefore it suffices to check that for all $x = x_i$ such that $i \in I_t$ $\hat{v}_{x,-1}\hat{v}_{x,+1} \geq 4\sqrt{\lambda}+2\lambda$. ■

The condition added in this theorem is that the best example in each iteration should induce a fairly balanced partition of the current version space. In our experiments we noticed that this is generally the case in practice. Moreover, the theorem shows that it is possible to verify that the condition holds while running the algorithm. Thus, the estimation procedure can easily be augmented with an additional verification step at the beginning of each iteration. On iterations that fail the verification, the algorithm will use the original black-box volume estimation procedure. We have used this simpler implementation in our experiments, which are reported below.

5.2 Handling Non-Separable Data and Kernel Representations

If the data pool X is not separable, but a small upper bound on the total hinge-loss of the best separator can be assumed, then ALuMA can be applied after a preprocessing step, which we describe in detail below. This preprocessing step maps the points in X to a set of points in a higher dimension, which are separable using the original labels of X. The dimensionality depends on the margin and on the bound on the total hinge-loss of the original representation. The preprocessing step also supports kernel representations, so that the original X can be represented by a kernel matrix as well. Applying ALuMA after this preprocessing steps results in an approximately optimal label complexity, however $\mathrm{OPT}_{\max}$ here is measured with respect to the new representation.

While some of the transformations we employ in the preprocessing step have been discussed before in other contexts (see, e.g., Balcan et al., 2006b), we describe and analyze the full procedure here for completeness. The preprocessing step is composed of two simple transformations. In the first transformation each example $x_i \in X$ is mapped to an example in dimension $d+m$, defined by $x'_i = (ax_i; \sqrt{1-a^2}\cdot e_i)$, where e_i is the i'th vector of the natural basis of $\mathbb{R}^m$ and $a > 0$ is a scalar that will be defined below. Thus the first d coordinates of x'_i hold the original vector times a, the rest of the coordinates are zero,except for $x'_i[d+i] = \sqrt{1-a^2}$. This mapping guarantees that the set $X' = (x'_1,\ldots,x'_m)$ is separable with the same labels as those of X, and with a margin that depends on the cumulative squared-hinge-loss of the data.

In the second transformation, a Johnson-Lindenstrauss random projection (Johnson and Lindenstrauss, 1984; Bourgain, 1985) is applied to X', thus producing a new set of points $\bar{X} = (\bar{x}_1,\ldots,\bar{x}_m)$ in a different dimension $\mathbb{R}^k$, where k depends on the original margin and on the amount of margin error. With high probability, the new set of points will be separable with a margin that also depends on the original margin and on the amount of margin error. If the input data is provided not as vectors in $\mathbb{R}^d$ but via a kernel matrix, then a simple decomposition is performed before the preprocessing begins.

The full preprocessing procedure is listed below as Alg. 3. The first input to the algorithm is the data for preprocessing, given as $X \subseteq \mathbb{R}^d$ or as a kernel matrix $K \in \mathbb{R}^{m\times m}$. The other inputs are γ—a margin parameter, H—an upper bound on the margin error relative to γ, and δ, which is the required confidence.

Algorithm 3 Preprocessing

```
1: **Input:** $X = \{x_1, \ldots, x_m\} \in \mathbb{R}^d$ or $K \in \mathbb{R}^{m\times m}$, $\gamma$, $H$, $\delta$
2: **if** input data is a kernel matrix $K$ **then**
3:     Find $U \in \mathbb{R}^{m\times m}$ such that $K = UU^T$
4:     $\forall i \in [m], x_i \leftarrow$ row $i$ of $U$
5:     $d \leftarrow m$
6: **end if**
7: $a \leftarrow \sqrt{\frac{1}{1+\sqrt{H}}}$
8: $\forall i \in [m], x'_i \leftarrow (ax_i; \sqrt{1-a^2}\cdot e_i)$
9: $k \leftarrow O\left(\frac{(H+1)\ln(m/\delta)}{\gamma^2}\right)$
10: $M \leftarrow$ a random $\{\pm 1\}$ matrix of dimension $k \times (d+m)$
11: **for** $i \in [m]$ **do**
12:     $\bar{x}_i \leftarrow Mx'_i$
13: **end for**
14: Return $(\bar{x}_1, \ldots, \bar{x}_m)$.
```

After the preprocessing step, $\bar{X}$ is used as input to ALuMA, which then returns a set of labels for the examples in $\bar{X}$. These are also the labels of the examples in the original X. To retrieve a halfspace for X with the least margin error, any passive learning algorithm can be applied to the resulting labeled sample. The full active learning procedure is described in Alg. 4.

Note that if ALuMA returns the correct labels for the sample, the usual generalization bounds for passive supervised learning can be used to bound the true error of the returned separator w. In particular, we can apply the support vector machine algorithm (SVM) and rely on generalization bounds for SVM.

Algorithm 4 Active Learning

```
1: **Input:** $X = \{x_1, \ldots, x_m\}$ or $K \in \mathbb{R}^{m\times m}$, $L : [m] \to \{-1, 1\}$, $N$, $\gamma$, $H$, $\delta$
2: **if** input has $X$ **then**
3:     Get $\bar{X}$ by running Alg. 3 with input $X, \gamma, H, \delta/2$.
4: **else**
5:     Get $\bar{X}$ by running Alg. 3 with input $K, \gamma, H, \delta/2$.
6: **end if**
7: Get $(y_1, \ldots, y_m)$ by running ALuMA with input $\bar{X}$, $L$, $N$, $\delta/2$.
8: Get $w \in \mathbb{R}^d$ by running SVM on the labeled sample $\{(x_1, y_1), \ldots, (x_m, y_m)\}$.
9: Return $w$.
```

The result of these transformations are summarized in the following theorem.

Theorem 17 *Let $X = \{x_1, \ldots, x_m\} \subseteq B$, where B is the unit ball in some Hilbert space. Let $H \geq 0$ and $\gamma > 0$, and assume there exists a $w^* \in B$ such that*

$$H \geq \sum_{i=1}^{m} \max(0, \gamma - L(i)\langle w^*, x_i\rangle)^2.$$

Let $\delta \in (0,1)$ be a confidence parameter. There exists an algorithm that receives X as vectors in $\mathbb{R}^d$ or as a kernel matrix $K \in \mathbb{R}^{m\times m}$, and input parameters γ and H, and outputs a set $\bar{X} = \{\bar{x}_1, \ldots, \bar{x}_m\} \subseteq \mathbb{R}^k$, such that

1. *$k = O\left(\frac{(H+1)\ln(m/\delta)}{\gamma^2}\right)$,*

2. *With probability $1-\delta$, $\bar{X} \subseteq \mathbb{B}_1^k$ and $(\bar{X}, L)$ is separable with a margin $\frac{\gamma}{2+2\sqrt{H}}$.*

3. *The run-time of the algorithm is polynomial in $d, m, 1/\gamma, \ln(1/\delta)$ if x_i are represented as vectors in d, and is polynomial in $m, 1/\gamma, \ln(1/\delta)$ if x_i are represented by a kernel matrix.*

The proof of Theorem 17 can be found in Appendix B. In Section 6.2 we demonstrate that in practice, this procedure provides good label complexity results on real data sets. Investigating the relationship between $\mathrm{OPT}_{\max}$ in the new representation and $\mathrm{OPT}_{\max}$ in the original representation is an important question for future work.

6. Other Approaches: A Theoretical and Empirical Comparison

We now compare the effectiveness of the approach implemented by ALuMA to other active learning strategies. ALuMA can be characterized by two properties: (1) its "objective" is to reduce the volume of the version space and (2) at each iteration, it aggressively selects an example from the pool so as to (approximately) minimize its objective as much as possible (in a greedy sense). We discuss the implications of these properties by comparing to other strategies. Property (1) is contrasted with strategies that focus on increasing the number of examples whose label is known. Property (2) is contrasted with strategies which are "mellow", in that their criterion for querying examples is softer.

Much research has been devoted to the challenge of obtaining a substantial guaranteed improvement of label complexity over regular "passive" learning for halfspaces in $\mathbb{R}^d$. Examples (for the realizable case) include the Query By Committee (QBC) algorithm (Seung et al., 1992; Freund et al., 1997), the CAL algorithm (Cohn et al., 1994), and the Active Perceptron (Dasgupta et al., 2005). These algorithms are not "pool-based" but rather use "selective-sampling": they sample one example at each iteration, and immediately decide whether to ask for its label. Out of these algorithms, CAL is the most mellow, since it queries any example whose label is yet undetermined by the version space. Its "objective" can be described as reducing the number of examples which are labeled incorrectly, since it has been shown to do so in many cases (Hanneke, 2007, 2011; Friedman, 2009). QBC and the active perceptron are less mellow. Their "objective" is similar to that of ALuMA since they decide on examples to query based on geometric considerations.

In Section 6.1 we discuss the theoretical advantages and disadvantages of different strategies, by considering some interesting cases from a theoretical perspective. In Section 6.2 we report an empirical comparison of several algorithms and discuss our conclusions.

6.1 Theoretical Comparison

The label complexity of the algorithms mentioned above is usually analyzed in the PAC setting, thus we translate our guarantees into the PAC setting as well for the sake of comparison. We define the (ϵ, m, D)-label complexity of an active learning algorithm to be the number of *label queries* that are required in order to guarantee that given a sample of m unlabeled examples drawn from D, the error of the learned classifier will be at most ϵ (with probability of at least $1-\delta$ over the choice of sample). A a pool-based active learner can be used to learn a classifier in the PAC model by first sampling a pool of m unlabeled examples from D, then applying the pool-based active learner to this pool, and finally running a standard passive learner on the labeled pool to obtain a classifier. For the class of halfspaces, if we sample an unlabeled pool of $m = \tilde{\Omega}(d/\epsilon)$ examples, then the learned classifier will have an error of at most ϵ (with high probability over the choice of the pool).

