Active Learning of Classifiers with Label and Seed Queries

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Abstract

We study exact active learning of binary and multiclass classifiers with margin. Given an n-point set $X \subset \mathbb{R}^m$, we want to learn any unknown classifier on X whose classes have finite *strong convex hull margin*, a new notion extending the SVM margin. In the standard active learning setting, where only *label* queries are allowed, learning a classifier with strong convex hull margin γ requires in the worst case $\Omega\big(1+\frac{1}{\gamma}\big)^{\frac{m-1}{2}}$ queries. On the other hand, using the more powerful *seed* queries (a variant of equivalence queries), the target classifier could be learned in $\mathcal{O}(m \log n)$ queries via Littlestone's Halving algorithm; however, Halving is computationally inefficient. In this work we show that, by carefully combining the two types of queries, a binary classifier can be learned in time $\mathrm{poly}(n+m)$ using only $\mathcal{O}(m^2 \log n)$ label queries and $\mathcal{O}\big(m \log \frac{m}{\gamma}\big)$ seed queries; the result extends to k-class classifiers at the price of a $k!k^2$ multiplicative overhead. Similar results hold when the input points have bounded bit complexity, or when only one class has strong convex hull margin against the rest. We complement the upper bounds by showing that in the worst case any algorithm needs $\Omega\big(\frac{km \log 1/\gamma}{\log m}\big)$ seed and label queries to learn a k-class classifier with strong convex hull margin γ.

1 Introduction

This work investigates efficient algorithms for exact active learning of binary and multiclass classifiers in the transductive setting. Given a set X of n points in $\mathbb{R}^m$, our goal is to learn a function $h : X \to [k]$ belonging to some class $\mathcal{H}$. In the classic active learning framework, h identifies a subset of X, and the algorithm learns h via queries $\textsc{label}(x)$ that return $h(x)$ for any given $x \in X$. In that case, it is well-known that h can be learned with $\mathcal{O}(\log n)$ $\textsc{label}$ queries if the *star number* of $\mathcal{H}$ is finite [Hanneke and Yang, 2015]. Unfortunately, even simple families such as linear classifiers have unbounded star number, in which case $\Omega(n)$ $\textsc{label}$ queries are needed in the worst case. To bypass this lower bound, it has become increasingly common to introduce *enriched queries*, that reveal additional information on h and are plausible in practice. One notable example is that of *comparison* queries for linear separators in $\mathbb{R}^m$ which, given any pair of points $x, y \in X$, reveal which one is closer to the decision boundary. As proven by Kane et al. [2017], under some margin assumptions the combination of $\textsc{label}$ and comparisons yields exponential savings, allowing one to learn linear separators with only $\mathcal{O}(\log n)$ queries.

In this work we combine $\textsc{label}$ queries with *seed queries*. For any $U \subset X$ and any $i \in [k]$, a query $\textsc{seed}(U, i)$ returns an abitrary point x in $U \cap C_i$, where $C_i = h^{-1}(i)$, or $\textsc{nil}$ if no such x exists. $\textsc{seed}$ queries are natural in certain settings like crowdsourcing—e.g., finding the image of a car, see also Beygelzimer et al. [2016]—and have been used implicitly or explicitly in several works [Hanneke, 2009, Balcan and Hanneke, 2012, Attenberg and Provost, 2010, Tong and Chang,

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2001, Doyle et al., 2011, Bressan et al., 2021b]. It is not hard to see that, using SEED alone, one can implement Littlestone's Halving algorithm and learn any $h \in \mathcal{H}$ with $\mathcal{O}(\log |\mathcal{H}|)$ queries[1]. For instance, linear separators in $\mathbb{R}^m$ can be learned with $\mathcal{O}(m \log n)$ SEED queries. The catch is that, save for special cases, it is not known how to run the Halving algorithm in polynomial time. Therefore, using SEED to obtain a computationally efficient active learning algorithm is less trivial than it seems at first glance.

The goal of this work is understanding whether one can actively learn binary and multiclass classifiers efficiently by using LABEL and SEED queries together. In line with Kane et al. [2017] and other previous works, we make assumptions on $\mathcal{H}$. Our main assumption is that every class C_i has *strong convex hull margin* $\gamma > 0$. This means that, for any $j \neq i$, C_i and C_j are linearly separable with a margin that is at least $\frac{\gamma}{2}$ times the diameter of C_i. Moreover, it is sufficient that this hold under some pseudometric d_i, unknown to the learner, that is homogeneous and invariant under translation (i.e., induced by a seminorm). This gives to every class its own personalized notion of distance that can be sensitive to the "scale" of the class. This assumption strictly generalizes the classical SVM margin; and, when suitably generalized, it captures stability properties of center-based clusterings Awasthi et al. [2012], Bilu and Linial [2012].

Using LABEL alone, Bressan et al. [2021a] showed that learning a multiclass classifier with (strong) convex hull margin $\gamma > 0$ requires between $\Omega\big(1+\frac{1}{\gamma}\big)^{(m-1)/2}$ and $\tilde{\mathcal{O}}\big(k^3 m^5 \big(1+\frac{1}{\gamma}\big)^m \log n\big)$ queries. This exponential dependence on m implies that, unless $m \ll \log n / \log \frac{1}{\gamma}$, one needs $\Theta(n)$ LABEL queries in the worst case. On the other hand our margin implies linear separability and thus, as noted above, a $\mathcal{O}(m \log n)$ SEED query bound for the binary case, but with a running time that can be superpolynomial. This leaves open the following problem, which is the subject of this work:

> Can one learn a multiclass classifier h with strong convex hull margin $\gamma > 0$ on $X \subset \mathbb{R}^m$ in time $\mathrm{poly}(n+m)$ using a number of queries that grows *polynomially* with m?

We solve the above question in the affirmative by proving that, with a careful combination of LABEL and SEED queries, one can do much better than using either query in isolation. For binary classification ($k = 2$), we show:

Theorem 1. *Any binary classifier h with strong convex hull margin $\gamma > 0$ over $X \subset \mathbb{R}^m$ can be learned in time $\mathrm{poly}(n+m)$ using in expectation $\mathcal{O}(m^2 \log n)$ LABEL queries and $\mathcal{O}\big(m \log \frac{m}{\gamma}\big)$ SEED queries.*[2]

Note that, unless γ is exceedingly small, Theorem 1 uses far fewer SEED than LABEL queries, which is a strength since SEED is arguably more expensive to implement. For instance, if $\gamma = \Omega(1/\mathrm{poly}(m))$ then we use $\mathcal{O}(m^2 \log n)$ LABEL queries but only $\mathcal{O}(m \log m)$ SEED queries. To prove Theorem 1 we design a novel algorithm that works in two phases. The first phase learns what we call an α-*rounding* of X w.r.t. h. Loosely speaking, this is a partition (X_1, X_2) of X such that each X_i lies inside $\alpha\,\mathrm{conv}(C_i)$ where $\mathrm{conv}(C_i)$ is the convex hull of C_i (see below for the formal definition). We show that, in polynomial time and using $\mathcal{O}(m^2 \log n)$ LABEL queries, one can compute an α-rounding of X_i for $\alpha = \mathcal{O}(m^3)$. This allows us to put X_i in near-isotropic position so that X_i has radius 1 and to separate $C_1 \cap X_i$ from $C_2 \cap X_i$ with margin $\eta = \Omega(\gamma/m^3)$. In the second phase, the algorithm uses SEED to implement a cutting plane algorithm that learns $C_1 \cap X_i$ and $C_2 \cap X_i$ using $\mathcal{O}\big(m \log \frac{1}{\eta}\big) = \mathcal{O}\big(m \log \frac{m}{\gamma}\big)$ queries in time $\mathrm{poly}(n+m)$.

Using a recursive approach, Theorem 1 can be extended to $k > 2$ at the price of a $k!k^2$ multiplicative overhead:

Theorem 2. *Any k-class classifier h with strong convex hull margin $\gamma > 0$ over $X \subset \mathbb{R}^m$ can be learned in time $\mathrm{poly}(n+m)$ using in expectation $\mathcal{O}(k!\ k^2 m^2 \log n)$ LABEL queries and $\mathcal{O}\big(k!\ k^2\, m \log \frac{m}{\gamma}\big)$ SEED queries.*

[1] Halving uses equivalence queries (testing if a given subset of X coincides with the target concept) each of which can be simulated using two SEED queries.

[2] This running time as well as those of Theorem 2 and 3 are actually in high probability as implied by Theorem 10; we have omitted this fact to keep the statements light.