To demonstrate the effect of the first property discussed above, consider again the simple case of thresholds on the line defined in Section 4. Compare two greedy pool-based active learners for $\mathcal{H}_{\text{line}}$: The first follows a binary search procedure, greedily selecting the example that increases the number of known labels the most. Such an algorithm requires $\lceil \log(m) \rceil$ queries to identify the correct labeling of the pool. The second algorithm queries the example that splits the version space as evenly as possible. Theorem 5 implies a label complexity of $O(\log(m)\log(1/\gamma(h)))$ for such an algorithm, since $\mathrm{OPT}_{\max} = \lceil \log(m) \rceil$. However, a better result holds for this simple case:

Theorem 18 *In the problem of thresholds on the line, for any pool with labeling L, the exact greedy algorithm requires at most $O(\log(1/\gamma(h)))$ labels. This is also the label complexity of any approximate greedy algorithm that outputs a majority vote.*

Proof First, assume that the algorithm is exactly greedy. A version space for $\mathcal{H}_{\text{line}}$ is described by a segment in $[a,b] \subseteq [0,1]$, and a query at point α results in a new version space, $[a,\alpha]$ or $[\alpha,b]$, depending on the label. We now show that for every version space $[a,b]$, at most two greedy queries suffice to either reduce the size of the version space by a factor of at least $2/3$, or to determine the labels of all the points in the pool.

Assume for simplicity that the version space is $[0,1]$, and denote the pool of examples in the version space by X. Assume w.l.o.g. that the greedy algorithm now queries $\alpha \leq \frac{1}{2}$. If $\alpha > 1/3$, then any answer to the query will reduce the version space size to less than $2/3$. Thus assume that $\alpha \leq 1/3$. If the query answer results in the version space $[0,\alpha)$ then we are done since this version space is smaller than $2/3$. We are left with the case that the version space after querying α is $[\alpha,1]$. Since the algorithm is greedy, it follows that for $\beta = \min\{x \in X \mid x \geq \alpha\}$, we have $\beta \geq 1-\alpha$: this is because if there was a point $\beta \in (\alpha, 1-\alpha)$, it would cut the version space more evenly than α, in contradiction to the greedy choice of α. Note further that $(\alpha, 1-\alpha)$ is larger than $[1-\alpha, 1]$ since $\alpha \leq 1/3$. Therefore, the most balanced choice for the greedy algorithm is β. If the query answer for β cuts the version space to $(\beta, 1]$ then we are done, since $1-\beta \leq \alpha \leq 1/3$. Otherwise, the query answer leaves us with the version space (α,β). This version space includes no more pool points, by the definition of β. Thus in this case the algorithm has determined the labels of all points.

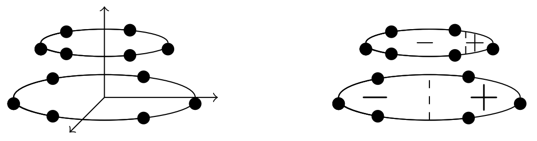
It follows that if the algorithm runs at least t iterations, then the size of the version space after t iterations is at most $(2/3)^{t/2}$. If the true labeling has a margin of γ, we conclude that $(2/3)^{t/2} \geq \gamma$, thus $t \leq O(\log(1/\gamma))$.

A similar argument can be carried for ALuMA, using a smaller bound on α and more iterations due to the approximation, and noting that if the correct answer is in $(\alpha, 1-\alpha)$ then a majority vote over thresholds drawn randomly from the version space will label the examples correctly. ■

Comparing the $\lceil \log(m) \rceil$ guarantee of the first algorithm to the $\log(1/\gamma(h))$ guarantee of the second, we reach the (unsurprising) conclusion, that the first algorithm is preferable when the true labeling has a small margin, while the second is preferable when the true labeling has a large margin. This simple example accentuates the implications of selecting the volume of the version space as an objective. A similar implication can be derived by considering the PAC setting, replacing the binary-search algorithm with CAL, and letting $m = \tilde{\Theta}(1/\epsilon)$. On the single-dimensional line, CAL achieves a label-complexity of $O(\log(1/\epsilon)) = O(\log(m))$, similarly to the binary search strategy we described. Thus when ϵ is large compared to $\gamma(h)$, CAL is better than being greedy on the volume, and the opposite holds when the condition is reversed. QBC will behave similarly to ALuMA in this setting.

To demonstrate the effect of the second property described above—being aggressive versus being mellow, we consider the following example, adapted slightly from Dasgupta (2006).

Example 19 *Consider two circles parallel to the (x,y) plane in $\mathbb{R}^3$, one at the origin and one slightly above it. For a given ϵ, fix $2/\epsilon$ points that are evenly distributed on the top circle, and $2/\epsilon$ points at the same angles on the bottom circle (see left illustration below). The distribution D_ϵ is an uneven mix of a uniform distribution over the points on the top circle and one over the points of the bottom circle: The top circle is given a much higher probability. All homogeneous separators label half of the bottom circle positively, but an unknown part of the top circle (see right illustration). The bottom points can be very helpful in finding the correct separator fast, but their probability is low.*



Dasgupta has demonstrated via this example that active learning can gain in label complexity from having significantly more unlabeled data. The following theorem shows that the aggressive strategy employed by

ALuMA indeed achieves an exponential improvement when there are more unlabeled samples. In many applications, unlabeled examples are virtually free to sample, thus it can be worthwhile to allow the active learner to sample more examples than the passive sample complexity and use an aggressive strategy.[3] In contrast, the mellow strategy of CAL does not significantly improve over passive learning in this case. We note that these results hold for any selective-sampling method that guarantees an error rate similar to passive ERM given the same sample size. This falls in line with the observation of Balcan et al. (2007), that in some cases a more aggressive approach is preferable.

Theorem 20 *For all small enough $\epsilon \in (0,1)$ the distribution D_ϵ in Example 19 satisfies*

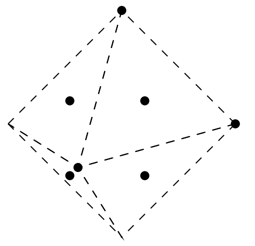
1. *For $m = O(1/\epsilon)$, the $(\epsilon, m, D_\epsilon)$-label complexity of* any active learner *is $\Omega(1/\epsilon)$.*
2. *For $m = \Omega(\log^2(1/\epsilon)/\epsilon^2)$, the $(\epsilon, m, D_\epsilon)$-label complexity of ALuMA is $O(\log^2(1/\epsilon))$.*
3. *For* any value *of m, the $(\epsilon, m, D_\epsilon)$-label complexity of CAL is $\Omega(1/\epsilon)$.*

The proof of Theorem 20 is provided in Appendix C. The example above demonstrated that more unlabeled examples can help ALuMA use less labels, whereas they do not help CAL. In fact, in some cases the label complexity of CAL can be significantly worse than that of the optimal algorithm, even when both CAL and the optimal algorithm have access to all the points in the support of the distribution. This is demonstrated in the following example. Note that in this example, a passive learner also requires access to all the points in the support of the distribution, thus CAL, passive learning, and optimal active learning all require the same size of a random unlabeled pool.

Example 21 *Consider a distribution in $\mathbb{R}^d$ that is supported by two types of points on an octahedron (see an illustration for $\mathbb{R}^3$ below).*

1. *Vertices: $\{e_1, \ldots, e_d\}$.*
2. *Face centers: z/d for $z \in \{-1,+1\}^d$.*

Consider the hypothesis class $\mathcal{W} = \{x \mapsto \mathrm{sgn}(\langle x, w\rangle - 1 + \frac{1}{d}) \mid w \in \{-1,+1\}^d\}$. Each hypothesis in $\mathcal{W}$, defined by some $w \in \{-1,+1\}^d$, classifies at most $d+1$ data points as positive: these are the vertices e_i for i such that $w[i] = +1$, and the face center w/d.



Theorem 22 *Consider Example 21 for $d \geq 3$, and assume that the pool of examples includes the entire support of the distribution. There is an efficient algorithm that finds the correct hypothesis from $\mathcal{W}$ with at most d labels. On the other hand, with probability at least $\frac{1}{e}$ over the randomization of the sample, CAL uses at least $\frac{2^d+d}{2d+3}$ labels to find the correct separator.*

3. In the limit of an infinite number of unlabeled examples, if the distribution has a non-zero support on the entire domain, the pool-based setting becomes identical to the setting of membership queries (Angluin, 1988). In contrast, we are interested in finite samples.

Proof First, it is easy to see that if $h^* \in \mathcal{W}$ is the correct hypothesis, then

$$w = (h^*(e_1), \ldots, h^*(e_d)).$$

Thus, it suffices to query the d vertices to discover the true w.

We now show that the number of queries CAL asks until finding the correct separator is exponential in d. CAL inspects the unlabeled examples sequentially, and queries any example whose label cannot be inferred from previous labels. Consider some run of CAL (determined by the random ordering of the sample). Assume w.l.o.g. that each data point appears once in the sample. Let S be the set that includes the positive face center and all the vertices. Note that CAL cannot terminate before either querying all the $2^d - 1$ negative face centers, or querying at least one example from S. Moreover, CAL will query all the face centers it encounters before encountering the first example from S. At each iteration t before encountering an example from S, there is a probability of $\frac{d+1}{2^d+d-t}$ that the next example is from S. Therefore, the probability that the first $T = \frac{2^d+d}{2d+3}$ examples are not from S is

$$\prod_{t=0}^{T-1} \left(1 - \frac{d+1}{2^d+d-t}\right) \geq \left(1 - \frac{d+1}{2^d+d-T}\right)^T \geq e^{-2T\frac{d+1}{2^d+d-T}} = e^{\frac{-2(d+1)}{\frac{2^d+d}{T}-1}} = \frac{1}{e} \,,$$

where in the second equality we used $1 - a \geq \exp(-2a)$ which holds for all $a \in [0, \frac{1}{2}]$. Therefore, with probability at least $\frac{1}{e}$ the number of queries is at least $\frac{2^d+d}{2d+3}$. ■

These examples show that in some cases an aggressive approach is preferable to a mellow approach such as employed by CAL. At the same time, it should be noted that CAL has a guaranteed label complexity for cases for which ALuMA currently has none. Its label complexity is bounded by $\tilde{O}(d\theta \log(1/\epsilon))$, where θ is the disagreement coefficient, a quantity that depends on the distribution and the target hypothesis (Hanneke, 2007, 2011). Specifically, if D is uniform over a sphere centered at the origin, then for all target hypotheses $\theta = \Theta(\sqrt{d})$. Thus CAL achieves an exponential improvement over passive learning for this canonical example. We do not have a similar analysis for ALuMA for the case of a uniform distribution.

6.2 Empirical Comparison

We carried out an empirical comparison between the algorithms discussed above. Our goal is twofold: First, to evaluate ALuMA in practice, and second, to compare the performance of aggressive strategies compared to mellow strategies. The aggressive strategies are represented in this evaluation by ALuMA and one of the heuristics proposed by Tong and Koller (2002). The mellow strategy is represented by CAL. QBC represents a middle-ground between aggressive and mellow. We also compare to a passive ERM algorithm—one that uses random labeled examples. We evaluated the algorithms over synthetic and real data sets and compared their label complexity performance.