We also consider the case where only one class has strong convex hull margin against the rest of the points w.r.t. a metric d induced by a norm $\|\cdot\|_d$. In this case we obtain a bound parameterized by the distortion κ_d of d (see Section 1.1):

Theorem 3. *Suppose $C \subset X$ has strong convex hull margin $\gamma \in (0,1]$ w.r.t. a metric d with distortion $\kappa_d < \infty$. Given only X, one can learn C in time $\mathrm{poly}(n+m)$ using $\mathcal{O}(\log n)$ LABEL queries and $\mathcal{O}\big(m \log \frac{\kappa_d}{\gamma}\big)$ SEED queries in expectation.*

As an application of our cutting-plane algorithm we also show that one can learn a k-class classifier whose classes are pairwise linearly separable in time $\mathrm{poly}(n+m)$ using, in expectation, $\mathcal{O}(k^2 m^3 B)$ SEED queries if every $x \in X$ has rational coordinates that can be encoded in B bits, and $\mathcal{O}(k^2 m(B + m \log m))$ SEED queries if every $x \in X$ lies on the grid over $[-1,1]^m$ with stepsize $2^{-B/m}$. It should be noted that, unlike most previous algorithms, all our algorithms do not need knowledge of γ. Moreover, all the bounds above can be turned from expectation to high probability.[3]

Finally, we show that the algorithms of Theorem 1 and 2 are nearly optimal:

Theorem 4. *For all $m \geq 2$, all $k \geq 2$, and all $\gamma \leq m^{-3/2}/16$ there exists a distribution of instances with k classes in $\mathbb{R}^m$ with strong convex hull margin γ where any randomized algorithm using* SEED *and* LABEL *queries that returns $\mathcal{C}$ with probability at least $\frac{1}{2}$ makes at least $\lfloor \frac{k}{2} \rfloor \frac{m}{24 \log m} \log \frac{1}{2\gamma}$ total queries in expectation.*

1.1 Preliminaries and notation

The input to our problem is a pair (X,k), where $X \subset \mathbb{R}^m$ and $k \in \mathbb{N}$ with $2 \leq k \leq n = |X|$. The algorithm has access to oracles O_{LABEL} and O_{SEED} which provide respectively LABEL and SEED queries. The oracles $O_{\text{LABEL}}, O_{\text{SEED}}$ behave consistently with some target classifier $h : X \to [k]$. For any $x \in X$, $\text{LABEL}(x)$ returns $h(x)$. For any $U \subseteq X$ and any $i \in [k]$, $\text{SEED}(U,i)$ returns an abitrary element $x \in U \cap C_i$ if $U \cap C_i \neq \emptyset$, and NIL otherwise, where $C_i = h^{-1}(i)$. We often think of h as of the partition $\mathcal{C} = (C_1, \ldots, C_k)$ and we call each C_i a *class* or *cluster*.

A pseudometric is a symmetric and subadditive function $d : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}_{\geq 0}$ such that $d(x,x) = 0$ for all $x \in \mathbb{R}^m$; unlike a metric, $d(x,y)$ need not be 0 for $x \neq y$. In this work d is always induced by a seminorm and thus homogeneous and invariant under translation: $d(u+ax, u+ay) = |a|\, d(x,y)$ for all $x,y,u \in \mathbb{R}^m$ and all $a \in \mathbb{R}$. For a pseudometric d and a set $A \subset \mathbb{R}^m$, we let $\phi_d(A) = \sup\{d(x,y) : x,y \in A\}$ denote the diameter of A under d. For $x \in \mathbb{R}^m$ and $r \geq 0$ we denote by $B_d^m(x,r)$ and $S_d^{m-1}(x,r)$ respectively the closed ball and the hypersphere with center x and radius r in $\mathbb{R}^m$ under d. When d is omitted we assume $d = d_{\text{euc}}$ where d_{euc} is the Euclidean metric. We may also omit the superscript if clear from the context. The distortion of a (pseudometric) d is $\kappa_d = \sup_{u,v \in S^{m-1}(0,1)} \|u\|_d / \|v\|_d$.

For any set $A \subset \mathbb{R}^m$, any $\mu \in \mathbb{R}^m$, and any $\lambda > 0$, let $\sigma(A,\mu,\lambda) = \mu + \lambda(A - \mu)$ be the scaling of A about μ by a factor of λ. For two sets $A, B \subset \mathbb{R}^m$, we write $A \leq \lambda B$ if $A \subseteq \sigma(B,z,\lambda)$ for some $z \in \mathbb{R}^m$. We may use x in place of A if $A = \{x\}$. If A is bounded, then $\mathrm{MVE}(A)$ denotes the minimum-volume enclosing ellipsoid (MVEE, or Löwner-John ellipsoid) of A. Our proofs repeatedly use John's theorem; that is, $\sigma(E,\mu,1/m) \subseteq \mathrm{conv}(A)$ where μ is the center of $E = \mathrm{MVE}(A)$ and $\mathrm{conv}(A)$ is the convex hull of A. Given $A, B \subseteq \mathbb{R}^m$, we say that A and B are linearly separable with margin r if there exist $u \in S^{m-1}(0,1)$ and $b \in \mathbb{R}$ such that $\langle u, x\rangle + b \leq -r$ for all $x \in A$ and $\langle u, x\rangle + b \geq r$ for all $x \in B$.

We consider classifiers satisfying the following property:[4]

Definition 5. *A class C_i has strong convex hull margin $\gamma > 0$ if there exists a pseudometric d_i induced by a seminorm over $\mathbb{R}^m$ such that $d_i(\mathrm{conv}(C_j), \mathrm{conv}(C_i)) > \gamma\, \phi_{d_i}(C_i)$ for all $j \in [k] \setminus \{i\}$. If this holds for all $i \in [k]$ then we say $\mathcal{C}$ has strong convex hull margin γ.*

Remarks. The margin of Definition 5 captures natural scenarios that SVM margin does not. For instance, suppose we are clustering fruits on the basis of weight and colour. First, a fruit weighting

[3] Formally, for some universal constant $a > 0$, each one of our bounds in the form $\mathbb{E}[Q] \leq q$, where Q is the number of queries, implies $\Pr(Q \geq q + \epsilon q) \leq \exp(-a\epsilon q)$ for all $\epsilon \geq 0$.

[4] Actually, all our upper bounds hold under a weaker condition: that for every i and every $j \in [k] \setminus \{i\}$ there is a d_{ij} giving the margin.

more than, say, 1.5 times the typical weight of a species probably does not belong to it; but the typical weight varies greatly across species. Our margin captures this scenario, as it is expressed as a fraction of the class' diameter. Second, different fruit species have different separating features; for instance, weight does not separate well oranges from bananas, but colour does. Our margin captures this aspect, too, by allowing the metric that determines the margin to be a function the class. It is also known that the SVM margin γ_{SVM} can be arbitrarily smaller than γ; for instance there are simple cases with $\gamma > 1$ but $\gamma_{\text{SVM}} < e^{-n}$ (see Bressan et al. [2021a]). Hence a large γ does not imply good bounds for standard algorithms based on SVM margin (e.g., the Perceptron).

2 Related work

It is well known that active learning may achieve exponential savings in label complexity. That is, there are natural concept classes that can be learned with a number of LABEL queries exponentially smaller than that of passive learning. Hanneke and Yang [2015] characterize the label complexity of concept classes in terms of their star number. However, the star number of many natural classes such as linear classifiers is unbounded, implying a strong lower bound of $\Omega(n)$ LABEL queries.

This and other negative results motivated research on enriched queries. Kane et al. [2017] prove that active learnability is characterized by the inference dimension of the concept class $\mathcal{H}$ under the set of allowed queries $\mathcal{Q}$, as long as those queries are local (i.e., are a function of a constant number of instances). This yields exponential savings when $\mathcal{H}$ is the class of linear separators and $\mathcal{Q}$ contains label queries and comparison queries (which, given two points, reveal which one is closer to the decision boundary), provided the classes have SVM margin or bounded bit complexity. Hopkins et al. [2020] give similar results under distributional assumptions. Unfortunately, bounded inference dimension does not automatically yield efficient algorithms, although it implies active learning algorithms with bounded memory [Hopkins et al., 2021].

SEED and their variants are motivated and used by Hanneke [2009] as *positive example queries*, by Balcan and Hanneke [2012] as *conditional class queries*, and by Beygelzimer et al. [2016], Attenberg and Provost [2010] as *search queries*. They are also used implicitly by Tong and Chang [2001], Doyle et al. [2011], and Vikram and Dasgupta [2016]. SEED queries have been used in cluster recovery [Bressan et al., 2021b] and yield exponential savings in non-realizable learning settings [Balcan and Hanneke, 2012]. It also easy to see that SEED queries are equivalent to *partial equivalence* queries of Maass and Turán [1992] and to *subset* plus *superset* queries of Angluin [1988]. To the best of our knowledge, no work combines LABEL and SEED as we do here.

Little is known about the SEED complexity of learning a concept class $\mathcal{H}$ actively in polynomial time. On the one hand, the inference dimension lower bounds of Kane et al. [2017] are inapplicable, as SEED queries are not local. On the other hand the Littlestone dimension of $\mathcal{H}$ yields an upper bound, but not necessarily an efficient algorithm; in fact, it is well known that (some sub-problem solved by) Halving is hard in general, see Gonen et al. [2013]. For $k = 2$, we can use SEED emulate *equivalence* queries, for which polynomial-time algorithms are known in some special cases. In particular, the algorithm of Maass and Turán [1994] could replace our cutting-planes subroutine under an implicit discretization of the space through a grid with step-size $\mathcal{O}(\gamma/m^4)$. However, this gives a polynomial-time algorithm that uses $\mathcal{O}(m^2 \log m/\gamma)$ SEED queries, which is $\mathcal{O}(m)$ times our bound. Moreover, Maass and Turán [1994] use *proper* equivalence queries (i.e., the queried concept must be in the class), for which they show a lower bound of $\Omega(m^2 \log m/\gamma)$. Finally, these techniques do not seem to extend to the case $k > 2$.