Our implementation of ALuMA uses hit-and-run samples instead of full-blown volume estimation, as described in Section 5.1. QBC is also implemented using hit-and-run, as described in Gilad-Bachrach et al. (2005). For both ALuMA and QBC, we used a fixed number of mixing iterations for hit-and-run, which we set to 1000. We also fixed the number of sampled hypotheses at each iteration of ALuMA to 1000, and used the same set of hypotheses to calculate the majority vote for classification. CAL and QBC examine the examples sequentially, thus the input provided to them was a random ordering of the example pool. The algorithm TK is the first heuristic proposed in Tong and Koller (2002), in which the example chosen at each iteration is the one closest to the max-margin solution of the labeled examples known so far. The graphs below compare the train and the test errors of the different algorithms.

In each of the algorithms, the classification of the training examples is done using the version space defined by the queried labels. The theory for CAL and ERM allows selecting an arbitrary predictor out of the version space. In QBC, the hypothesis should be drawn uniformly at random from the version space. We have found that all the algorithms show a significant improvement in classification error if they classify using

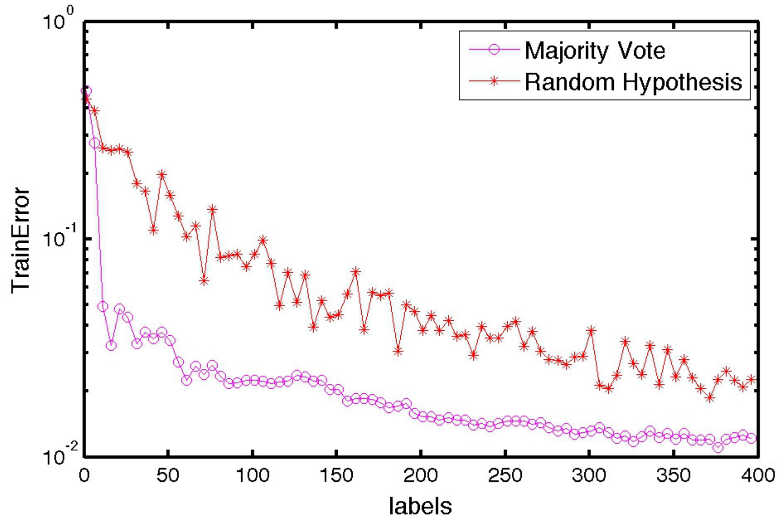


Figure 1: QBC (MNIST 4 vs. 7) - Random hypothesis Vs. Majority vote

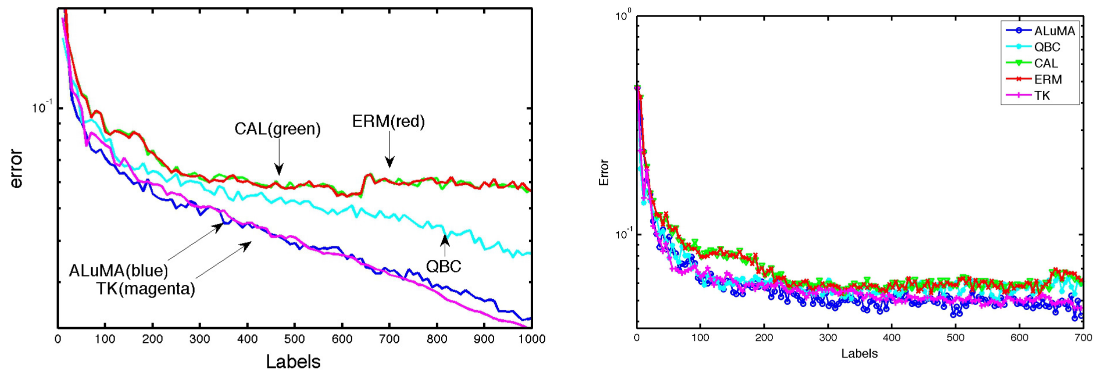


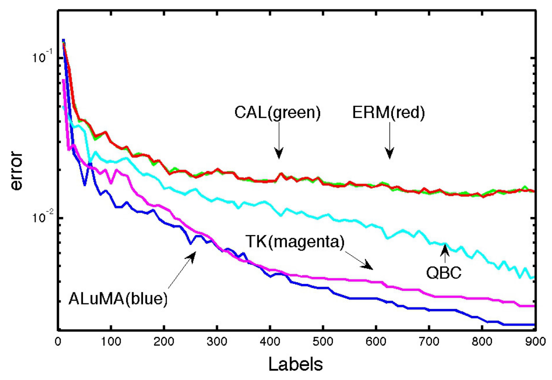
Figure 2: MNIST 3 vs. 5. Train error (left) and test error (right)

the majority vote classification proposed for ALuMA. This observation is demonstrated in Figure 1, which shows the rate of error of QBC (on MNIST data which is described below) using a random hypothesis and a majority vote. Therefore, in all of our experiments below, the results for all the algorithms are based on a majority vote classification.

Our first data set is MNIST.[4] The examples in this data set are gray-scale images of handwritten digits in dimension 784. Each digit has about 6,000 training examples. We performed binary active learning by pre-selecting pairs of digits. Figure 2 and Figure 3 depict the error as a function of the label budget for two pairs of digits: 3 vs. 5 and 4 vs. 7. It is striking to observe that CAL provides no improvement over passive ERM in the first 1000 examples, while this budget suffices to reach zero training error for ALuMA and TK.

We also tested the algorithms on the PCMAC data set.[5] This is a real-world data set, which represents a two-class categorization of the 20-Newsgroup collection. The examples are web-posts represented using bag-of-words. The original dimension of examples is 7511. We used the Johnson-Lindenstrauss projection to reduce the dimension to 300, which kept the data still separable. We used a training set of 1000 examples.

4. The data set is available at `http://yann.lecun.com/exdb/mnist/`.
5. The data set is available at `http://vikas.sindhwani.org/datasets/lskm/matlab/pcmac.mat`.



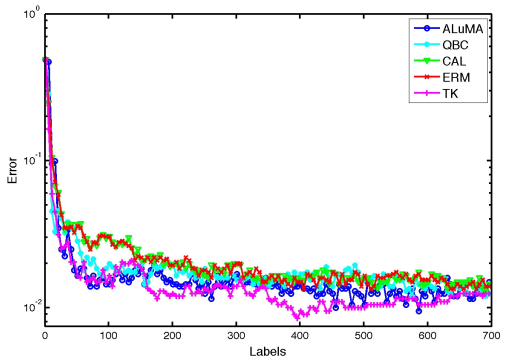
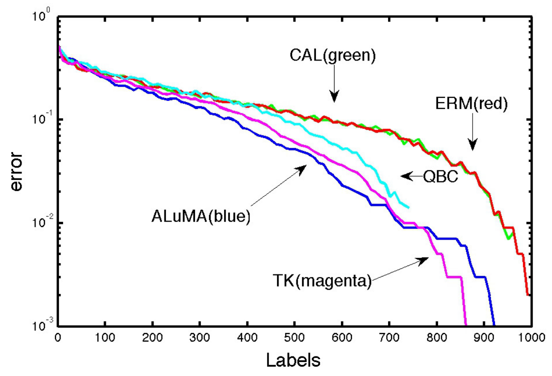


Figure 3: MNIST 4 vs. 7. Train error (left) and test error (right)



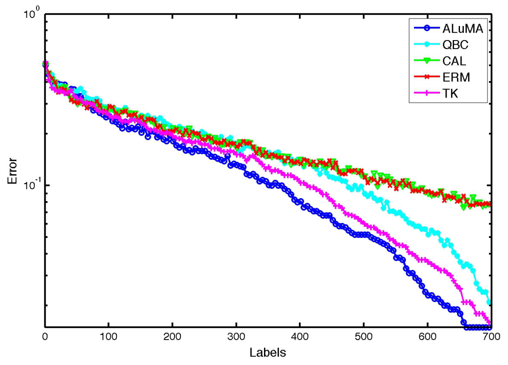
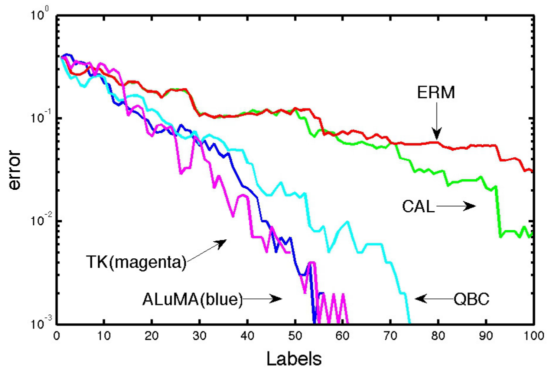


Figure 4: PCMAC. Train error (left) and test error (right)

Figure 4 depicts the results. We were not able to run QBC long enough to use its entire label budget, as it tends to become slower when the training error becomes small.

The following experiments show that ALuMA and TK outperform CAL and QBC even on a data sampled from the uniform distribution on a sphere in $\mathbb{R}^d$. Figure 5 and Figure 6 depict the error as a function of the label budget when learning a random halfspace over the uniform distribution in $\mathbb{R}^{10}$ and $\mathbb{R}^{100}$ respectively.