Our notion of margin strengthens the convex hull margin of Bressan et al. [2021a] by requiring $d(\text{conv}(C_j), \text{conv}(C_i)) > \gamma\phi(C_i)$ rather than $d(C_j, C_i) > \gamma\phi(C_i)$. It is not hard to see that the convex hull margin can be arbitrarily smaller than our strong convex hull margin. Finally, the polytope margin of Gottlieb et al. [2018] assumes that each class is in the intersection of a finite number of halfspaces with margin. It is easy to see that this condition is strictly stronger than ours.

3 Upper Bounds

This section gives the proofs of Theorem 1 and Theorem 2. The algorithm behind both theorems has two phases which are described in the next subsections. The case $k > 2$ is essentially the same as for $k = 2$, except for an adaptation in the second phase.

3.1 The First Phase: Rounding the Classes

The first phase of our algorithms learns what we call an α-rounding of X.

Definition 6. *An α-rounding of X (w.r.t. h) is a sequence of pairs $((X_i, E_i))_{i\in[k]}$ where $(X_i)_{i\in[k]}$ is a partition of X, and where E_i for $i \in [k]$ is an ellipsoid such that $X_i \subseteq E_i$ and $E_i \leq \alpha \operatorname{conv}(C_i)$.*

The idea is that, if $((X_i, E_i))_{i\in[k]}$ is an α-rounding of X, then E_i gives an approximation of the pseudometric d_i witnessing the strong convex hull margin of C_i. Indeed, let p_i be the pseudometric induced by E_i, the one such that $E_i = B_{p_i}(\mu_i, 1)$ where μ_i is the center of E_i; it is not hard to prove (see Appendix A):

Lemma 7. *If $((X_i, E_i))_{i\in[k]}$ is an α-rounding of X then $p_i(\operatorname{conv}(X_i \cap C_i), \operatorname{conv}(X_i \cap C_j)) \geq \frac{\gamma}{\alpha}$ for all distinct $i, j \in [k]$.*

We will use Lemma 7 in the second phase. First, we show how to compute an α-rounding of X efficiently. We sample points independently and uniformly at random from X until we find $\Theta(m^2)$ points S_i with the same label i. As the VC dimension of ellipsoids in $\mathbb{R}^m$ is $\mathcal{O}(m^2)$, by standard generalization error bounds with constant probability the MVE of S_i contains at least half of C_i. We then store that MVE together with the index i, remove S_i from X, and repeat until X becomes empty. At that point for each $i \in [k]$ we "merge" together all points in the MVEs that were computed for class i, and compute the MVE of this merged set. We show that this produces an α-rounding of X after $\mathcal{O}(k \log n)$ rounds in expectation.[5] The resulting algorithm Round is listed below; Figure 1 depicts its behaviour on a toy example.

Algorithm 1: $\mathrm{Round}(X, k)$

for $i \in [k]$ **do** $h_i \leftarrow 0$
while $X \neq \emptyset$ **do**
  draw points independently u.a.r. from X and LABEL them until for some $i \in [k]$ we draw a (multi)set of cm^2 points from C_i
  $h_i \leftarrow h_i + 1$
  $S_i^{h_i} \leftarrow$ the sample of cm^2 points from C_i
  $X_i^{h_i} \leftarrow X \cap \mathrm{MVE}(S_i^{h_i})$
  $X \leftarrow X \setminus X_i^{h_i}$
for $i \in [k]$ **do**
  $X_i \leftarrow X_i^1 \cup \ldots \cup X_i^{h_i}$ (set to $\emptyset$ if $h_i = 0$)
  $E_i \leftarrow \mathrm{MVE}(X_i)$ (set to $\emptyset$ if $X_i = \emptyset$)
return $((X_i, E_i))_{i\in[k]}$

Lemma 8. $\mathrm{Round}(X, k)$ *returns an $m^2(m+1)$-rounding of X in time $\mathrm{poly}(n+m)$ using $\mathcal{O}(k^2 m^2 \log n)$ LABEL queries in expectation.*

Proof. (*Sketch*) First we show that $E_i \leq m^2(m+1)\operatorname{conv}(C_i)$ for all $i \in [k]$. This is trivial if $E_i = \emptyset$, so let $E_i \neq \emptyset$ and let $\ell_i \geq 1$ be the value of h_i at return time. For every $h = 1, \ldots, \ell_i$ let $E_i^h = \mathrm{MVE}(S_i^h)$ and let μ_i^h be the center of E_i^h. Using John's theorem one can show that $\sigma\big(E_i, \mu_i, \frac{1}{m}\big) \subseteq \operatorname{conv} \bigcup_{h=1}^{\ell_i} \sigma\big(\operatorname{conv}(S_i^h), \mu_i^h, m\big)$ and $\sigma\big(\operatorname{conv}(S_i^h), \mu_i^h, m\big) \subseteq \sigma(\operatorname{conv}(C_i), \mu, m(m+1))$. By taking the union over all $h \in [\ell_i]$ we conclude that $\sigma\big(E_i, \mu_i, \frac{1}{m}\big) \subseteq \sigma(\operatorname{conv}(C_i), \mu, m(m+1))$, that is, $E_i \leq m^2(m+1)\operatorname{conv}(C_i)$. It is also easy so see that $(X_i)_{i\in[k]}$ is a partition of X, hence $((X_i, E_i))_{i\in[k]}$ is an $m^2(m+1)$-rounding of X.

For the running time, the **for** loops perform $k \leq n$ iterations, and the **while** loop performs at most n iterations as each iteration strictly decreases the size of X. The running time of any iteration is dominated by the computation of $\mathrm{MVE}(S_i)$ or $\mathrm{MVE}(X_i)$, which takes time $\mathrm{poly}(n+m)$, see

[5] What we actually want is, given a finite set $S \subset \mathbb{R}^m$, an ellipsoid $\mathcal{E}$ such that $\frac{1}{(1+\epsilon)d}\mathcal{E} \subset \operatorname{conv}(S) \subset \mathcal{E}$. This can be computed in $\mathcal{O}(|S|^{3.5} \ln(|S|/\epsilon))$ operations in the real number model of computation, see Khachiyan [1996]. For simplicity however we just assume that we can compute $\mathcal{E} = \mathrm{MVE}(S)$ in polytime.

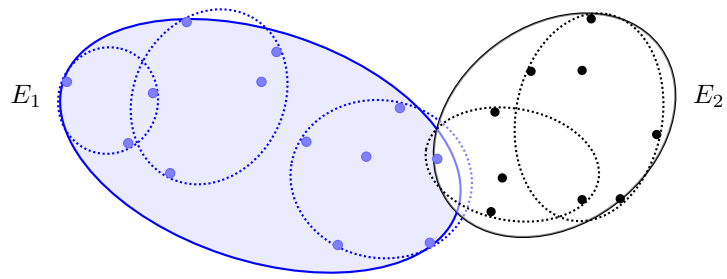

Figure 1: A toy example in $\mathbb{R}^2$ with $k = 2$; black points are in C_1, blue points in C_2. $\mathrm{Round}(X, 2)$ computes first the ellipsoids E_2^1, E_2^2 (dotted black, from left to right), and then the ellipsoids E_1^1, E_1^2, E_1^3 (dotted blue, from left to right). Finally it computes E_1 (solid blue) and E_2 (solid black). X_1 and X_2 consist of the points in the blue and white areas respectively. Note that X_2 contains a point of C_1.

above. Hence $\mathrm{Round}(X, k)$ runs in time $\mathrm{poly}(n + m)$. For the query bounds, the **while** loop makes $\mathcal{O}(m^2 k)$ LABEL queries per iteration. By standard generalization bounds, since the VC dimension of ellipsoids in $\mathbb{R}^m$ is $\mathcal{O}(m^2)$, E_i^h contains at least half of $X \cap C_i$ with probability at least $\frac{1}{2}$, and thus the expected number of rounds before X becomes empty is in $\mathcal{O}(k \lg n)$, see Bressan et al. [2021a]. We conclude that $\mathrm{Round}(X, k)$ uses $\mathcal{O}(m^2 k^2 \lg n)$ LABEL queries in expectation. □

3.2 The Second Phase: Finding a Separator via Cutting Planes

Let $((X_i, E_i))_{i \in [k]}$ be the output of $\mathrm{Round}(X, k)$, and fix $i \in [k]$. For each $j \in [k] \setminus \{i\}$, we want to separate $X_i \cap C_i$ from $X_i \cap C_j$. To this end, first we use E_i to perform a change of coordinates; this puts X_i inside the unit ball and ensures that $X_i \cap C_i$ and $X_i \cap C_j$ are linearly separated with margin $\gamma_{\text{SVM}} = \Omega(\gamma m^{-3})$. Next, by calling C_i the positive class $(+1)$ and C_j the negative class (-1), and letting $X = X_i$ for simplicity, one can reduce the task to the following problem. Consider a *partial* classifier $h : X \to \{+1, -1, *\}$. The algorithm has access to an oracle answering queries SEED(U, y) where $U \subseteq X$ and $y \in \{+1, -1\}$, and its goal is to compute a separator of X:

Definition 9. *Let $X \subset \mathbb{R}^m$ and $h : X \to \{+1, -1, *\}$. A* separator *of X (w.r.t. h) is a partition (X_+, X_-) of X such that, for every $x \in X$, if $h(x) = +1$ then $x \in X_+$ and if $h(x) = -1$ then $x \in X_-$.*

A separator of X can be learned, for instance, by the Perceptron (using SEED to find counterexamples). However, this would yield a query and running time bound of $\mathcal{O}(1/\gamma_{\text{SVM}}^2) = \mathcal{O}(m^6/\gamma^2)$. We provide CPLearn, a cutting-plane algorithm based on SEED that is much more query-efficient (in fact, near-optimal):

Theorem 10. *Let $X \subset \mathbb{R}^m$ and $h : X \to \{+1, -1, *\}$, and suppose $h^{-1}(+1)$ and $h^{-1}(-1)$ are linearly separable with margin r. Given X and access to* SEED *for labels $\{+1, -1\}$,* CPLearn(X) *computes a separator of X w.r.t. h using $\mathcal{O}(m \log \frac{R}{r})$* SEED *queries in expectation, where $R = \max_{x \in X} \|x\|_2$, and running with high probability*[6] *in time* $\mathrm{poly}(m + |X|)$.

Proof. (*Sketch*) First, we lift X to $\mathbb{R}^{m+1}$. This reduces the problem to finding a homogeneous linear separator. To this end we let $X' = \{x' : x \in X\}$ where x' is obtained by appending to x an $(m+1)$-th coordinate that is equal to R, and we extend h to X' in the obvious way. It is easy to prove that X' has radius at most $2R$ and that in X' the two classes are linearly separable with margin $\frac{r}{2}$.

Next, we learn a separator of X' w.r.t. h via cutting planes—see, e.g., Mitchell [2003]. Let $V_0 = B^{m+1}(0, 1)$. Every point $u \in V_0$ identifies the halfspace $H(u) = \{z \in \mathbb{R}^{m+1} : \langle u, z \rangle \geq 0\}$. For $i = 1, 2, \ldots$, V_i will be our version space, and we compute V_{i+1} from V_i as follows. Let μ_i be the center of mass of V_i, and let $X_i' = X' \cap H(\mu_i)$. By issuing SEED$(X_i', -1)$ and SEED$(X' \setminus X_i', +1)$ we learn whether $(X_i', X' \setminus X_i')$ is a separator of X' w.r.t. h, in which case we return the corresponding partition of X, or we obtain a point u_i. In the second case, we let $V_{i+1} = V_i \cap U_i$ where $U_i = \{x \in$

[6] This means that the running time can be brought in $\mathrm{poly}(m + |X|)$ with probability $1 - \exp(-(m + |X|))$.

$\mathbb{R}^{m+1} : h(u_i) \cdot \langle u_i, x \rangle \geq 0\}$. By [Gilad-Bachrach et al., 2004, Theorem 2] this procedure returns a separator of X' w.r.t. h using at most $\frac{2m}{\log \frac{e}{e-1}} \log \frac{4R}{r/2} = \mathcal{O}\big(m \log \frac{R}{r}\big)$ queries.

Unfortunately, computing μ_i is hard in general [Rademacher, 2007]. We instead compute an estimate $\hat{\mu}_i$ that, used in place of μ_i, ensures $\frac{\mathrm{vol}(V_{i+1})}{\mathrm{vol}(V_i)}$ is bounded away from 1 with high probability; the expected query bound follows by adapting the proof of [Gilad-Bachrach et al., 2004]. Assume for the moment that V_i is well-rounded—that is, it contains a ball of radius $r = \mathrm{poly}(m)$ and is contained in a ball of radius 1. To compute $\hat{\mu}_i$ we average over $\mathrm{poly}(n+m)$ independent uniform points from V_i, which can be draw efficiently thanks to the rounding condition. At this point we use $\hat{\mu}_i$ in place of μ_i to invoke SEED and obtain a violated constraint U_i. However, setting $V_{i+1} = V_i \cap U_i$ could make V_{i+1} far from rounded (too "thin"), making sampling inefficient at the next round. Therefore we rotate U_i so to obtain a weaker constraint U_i^*, one that still contains $V_i \cap U_i$ but that has $\hat{\mu}_i$ on its boundary, and let $V_{i+1} = V_i \cap U_i^*$. By the assumption on $\hat{\mu}_i$ this implies that $\mathrm{vol}(V_{i+1}) \geq \frac{1}{3}\,\mathrm{vol}(V_i)$; therefore by sampling uniform points from V_i we can obtain a large sample in V_{i+1}, from which we can put V_{i+1} in a rounding position. See the full proof for all the details. □

To the best of our knowledge, CPLearn is the first efficient algorithm that achieves the query upper bound of Theorem 10, even for the special case of SVM margin.