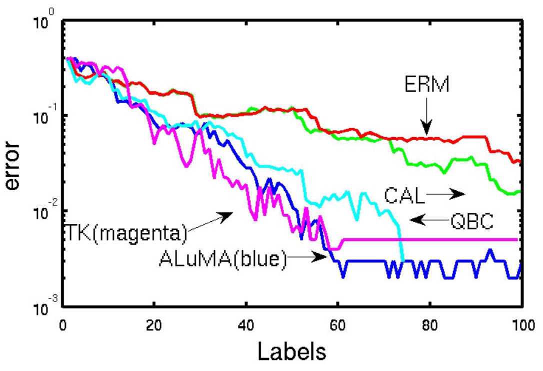


Figure 5: Uniform distribution ($d = 10$). Train error (left) and test error (right)

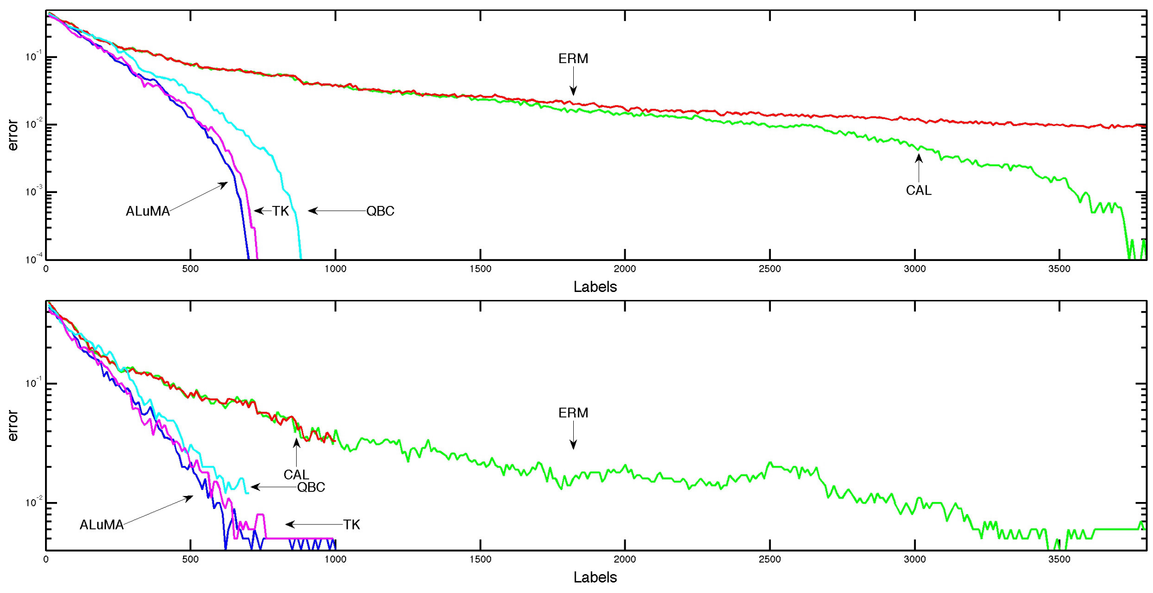


Figure 6: Uniform distribution ($d = 100$). Train error (up) and test error (down)

The difference between the performance of the different algorithms is less marked for $d = 10$ than for $d = 100$, suggesting that the difference grows with the dimension. This result suggests that ALuMA might have a better guarantee than the general relative analysis in the case of the uniform distribution. Achieving such an analysis is an open question which is left for future work.

In the experiments reported so far, TK and ALuMA perform about the same, showing that the TK heuristic is very successful. However, there are cases where TK performs much worse than ALuMA, as the following synthetic experiment demonstrates. In this experiment the pool of examples is taken to be the support of the distribution described in Example 21, with an additional dimension to account for halfspaces with a bias. We also added the negative vertices $-e_i$ to the pool. Similarly to the proof of Theorem 22, it suffices to query the vertices to reach zero error. Table 1 lists the number of iterations required in practice to achieve zero error by each of the algorithms. In this experiment, unlike the rest, ALuMA is not only much better than QBC and CAL, it is also much better than TK, which is worse even than QBC here. This suggests that TK might not have guarantees similar to those of ALuMA, despite the fact that they both attempt to minimize the same objective. The number of queries ALuMA requires is indeed close to the number of vertices.

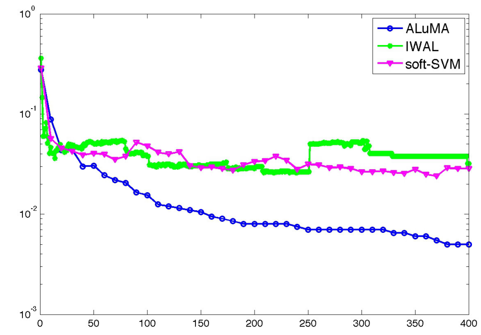
d	ALuMA	TK	QBC	CAL	ERM
10	**29**	156	50	308	1008
12	**38**	735	113	862	3958
15	**55**	959	150	2401	> 20000

Table 1: Octahedron: number of queries to achieve zero error

To summarize, in all of the experiments above, aggressive algorithms performed better than mellow ones. These results are not fully explained by current theory. The experiments also show that ALuMA and TK have comparable success in practice, but also that there are cases where TK is much worse than ALuMA.

6.3 Non-Separable Data

We now turn to evaluate ALuMA on non-separable data, based on the procedure described in Section 5.2. We compare to IWAL (Beygelzimer et al., 2009), which is a state-of-the-art active learning algorithm for the agnostic case. We compared ALuMA and IWAL to the passive soft-SVM, which selects random labeled examples from the training set as input.



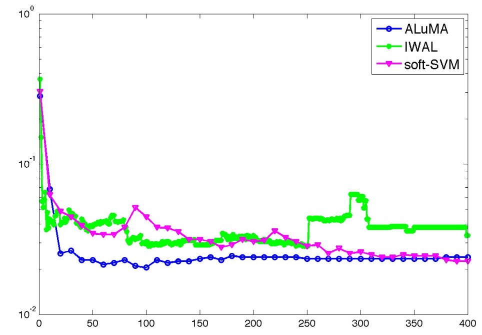
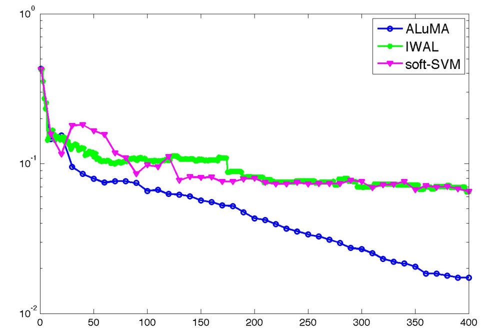


Figure 7: MNIST 4 vs. 7. (non-separable) training error (left) and test error (right)



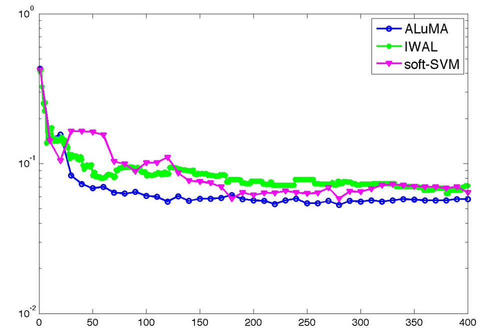


Figure 8: MNIST 3 vs. 5. (non-separable), training error (left) and test error (right)

In our first experiment, we tested the algorithms on the MNIST data, pairs 3 vs. 5 and 4 vs. 7 again, by first reducing the dimension. Following the experimental procedure in Beygelzimer et al. (2009), we projected the 784-dimensional data to a 25-dimensional space using PCA. This renders the two pairs of digits we tested in Section 6.2 non-separable. Using model selection, we set the regularization parameter of soft-SVM to $\lambda = 10^{-3}$ and the maximal norm of the separator in IWAL to $\sqrt{1000}$. For ALuMA, the noise parameter was set to $H = 0.02$ and the dimension after preprocessing was 240. The results are presented in Figures 7 and 8. It can be seen that ALuMA enjoys a faster improvement in error compared to IWAL. This improvement might be attributed to the fact that we assume an upper bound on the hinge-loss in this case, while IWAL must be prepared to handle any amount of label error.

Our second experiment is for the W1A data set.[6] The original data contains a (sparse representation of) more than 2000 train instances and more than $47,000$ test instances in dimension 300. Our preprocessing step used $H = 10^{-2}$ and projected the data to dimension 260. The other parameters were the same as in the previous experiments. The results are shown in Figure 9. It can be seen that in this data set IWAL and ALuMA are comparable, both offering improvement over soft SVM. Unlike MNIST, here ALuMA does not show a consistent improvement over IWAL. We suspect that this is due to the fact that the best achievable error for this data is larger, thus decreasing ALuMA's advantage.

6. The data set is available at `http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/`.

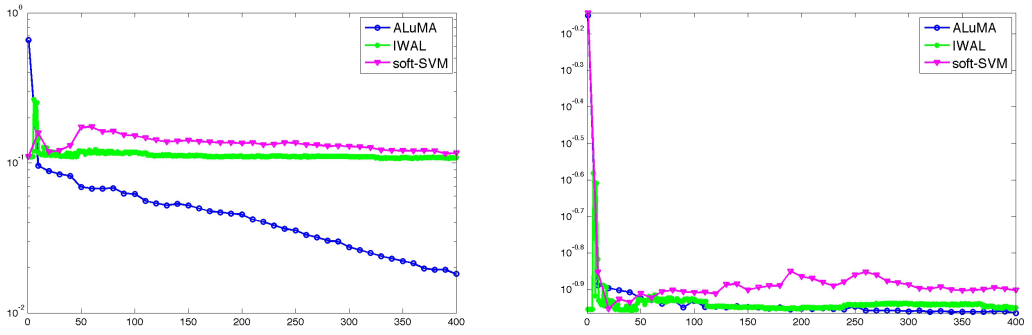


Figure 9: W1A training error (left) and test error (right)

7. Discussion

In this work we have shown that the aggressive approach for active learning can be implemented efficiently and successfully for learning halfspaces. Our theoretical results shed light on the relationship between the margin of the true separator and the number of active queries that the algorithm requires. The experiments show that this approach is practical to implement, and results in improved performance compared to mellow approaches.

Many questions remain open. First, while our analysis guarantees an approximation factor of $O(d\log(m))$, in practice our experiments for the uniform distribution show that in this case the approach performs as well or better than algorithms which are known to achieve almost optimal rates, such as QBC, even in high dimensions. Providing a tight analysis for the label complexity of the aggressive approach for the uniform distribution is thus an interesting open question. Further, while our guarantees only bound the number of queries required to achieve zero error, in practice the algorithm performs well compared to other algorithms even if the goal is only to reach some small non-zero error. Characterizing the behavior of the aggressive approach in this regime is another important open question. Lastly, our work shows that for low-error settings, the aggressive approach can be preferable to the mellow approach. On the other hand, the mellow approach is clearly preferable when error levels are very high. Thus we posit the following open problem for further research: Characterizing the best active learning algorithm one should choose, given a numerical upper bound on the amount of error in the given learning problem.

Appendix A. Proof of Theorem 5

In this section we provide the complete proof of Theorem 5. We will follow Golovin and Krause (2010) and rely on the notion of adaptive sub-modularity.

Denote the product space of partial realizations by $\mathcal{L}_{X,\mathcal{H}}$. Let $f : \mathcal{L}_{X,\mathcal{H}} \to \mathbb{R}_+$ be any utility function from the set of possible partial labelings of X to the non-negative reals. We define the notions of *adaptive monotonicity* and *adaptive submodularity* of a utility function using the following notation: For an element $x \in X$, a subset $Z \subseteq X$ and a hypothesis $h \in \mathcal{H}$, we define the conditional expected marginal benefit of x, conditioned on having observed the partial labeling $h|_Z$, by

$$\Delta(h|_Z, x) = \mathbb{E}_g\left[f(g|_{Z\cup\{x\}}) - f(g|_Z) \,\middle|\, g|_Z = h|_Z\right].$$

Put another way, $\Delta(h|_Z, x)$ is the expected improvement of f if we add to Z the element x, where expectation is over a choice of a hypothesis g taken uniformly at random from the set of hypotheses that agree with h on Z.

Definition 23 (Adaptive Monotonicity) *A utility function $f : \mathcal{L}_{X,\mathcal{H}} \to \mathbb{R}_+$ is* adaptive monotone *if the conditional expected marginal benefit is always non-negative. That is, if for all $h \in \mathcal{H}, Z \subseteq X$ and $x \in X$, $\Delta(h|_Z, x) \geq 0$.*

Definition 24 (Adaptive Submodularity) *A function $f : \mathcal{L}_{X,\mathcal{H}} \to \mathbb{R}_+$ is* adaptive submodular *if the conditional expected marginal benefit of a given item does not increase if the partial labeling is extended. That is, if for all $h \in \mathcal{H}$, for all $Z_1 \subseteq Z_2 \subseteq X$,and for all $x \in X$,*

$$\Delta(h|_{Z_1}, x) \geq \Delta(h|_{Z_2}, x).$$

Any (deterministic) pool-based algorithm is associated with a policy function, which we usually denote by π, which maps each partial realization $h|_S$ to an element x of X, namely, the element x queried by the algorithm after observing $h|_S$. It is natural to consider a greedy algorithm which always selects an item that maximizes the marginal utility. Since it is often computationally hard to choose the element which maximizes the marginal utility, we introduce the notion of an approximately-greedy algorithm, following Golovin and Krause (2010).

Definition 25 (Approximate Greedy) *Let $\alpha \geq 1$. An algorithm which is associated with policy $\pi : \mathcal{L}_{X,\mathcal{H}} \to X$ is* α-approximately greedy *with respect to a utility function f if for every h and for every $Z \subseteq X$*

$$\Delta(h|_Z, \pi(h|_Z)) \geq \frac{1}{\alpha} \max_{x \in X} \Delta(h|_Z, x). \tag{7}$$

If an algorithm $\mathcal{A}$ is 1-approximately greedy *with respect to a utility function f, we simply say that $\mathcal{A}$ is greedy w.r.t. f.*

We denote by $S(\mathcal{A}, h, k)$ the first k pairs of instances along with their labels observed by $\mathcal{A}$, under the assumption that $L \Leftarrow h$. Following this notation, the utility of running $\mathcal{A}$ for k steps under the assumption that $L \Leftarrow h$ is denoted by $f(S(\mathcal{A}, h, k))$. The expected utility of running $\mathcal{A}$ for k steps is defined by

$$f_{\text{avg}}(\mathcal{A}, k) = \mathbb{E}_{h \sim P}[f(S(\mathcal{A}, h, k)].$$

The central theorem of adaptive submodularity, stated below as Theorem 26, links the expected utility of the optimal policy for maximizing f_{avg} with the expected utility of the associated approximately-greedy algorithm.

Theorem 26 (Golovin and Krause (2010)) *Let $f : \mathcal{L}_{X,\mathcal{H}} \to \mathbb{R}_+$ be a utility function, and let $\mathcal{A}$ be a (deterministic) active learning algorithm. If f is adaptive monotone and adaptive submodular, and $\mathcal{A}$ is α-approximately greedy, then for any deterministic algorithm $\mathcal{A}^*$ and for all positive integers t, k,*

$$f_{\text{avg}}(\mathcal{A}, t) \geq (1 - e^{-\frac{t}{\alpha k}}) f_{\text{avg}}(\mathcal{A}^*, k).$$

Let P be a distribution over $\mathcal{H}$. For any algorithm alg, denote by $V_t(\text{alg}, h)$ the version space induced by the first t labels it queries if the true labeling of the pool is consistent with h. Denote the version space reduction of alg after t queries in the case that $L \Leftarrow h$ by

$$f(\text{alg}, t, h) = 1 - P(V_t(\text{alg}, h)). \tag{8}$$

The average version space reduction of alg after t queries is

$$f_{\text{avg}}(\text{alg}, t) = 1 - \mathbb{E}_{h \sim P}[P(V_t(\text{alg}, h))].$$

In the active learning setting, we define the utility function f as in Equation (8) and have the following result:

Lemma 27 (Golovin and Krause (2010)) *The function f defined in Equation (8) is adaptive monotone and adaptive submodular.*

Corollary 28 *Let $X = \{x_1, \ldots, x_m\}$. Let $\mathcal{H}$ be a hypothesis class, and let P be a distribution over $\mathcal{H}$. Suppose that $\mathcal{A}$ is α-approximately greedy with respect to P, and let $\mathcal{A}^*$ be a (deterministic) algorithm that achieves* $\mathrm{OPT}_{\max}$*, that is $c_{wc}(\mathcal{A}^*) = \mathrm{OPT}_{\max}$. Then, for all positive integers t, k,*

$$f_{\mathrm{avg}}(\mathcal{A}, t) \geq (1 - e^{-\frac{t}{\alpha k}}) f_{\mathrm{avg}}(\mathcal{A}^*, k).$$

The following lemma will allow us to show that the version space of an α-approximately greedy algorithm is relatively pure.

Lemma 29 *Let $\mathcal{A}^*$ be an algorithm that achieves* $\mathrm{OPT}_{\max}$*. For any $h \in \mathcal{H}$, any active learner $\mathcal{A}$, and any t,*

$$f_{\mathrm{avg}}(\mathcal{A}^*, \mathrm{OPT}_{\max}) - f_{\mathrm{avg}}(\mathcal{A}, t) \geq P(V(h|_X))\,(P(V_t(\mathcal{A}, h)) - P(V(h|_X)))\ .$$

Proof Since $\mathcal{A}^*$ acheives the optimal worst-case cost, the version space induced by the labels that $\mathcal{A}^*$ queries within the first $\mathrm{OPT}_{\max}$ iterations must be exactly the set of hypotheses which are consistent with the true labels of the sample. Therefore, for any $h \in \mathcal{H}$.

$$P(V_{\mathrm{OPT}_{\max}}(\mathcal{A}^*, h)) = P(V(h|_X)).$$

By definition of f_{avg},

$$\begin{aligned} f_{\mathrm{avg}}(\mathcal{A}^*, \mathrm{OPT}_{\max}) - f_{\mathrm{avg}}(\mathcal{A}, t) &= \mathbb{E}_{h \sim P}[P(V_t(\mathcal{A}, h)) - P(V_{\mathrm{OPT}_{\max}}(\mathcal{A}^*, h))] \\ &= \mathbb{E}_{h \sim P}[P(V_t(\mathcal{A}, h)) - P(V(h|_X))]. \end{aligned}$$

Since $S(\mathcal{A}, h, t)$ does not depend on the value of h outside of X, we can sum over the possible labelings of X to have

$$f_{\mathrm{avg}}(\mathcal{A}^*, \mathrm{OPT}_{\max}) - f_{\mathrm{avg}}(\mathcal{A}, t) = \sum_{h|_X : h \in \mathcal{H}} P(V(h|_X))(P(V_t(\mathcal{A}, h)) - P(V(h|_X))).$$

Now, it is easy to see that for any $h \in \mathcal{H}$, $V_t(\mathcal{A}, h) \supseteq V(h|_X)$, thus

$$P(V_t(\mathcal{A}, h)) - P(V(h|_X)) \geq 0.$$

It follows that for any $h \in \mathcal{H}$

$$f_{\mathrm{avg}}(\mathcal{A}^*, \mathrm{OPT}_{\max}) - f_{\mathrm{avg}}(\mathcal{A}, t) \geq P(V(h|_X))(P(V_t(\mathcal{A}, h)) - P(V(h|_X))).$$

■

Combining Corollary 28 and Lemma 29, the following corollary is immediate.

Corollary 30 *For any α-approximate greedy algorithm $\mathcal{A}$,*

$$\forall h \in \mathcal{H}, \quad P(V(h|_X))(P(V_t(\mathcal{A}, h)) - P(V(h|_X))) \ \leq\ e^{-\frac{t}{\alpha \mathrm{OPT}_{\max}}}\ ,$$

which yields

$$\forall h \in \mathcal{H}, \quad \frac{P(V(h|_X))}{P(V_t(\mathcal{A}, h))} \geq \frac{P(V(h|_X))^2}{e^{-\frac{t}{\alpha \mathrm{OPT}_{\max}}} + P(V(h|_X))^2}. \tag{9}$$

Proof (Of Theorem 5) Let $\mathcal{A}$ be α-approximately greedy algorithm which outputs a β-approximate majority vote. Corollary 30 holds for $\mathcal{A}$. Let h be the target hypothesis. Substituting $T \geq \alpha(2\ln(1/P(h)) + \ln(\frac{\beta}{1-\beta})) \cdot \mathrm{OPT}_{\max}$ into Equation (9) implies that

$$\frac{P(V(h|_X))}{P(V_T(\mathcal{A},h))} \geq \beta .$$

The proof now follows from the fact that $\mathcal{A}$ outputs a β-approximate majority vote. ■

Appendix B. Handling Non-Separable Data and Kernel Representations

We now prove Theorem 17 by showing that Alg. 3 satisfies the claims of the theorem. It is clear that Alg. 3 is polynomial as required in item (3). In addition, item (1) holds from the definition of Alg. 3. We have left to prove item (2). We first prove that it holds for the case where the input is represented directly as $X \subseteq \mathbb{R}^d$.

We start by showing that under the assumption of Theorem 17, the set $\{x'_1, \ldots, x'_m\}$, which is generated in step 8, is separated with a bounded margin by the original labels of x_i. Fix $\gamma > 0$ and $w^* \in \mathbb{B}_1^d$. For each $i \in [m]$, define

$$\ell_i = \max(0, \gamma - L(i)\langle w^*, x_i\rangle).$$

Thus, ℓ_i quantifies the margin violation of example x_i by w^*, relative to its true label $L(i)$.

Lemma 31 *If $H \geq \sum_{i=1}^m \ell_i^2$, where H is the input to Alg. 3, then there is a $w \in \mathbb{B}_1^{d+m}$ such that for all $i \in [m]$, $L(i)\langle w, x'_i\rangle \geq \frac{\gamma}{1+\sqrt{H}}$.*

Proof By step 8 in Alg. 3, $x'_i = (a \cdot x_i; \sqrt{1-a^2} \cdot e_i)$, where $a = \sqrt{\frac{1}{1+\sqrt{H}}}$. Define

$$w' = (w^*; \frac{a}{\sqrt{1-a^2}}(L(1)\ell_1, \ldots, L(m)\ell_m)).$$

Then

$$L(i)\langle w', x'_i\rangle = aL(i)\langle w^*, x_i\rangle + a\ell_i \geq a(\gamma - \ell_i) + a\ell_i = a\gamma.$$

Let $w = \frac{w'}{\|w'\|}$. Then $w \in \mathbb{B}_1^{d+m}$, and

$$L(i)\langle w, x'_i\rangle = \frac{L(i)\langle w', x'_i\rangle}{\|w'\|} \geq \frac{a\gamma}{\sqrt{1 + \frac{a^2}{1-a^2}\sum_{i=1}^m \ell_i^2}} = \frac{\gamma}{\sqrt{\frac{1}{a^2} + \frac{1}{1-a^2}\sum_{i=1}^m \ell_i^2}}.$$

Set $a^2 = \frac{1}{1+\sqrt{H}}$, and assume $H \geq \sum_{i=1}^m \ell_i^2$. Then

$$L(i)\langle w, x'_i\rangle \geq \frac{\gamma}{1+\sqrt{H}}.$$

■

The set $\{\bar{x}_1, \ldots, \bar{x}_m\}$ returned by Alg. 3 is a Johnson-Lindenstrauss projection of $\{x'_1, \ldots, x'_m\}$ on $\mathbb{R}^k$. It is known (see, e.g., Balcan et al., 2006b) that if a set of m points is separable with margin η and $k \geq O\left(\frac{\ln(m/\delta)}{\eta^2}\right)$, then with probability $1-\delta$, the projected points are separable with margin $\eta/2$. Setting $\eta = \frac{\gamma}{1+\sqrt{H}}$, it is easy to see that step 12 in Alg. 3 indeed maintains the desired margin. This completes the proof of item (2) of Theorem 17 for the case where the input is $X \subseteq \mathbb{R}^m$.

We now show that if the input is a kernel matrix K, then the decomposition step 3 preserves the separation properties of the input data, thus showing that item (2) holds in this case as well. To show that our decomposition step does not change the properties of the original data, we first use the following lemma, which indicates that separation properties are conserved under different decompositions of the same kernel matrix.

Lemma 32 (Sabato et al. (2010), Lemma 6.3) *Let $K \in \mathbb{R}^{m\times m}$ be a positive definite matrix and let $V \in \mathbb{R}^{m\times n}, U \in \mathbb{R}^{m\times k}$ be matrices such that $K = VV^T = UU^T$. For any vector $w \in \mathbb{R}^n$ there exists a vector $u \in \mathbb{R}^k$ such that $Vw = Uu$ and $\|u\| \leq \|w\|$.*

The next lemma extends the above result, showing that the property holds even if K is not invertible.

Lemma 33 *Let $K \in \mathbb{R}^{m\times m}$ be a positive definite matrix and let $V \in \mathbb{R}^{m\times n}, U \in \mathbb{R}^{m\times k}$ be matrices such that $K = VV^T = UU^T$. For any vector $w \in \mathbb{R}^n$ there exists a vector $u \in \mathbb{R}^k$ such that $Vw = Uu$ and $\|u\| \leq \|w\|$.*

Proof For a matrix A and sets of indexes I, J let $A[I]$ be the sub-matrix of A whose rows are the rows of A with an index in I. Let $A[I,I]$ be the sub-matrix of A whose rows and columns are those that have index I in A.

If K is invertible, the claim holds by Lemma 32. Thus, assume K is singular. Let $I \subseteq [m]$ be a maximal subset such that the matrix $K[I;I]$ is invertible.[7] Then by Lemma 32, $K[I;I] = V[I](V[I])^T = U[I](U[I])^T$, and there exists a vector u such that $V[I]w = U[I]u$, and $\|u\| \leq \|w\|$. We will show that for any $i \notin I$, $V[i]w = U[i]u$ as well.

For any $i \notin I$, $K[I\cup\{i\}; I\cup\{i\}]$ is singular. Therefore $V[I\cup\{i\}]$ is singular, while $V[I]$ is not. Thus there is some vector $\lambda \in \mathbb{R}^{|I|}$ such that $V[i]^T = V[I]^T\lambda$. By a similar argument there is some vector $\eta \in \mathbb{R}^{|I|}$ such that $U[i]^T = U[I]^T\eta$. We have $K[I,i] = V[I]V[i]^T = V[I]V[I]^T\lambda = K[I,I]\lambda$. Similarly for U, $K[I,i] = K[I,I]\eta$. Therefore $K[I,I](\lambda - \eta) = 0$. Since $K[I,I]$ is invertible, it follows that $\lambda = \eta$. Therefore, $U[i]u = \eta^T U[I]u = \lambda^T V[I]w = V[i]w$. ■

We now use this lemma to show that the decomposition step does not change the upper bound on the margin loss which is assumed in Theorem 17.

Theorem 34 *Let $\psi_1, \ldots, \psi_m$ be a set of vectors in a Hilbert space S, and let $K \in \mathbb{R}^{m\times m}$ such that for all $i, j \in [m]$, $K_{i,j} = \langle \psi_i, \psi_j \rangle$. suppose there exists a $w \in S$ with $\|w\| \leq 1$ such that*

$$H \geq \sum_{i=1}^{m} \max(0, \gamma - y_i\langle w, \psi_i \rangle)^2. \tag{10}$$

Let $U \in \mathbb{R}^{m\times k}$ such that $K = UU^T$ and let x_i be row i of U. Then there exists a $u \in \mathbb{B}_1^k$ such that

$$H \geq \sum_{i=1}^{m} \max(0, \gamma - y_i\langle u, x_i \rangle)^2. \tag{11}$$

Proof Let $\alpha_1, \ldots, \alpha_n \in S$ be an orthogonal basis for the span of $\psi_1, \ldots, \psi_m$ and w, and let $v_1, \ldots, v_m, v_w \in \mathbb{R}^n$ such that $\sum_{l=1}^n v_i[l]\alpha_l = \psi_i$ and $\sum_{l=1}^n v_w[l]\alpha_l = w$. Let $V \in \mathbb{R}^{m\times n}$ be a matrix such that row i of the matrix is v_i. Then $K = VV^T$, and $Vv_w = r$, where $r[i] = \langle v_w, v_i \rangle = \langle w, \psi_i \rangle$. By Lemma 33, there exists a $u \in \mathbb{R}^k$ such that $Uu = r$. Then we have $\langle u, x_i \rangle = r[i]$. Therefore for all $i \in [m]$, $\langle w, \psi_i \rangle = \langle u, x_i \rangle$, thus Equation (10) implies Equation (11). In addition, $\|u\| \leq \|v_w\| = \|w\| \leq 1$, therefore $u \in \mathbb{B}_1^k$. ■

7. If no such subset exists then K, V, U are all zero and the claim is trivial.

Appendix C. Proof of Theorem 20

Proof [of Theorem 20] Assume that $1/(2\epsilon)$ is an odd integer and $\epsilon < 1/8$. Let D_a be the uniform distribution over points on the top circle, defined by

$$S_a = \{a_n \overset{\text{def}}{=} (\frac{1}{\sqrt{2}}\cos 2\pi\epsilon n, \frac{1}{\sqrt{2}}\sin 2\pi\epsilon n, \frac{1}{\sqrt{2}}) : n \in \{0,1,\ldots,1/\epsilon - 1\}\} .$$

Let D_b be the uniform distribution over points on the bottom circle, defined by

$$S_b = \{b_n \overset{\text{def}}{=} (\cos 2\pi\epsilon n, \sin 2\pi\epsilon n, 0) : n \in \{0,1,\ldots,1/\epsilon - 1\}\} .$$

Let $D_{\epsilon/2}$ be the distribution $(1-\tau)D_a + \tau D_b$, where $\tau = \frac{\epsilon}{4\log(4/\epsilon)}$. Note that in order to label $D_{\epsilon/2}$ correctly with error no more than $\epsilon/2$, all the labels of points in S_a need to be determined. We prove each of the theorem statements in order. We consider the label complexity with high probability over the choice of unlabeled sample, where high probability is $1-\delta$ for some fixed $\delta \in (0, 1/2)$.

First, we prove claim (1). If the unlabeled sample contains only points from S_a, then an active learner has to query all the points in S_a to distinguish between a hypothesis that labels all of S_a positively and one that labels positively all but one point in S_a. Since the probability of the entire set S_b is $o(\epsilon)$, an i.i.d. sample of size $O(1/\epsilon)$, will not contain a point from S_b, thus any active learner will require $\Omega(1/\epsilon)$ labels.

More formally, assume that there exists a constant C and $\epsilon_0 > 0$ such that if $\epsilon < \epsilon_0$, then at most C/ϵ examples are drawn. Assume from now that $\epsilon < \epsilon_0$ and that $\frac{C}{4\log(4/\epsilon)} \le 1/2$. Let A be the event that an i.i.d. sample of size $m(\epsilon) \le C/\epsilon$ contains any element from S_b. Then, using the union bound, we obtain

$$\mathbb{P}(A) \le \frac{C}{\epsilon}\frac{\epsilon}{4\log(4/\epsilon)} \le 1/2 \le 1-\delta .$$

We now turn to prove claim (2). Assume that the size of the sample is at least $\frac{4\log(4/\epsilon)\log(1/(\epsilon\delta))}{\epsilon^2}$. It is easy to check that with probability at least $1-\delta$, the sample contains all the points in $S_a \cup S_b$. More formally,let $\delta > 0$ be any given confidence parameter. Let B be the event that the sample doesn't contain all the points of D_b and let A the event that the sample doesn't contain all the points of D_a. For $n \in \{0,1,\ldots,1/\epsilon - 1\}$ let B_n be the event that the sample doesn't contain the element b_n. Then,

$$\mathbb{P}(B_n) = \left(1 - \frac{\epsilon^2}{4\log(4/\epsilon)}\right)^{\frac{4\log(4/\epsilon)\log(2/(\epsilon\delta))}{\epsilon^2}} \le \epsilon\delta/2 .$$

Using the union bound, we obtain that

$$\mathbb{P}(B) \le \frac{1}{\epsilon}\mathbb{P}(A_0) \le \delta/2 .$$

Obviously, $\mathbb{P}(A) \le \mathbb{P}(B)$. Using the union bound, we obtain that with probability at least $1-\delta$, both A and B don't occur.

Given such a sample as a pool, we now show that $\mathrm{OPT}_{\max} = O(\log(1/\epsilon))$, by describing an active learning algorithm that achieves this label complexity:

1. For all possible separators, the points $b_0 = (1,0,0)$ and $b_{1/2\epsilon} = (-1,0,0)$ have different labels. The algorithm will first query these initial points, and then apply a binary search to find the boundary between negative and positive labels in S_b. This identifies the labels of all the points in S_b using $O(\log(1/\epsilon))$ queries.

2. Of the points in S_b, half are labeled positively and half negatively. Moreover, there are n_1, n_2 and $y \in \{-1,1\}$ such that $b_{n_1},\ldots,b_{n_2}$ are all labeled by y, and $n_2 - n_1 + 1 = |S_b|/2 = \frac{1}{2\epsilon}$ (see illustration in Figure 10). Let $n_3 = \frac{n_2+n_1}{2}$ (this is the middle point with label y). n_3 is an integer because $n_2 - n_1$ is even, thus their sum is also even. Let $n_4 = \mod(n_3 + 1/2\epsilon, 1/2\epsilon)$. Query the points a_{n_3} and a_{n_4} for their label.

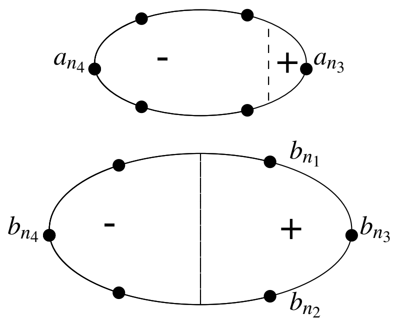


Figure 10: Illustration for the proof of Theorem 20.

3. If a_{n_3} and a_{n_4} each have a different label, apply a binary search starting from these points to find the boundaries between positive and negative labels in S_a, using $O(\log(1/\varepsilon))$ queries. Otherwise, label all the examples in S_a by the label of a_{n_3}.

This algorithm uses $O(\log(1/\varepsilon))$ queries to label the sample. If a_{n_3} and a_{n_4} have different labels, it is clear that the algorithm labels all the examples correctly. We only have left to prove that if they both have the same label, then all the examples in S_a also share that label. Let h^* be the true hypothesis, defined by some homogeneous separator, and assume w.l.o.g that $\{b_n \mid h^*(b_n) = 1\} = \{b_n \in S_b \mid b_n[1] > 0\}$ (note that no point has $b_n[1] = 0$ since $1/2\varepsilon$ is odd). It follows that $n_3 = 0$ and $n_4 = 1/2\varepsilon$, thus $a_{n_3} = (1/\sqrt{2}, 0, 1/\sqrt{2})$ and $a_{n_4} = (-1/\sqrt{2}, 0, 1/\sqrt{2})$ (see illustration in Figure 10). We use the following lemma, whose proof can be found in Appendix D:

Lemma 35 *Assume* $1/2\varepsilon$ *is odd. If* $\{b_n \in S_b \mid h^*(b_n) = 1\} = \{b_n \mid b_n[1] > 0\}$ *and* $h^*(a_0) = h^*(a_{1/2\varepsilon}) = y$ *then* $\forall a_n \in S_a, \quad h^*(a_n) = y$.

If follows that $\mathrm{OPT}_{\max} = O(\log(1/\varepsilon))$.

To bound the label complexity of ALuMA, it suffices to bound from below the minimal margin of possible separators over the given sample. Let h^* be the correct hypothesis. By the same argument as in the proof of Lemma 10, there exists some $w \in \mathbb{R}^3$ that labels the sample identically to h^* and attains its maximal margin on three linearly independent points a, b, c from our sample. Hence, $Aw = \mathbf{1}$ where $A \in \mathbb{R}^{3\times 3}$ is the matrix whose rows are $a, b, c \in S_a \cup S_b$. By Cramer's rule, for every $i \in [3]$

$$w[i] = \frac{\det A_i}{\det A},$$

where A_i is the matrix obtained from A by replacing the ith column with the vector $\mathbf{1}$. Recall that the absolute value of the determinant of A is the volume of the parallelepiped whose sides are a, b and c. Since a, b, c are linearly independent, each of S_a and S_b includes at most two of them. Assume that $a, b \in S_a$ and $c \in S_b$. In this case, the surface area of the basis of this parallelepiped, defined by a and b, is at least $\frac{\sin 2\pi\varepsilon}{\sqrt{2}}$, and the height is $1/\sqrt{2}$. Hence,

$$|\det A| \geq \frac{\sin 2\pi\varepsilon}{2} = \Omega(\varepsilon) .$$

The case where two of the points are in S_b leads to an even larger lower bound. Since the elements in each A_i are in $[-1, 1]$, we also have that $|\det A_i| \leq 3! = 6$. Thus, for $i \in [3]$ we obtain that $w_i = O(1/\varepsilon)$. All in all, we get $\|w\|_2 = O(1/\varepsilon)$, and thus $\gamma(h^*) = \Omega(\varepsilon)$. Applying Corollary 9, we obtain that ALuMA classifies all the points correctly using $O(\log(1/\gamma(h^*)) \cdot \mathrm{OPT}_{\max}) = O(\log^2(1/\varepsilon))$ labels.

Finally, we prove claim (3). CAL examines the examples sequentially at a random order, and queries the label of any point whose label is not determined by previous examples. Thus, if the true hypothesis is all-positive on S_a, and CAL sees all the points in S_a before seeing any point in S_b, it will request $\Omega(1/\varepsilon)$ labels. Hence, it suffices to show that there is a large probability that CAL will indeed examine all of S_a before examining any point from S_b. Let A be the event that the first $\frac{1}{\varepsilon}\log\frac{4}{\varepsilon}$ examples of an i.i.d. sample contain any element from S_b. Then, by the union bound, $\mathbb{P}(A) \le \frac{1}{\varepsilon}\log(\frac{4}{\varepsilon}) \cdot \frac{\varepsilon}{4\log\frac{4}{\varepsilon}} = 1/4$. Assume now that A does not occur. Let B be the event that the first $\frac{1}{\varepsilon}\log\frac{1}{\varepsilon}$ examples do not contain all the elements in S_a. Then, by the union bound, $\mathbb{P}(B) \le \frac{1}{\varepsilon}(1-\varepsilon)^{\frac{1}{\varepsilon}\log\frac{4}{\varepsilon}} \le 1/4$. All in all, with probability at least $1/2$, CAL see all the points in S_a before seeing any point in S_b and thus its label complexity is $\Omega(1/\varepsilon)$. ■

Appendix D. Other Proofs

In this section we provide proofs omitted from the text.

Proof [of Lemma 8] Fix $h \in \mathcal{W}$ and let $V = \{h' \in \mathcal{H} : \forall i, h'(x_i) = h(x_i)\}$. Assume w.l.o.g. that $\|x\| = 1$ for all $x \in X$. Denote for brevity $\gamma = \gamma(h)$. Choose $w \in \mathbb{B}_1^d$ such that $\forall x \in X, h(x)\langle w,x\rangle \ge \gamma$. For a given $v \in \mathbb{B}_1^d$, denote by $h_v \in \mathcal{H}$ the mapping $x \mapsto \operatorname{sgn}(\langle v,x\rangle)$. Note that for all $v \in \mathbb{B}_1^d$ such that $\|w-v\| < \gamma$, $h_v \in V$. This is because for all $x \in X$,

$$h(x)\langle v,x\rangle = \langle v-w, h(x)\cdot x\rangle + h(x)\langle w,x\rangle \ge -\|w-v\|\cdot\|h(x)\cdot x\| + \gamma > -\gamma+\gamma = 0,$$

Since $h_v(x) = \operatorname{sgn}(\langle v,x\rangle)$ it follows that $h_v(x) = h(x)$. We conclude that $\{v \mid h_v \in V\} \supseteq \mathbb{B}_1^d \cap B(w,\gamma)$, where $B(z,r)$ denotes the ball of radius r with center at z. Let $u = (1-\gamma/2)w$. Then for any $z \in B(u,\gamma/2)$, we have $z \in \mathbb{B}_1^d$, since

$$\|z\| = \|z-u+u\| \le \|z-u\| + \|u\| \le \gamma/2 + 1 - \gamma/2 = 1.$$

In addition, $z \in B(w,\gamma)$ since

$$\|z-w\| = \|z-u+u-w\| \le \|z-u\| + \|u-w\| \le \gamma/2 + \gamma/2 = \gamma.$$

Therefore $B(u,\gamma/2) \subseteq \mathbb{B}_1^d \cap B(w,\gamma)$. We conclude that $\{v \mid h_v \in V\} \supseteq B(u,\gamma/2)$. Thus,

$$P(h) = P(V) \ge \operatorname{Vol}(B(u,\gamma/2))/\operatorname{Vol}(\mathbb{B}_1^d) \ge \left(\frac{\gamma}{2}\right)^d.$$

■

Proof (of Lemma 10) Let us multiply all examples in the pool by $1/c$. Then, all the elements of all examples in the pool are integers. Choose a labeling L which is consistent with some w^*. Consider the optimization problem:

$$\min_w \|w\|^2 \text{ s.t. } \forall i,\ L(i)\langle w,x_i\rangle \ge 1 .$$

For simplicity assume that the pool of examples span all of $\mathbb{R}^d$. Then, it is easy to show that if w the solution to the above problem then there exist d linearly independent examples from the pool, denoted w.l.o.g. by $x_1,\ldots,x_d$, such that $L(i)\langle w,x_i\rangle = 1$ for all i. In other words, w is the solution of the linear system $Aw = b$ where the rows of A are $x_1,\ldots,x_d$ and $b = (L(1),\ldots,L(m))^T$.

By Cramer's rule, $w_i = \det(A_i)/\det(A)$, where A_i is obtained by replacing column i of A by the vector b. Since all elements of A are integers and A is invertible, we must have that $|\det(A)| \ge 1$. Therefore, $|w_i| \le |\det(A_i)|$. Furthermore, by Hadamard's inequality, $|\det(A_i)|$ is upper bounded by the product of the norms of the columns of A_i. Since each element of A_i is upper bounded by $1/c$, we obtain that the norm of each column is at most $\frac{\sqrt{d}}{c}$, hence $|\det(A_i)| \le (\sqrt{d}/c)^d$. It follows that $\|w\| \le \sqrt{d}\,(\sqrt{d}/c)^d$. Hence, the margin is

$$\frac{1}{\|w\|\max_i\|x_i\|} \ge \frac{1}{\sqrt{d}\,(\sqrt{d}/c)^d\cdot\sqrt{d}/c} = \frac{1}{\sqrt{d}\,(\sqrt{d}/c)^{d+1}} .$$

■

Proof (of Theorem 11) Set $m = \lfloor \ln(1/\gamma) \rfloor$ such that m is a power of 2. Let $x'_0 = (1,0) \in \mathbb{R}^2$. For all $i \in [m-1]$, define $x'_i = (\cos(\pi/2^i), \sin(\pi/2^i))$. Fix $c > 0$, and define $S = \mathbb{B}^2_1 \cap \{-1, -1+c, \ldots, 1-c, 1\}^2$. For each $i \in \{0,1,\ldots,m-1\}$, let x_i be the nearest neighbor of x'_i in S, that is $x_i = \arg\min_{x \in S} \|x - x'_i\|_2$. It can be easily seen that if $c = \Theta(\gamma)$ then $\forall i$, $\|x_i - x'_i\| = O(\gamma)$.

Consider an exact greedy algorithm that always selects x_0 first (this is possible since on the first round of the algorithm, any query halves the version space). Suppose that the target hypothesis h^* satisfies

$$h^*(x_i) = \begin{cases} -1 & i = 0 \\ 1 & \text{otherwise} \end{cases}$$

By setting a small enough c we get that $\gamma(h^*) = \Omega(\gamma)$.

If c is small enough compared to γ, then after querying x_0 the algorithm will query $x_1, \ldots, x_{m-1}$ in order. In addition, on every round $t < m-1$ the majority vote would lead to the wrong labeling, since only a small fraction of the version space belongs to the correct hypothesis. Thus the algorithm queries all the examples (except perhaps one) before reaching the correct answer. ■

Proof [of Lemma 35] We prove the lemma for the case $h^*(a_{1/2\varepsilon}) = 1$. The case $h^*(a_0) = -1$ can be proved similarly. Let w^* be any hyperplane which is consistent with h^*. Let $n_1 = \frac{1}{4\varepsilon} - \frac{1}{2}$ and let $n_2 = n_1 + 1$. Then

$$\begin{aligned} b_{n_1} &= (\cos(\pi/2 - \pi\varepsilon), \sin(\pi/2 - \pi\varepsilon), 0), \text{ and} \\ b_{n_2} &= (\cos(\pi/2 + \pi\varepsilon), \sin(\pi/2 + \pi\varepsilon), 0). \end{aligned}$$

By the assumption of the lemma, $\langle w^*, b_{n_1} \rangle > 0$ and $\langle w^*, b_{n_2} \rangle < 0$. It follows that $w^*[1]\sin\pi\varepsilon > w^*[2]\cos\pi\varepsilon$ and $-w^*[1]\sin\pi\varepsilon < w^*[2]\cos\pi\varepsilon$. As a consequence, we obtain that $|w^*[2]| < w^*[1]\tan(\pi\varepsilon)$.

Now, choose some $n \in \{0, \ldots, 1/\varepsilon - 1\}$. We show that the corresponding element in S_a is labeled positively. First, from the last inequality, we obtain

$$\begin{aligned} \langle w^*, a_n \rangle &= \frac{1}{\sqrt{2}} \langle w^*, (\cos 2\pi\varepsilon n, \sin 2\pi\varepsilon n, 1) \rangle \\ &\geq \frac{1}{\sqrt{2}} (w^*_1(\cos 2\pi\varepsilon n - \tan(\pi\varepsilon)\sin(2\pi\varepsilon n)) + w^*_3). \end{aligned} \tag{12}$$

We will now show that

$$\forall n \in \{0,1,\ldots,1/\varepsilon - 1\}, \ \cos 2\pi\varepsilon n - \tan(\pi\varepsilon)\sin(2\pi\varepsilon n) \geq -1. \tag{13}$$

From symmetry, it suffices to prove this for every $n \in \{0,1,\ldots,1/(2\varepsilon)-1\}$. We divide our range and conclude for each part separately; since $\varepsilon < 1/8$, we have that $\tan\varepsilon\pi < 1$. Then, $\cos\alpha - \tan(\pi\varepsilon)\sin\alpha \geq -1$ in the range $\alpha \in [0, \pi/2]$. For $\alpha \in [\pi/2, \pi - \pi\varepsilon]$, it can be shown that the function $\cos\alpha - \tan(\pi\varepsilon)\sin\alpha$ is monotonically decreasing, thus it suffices to show that the inequality holds for $n = 1/(2\varepsilon) - 1$. Indeed,

$$\begin{aligned} \cos(\pi - 2\varepsilon\pi) - \tan(\varepsilon\pi)\sin(\pi - 2\varepsilon\pi) &= -\cos(2\pi\varepsilon) - 2\sin^2(\pi\varepsilon) \\ &= -\cos^2(\pi\varepsilon) - \sin^2(\pi\varepsilon) \\ &= -1 \,. \end{aligned}$$

Therefore, we obtain from Equation (12) and Equation (13) that

$$\frac{1}{\sqrt{2}} \langle w^*, a_n \rangle \geq \frac{1}{\sqrt{2}} (-w^*[1] + w^*[3]) = \langle w^*, (-1/\sqrt{2}, 0, 1/\sqrt{2}) \rangle = \langle w^*, a_{1/2\varepsilon} \rangle > 0,$$

where the last inequality follows from the assumption that $h^*(a_{1/2\varepsilon}) = 1$. ■

References

D. Angluin. Queries and concept learning. *Machine Learning*, 2(4):319–342, 1988.

E. M. Arkin, H. Meijer, J.S.B. Mitchell, D. Rappaport, and S.S. Skiena. Decision trees for geometric models. In *Proceedings of the Ninth Annual Symposium on Computational Geometry*, pages 369–378. ACM, 1993.

M. F. Balcan, A. Beygelzimer, and J. Langford. Agnostic active learning. In *Proceedings of the 23rd International Conference on Machine Learning*, pages 65–72. ACM, 2006a.

M. F. Balcan, A. Blum, and S. Vempala. Kernels as features: On kernels, margins, and low-dimensional mappings. *Machine Learning*, 65(1):79–94, 2006b.

M. F. Balcan, A. Broder, and T. Zhang. Margin based active learning. *Learning Theory*, pages 35–50, 2007.

A. Beygelzimer, S. Dasgupta, and J. Langford. Importance weighted active learning. In *Proceedings of the 26th Annual International Conference on Machine Learning*, pages 49–56. ACM, 2009.

J. Bourgain. On lipschitz embedding of finite metric spaces in hilbert space. *Israel Journal of Mathematics*, 52(1):46–52, 1985.

G. Brightwell and P. Winkler. Counting linear extensions is #p-complete. In *Proceedings of the Twenty-third Annual ACM Symposium on Theory of Computing*, STOC '91, pages 175–181, 1991.

D. Cohn, L. Atlas, and R. Ladner. Improving generalization with active learning. *Machine Learning*, 15(2): 201–221, 1994.

S. Dasgupta. Analysis of a greedy active learning strategy. *Advances in Neural Information Processing Systems*, 17:337–344, 2005.

S. Dasgupta. Coarse sample complexity bounds for active learning. *Advances in Neural Information Processing Systems*, 18:235, 2006.

S. Dasgupta, A. Kalai, and C. Monteleoni. Analysis of perceptron-based active learning. *Learning Theory*, pages 889–905, 2005.

S. Dasgupta, D. Hsu, and C. Monteleoni. A general agnostic active learning algorithm. *Advances in Neural Information Processing Systems*, 20:353–360, 2007.

R. El-Yaniv and Y. Wiener. Active learning via perfect selective classification. *The Journal of Machine Learning Research*, 13:255–279, 2012.

Y. Freund, H.S. Seung, E. Shamir, and N. Tishby. Selective sampling using the query by committee algorithm. *Machine Learning*, 28(2):133–168, 1997.

E. Friedman. Active learning for smooth problems. In *Proceedings of the 22nd Conference on Learning Theory*, volume 1, pages 3–2, 2009.

R. Gilad-Bachrach, A. Navot, and N. Tishby. Query by committee made real. *Advances in Neural Information Processing Systems (NIPS)*, 19, 2005.

D. Golovin and A. Krause. Adaptive submodularity: A new approach to active learning and stochastic optimization. In *Proceedings of International Conference on Learning Theory (COLT)*, 2010.

S. Hanneke. A bound on the label complexity of agnostic active learning. In *The 24th Annual International Conference on Machine Learning (ICML)*, 2007.

S. Hanneke. Rates of convergence in active learning. *The Annals of Statistics*, 39(1):333–361, 2011.

J. Håstad. On the size of weights for threshold gates. *SIAM Journal on Discrete Mathematics*, 7:484, 1994.

W. Johnson and J. Lindenstrauss. Extensions of lipschitz mapping into hilbert space. *Contemporary Mathematics*, 26:189–206, 1984.

R. Kannan, L. Lovász, and M. Simonovits. Random walks and an $o*(n^5)$ volume algorithm for convex bodies. *Random Structures and Algorithms*, 11(1):1–50, 1997.

L. Lovász. Hit-and-run mixes fast. *Mathematical Programming*, 86(3):443–461, 1999.

J. Matoušek. *Lectures on Discrete Geometry*, volume 212. Springer Verlag, 2002.

A. McCallum and K. Nigam. Employing em in pool-based active learning for text classification. In *Proceedings of ICML-98, 15th International Conference on Machine Learning*, pages 350–358, 1998.

S. Muroga, I. Toda, and S. Takasu. Theory of majority decision elements. *Journal of the Franklin Institute*, 271(5):376–418, 1961.

S. Sabato, N. Srebro, and N. Tishby. Tight sample complexity of large-margin learning. In *Advances in Neural Information Processing Systems 23 (NIPS)*, pages 2038–2046, 2010.

H. S. Seung, M. Opper, and H. Sompolinsky. Query by committee. In *Proceedings of the Fifth Annual Workshop on Computational Learning Theory*, pages 287–294. ACM, 1992.

C. E. Shannon. Probability of error for optimal codes in a gaussian channel. *Bell System Technical Journal*, 38:611–656, 1959.

S. Tong and D. Koller. Support vector machine active learning with applications to text classification. *The Journal of Machine Learning Research*, 2:45–66, 2002.