3.3 Wrap-Up

We wrap up our algorithms, starting with the case $k = 2$; the case $k \geq 2$ is slightly more involved.

Algorithm 2: $\mathrm{BinLearn}(X)$

$((X_1, E_1), (X_2, E_2)) \leftarrow \mathrm{Round}(X)$
for $i \leftarrow 1, 2$ **do**
  change system of coordinates so that E_i becomes the unit ball
  $(X_{i+}, X_{i-}) \leftarrow \mathrm{CPLearn}(X_i)$ with $h : X_i \to \{1, 2\}$
return $(X_{1+} \cup X_{2-}, X_{2+} \cup X_{1-})$

Theorem 11. *Suppose $k = 2$. Then $\mathrm{BinLearn}(X)$ returns $\mathcal{C} = (C_1, C_2)$ in time $\mathrm{poly}(n+m)$ using in expectation $\mathcal{O}(m^2 \log n)$ LABEL queries and $\mathcal{O}(m \log \frac{m}{\gamma})$ SEED queries.*

Proof. By Lemma 8, $\mathrm{Round}(X)$ runs in time $\mathrm{poly}(n+m)$, makes $\mathcal{O}(m^2 \log n)$ LABEL queries in expectation, and returns an $\mathcal{O}(m^3)$-rounding of X. It is immediate to see that, after the change of coordinates, X_i has radius $R \leq 1$, while $C_1 \cap X_1$ and $C_2 \cap X_1$ are separated linearly with margin $r = \Omega(\gamma m^{-3})$. By Theorem 10 then, $\mathrm{CPLearn}(X_i)$ returns the partition of X_i induced by h in time $\mathrm{poly}(|X_i| + m) = \mathrm{poly}(n+m)$ using $\mathcal{O}\big(m \log \frac{R}{r}\big) = \mathcal{O}\big(m \log \frac{m}{\gamma}\big)$ expected SEED queries. □

For $k \geq 2$ we proceed as follows. Let $\mathbf{k} = [k]$. We take X_i for each $i \in \mathbf{k}$ in turn, and for each $j \in \mathbf{k} \setminus i$, we use CPLearn to compute a separator for i, j in X_i. By intersecting the left side of all those separators we obtain $X_i \cap C_i$. Then we recurse on $X_i \setminus C_i$, updating $\mathbf{k}$ to $\mathbf{k} \setminus i$. The resulting algorithm KClassLearn is listed below and yields:

Theorem 12. $\mathrm{KClassLearn}(X, [k])$ *returns $\mathcal{C}$ in time $\mathrm{poly}(n+m)$ using in expectation $\mathcal{O}(k!k^2\, m^2 \log n)$ LABEL queries and $\mathcal{O}\big(k!k^2\, m \log \frac{m}{\gamma}\big)$ SEED queries.*

Proof. We adapt the proof of Theorem 11. Observe that $\mathrm{KClassLearn}(X, [k])$ makes at most $\min(k!, n)$ recursive calls; the n in the min comes from the fact that any given (recursive) call learns the label of at least one unlabeled point. Now, every (recursive) call makes one invocation to $\mathrm{Round}(X)$, which by Lemma 8 uses time $\mathrm{poly}(n+m)$ and $\mathcal{O}(k^2 m^2 \log n)$ LABEL queries, and $\mathcal{O}(k^2)$ invocations to $\mathrm{CPLearn}(X_i)$, each of which by Theorem 10 uses $\mathrm{poly}(n+m)$ time and $\mathcal{O}\big(m \log \frac{m}{\gamma}\big)$ SEED queries. □

Algorithm 3: $\mathrm{KClassLearn}(X, \mathbf{k})$

$k \leftarrow |\mathbf{k}|$
if $k = 1$ **then** query any point of X and label all of X accordingly
else
  $((X_i, E_i))_{i \in [k]} \leftarrow \mathrm{Round}(X)$
  for $i \in \mathbf{k}$ **do**
    change system of coordinates so that E_i becomes the unit ball
    for $j \in \mathbf{k} \setminus i$ **do**
      $(C_{ij}, \overline{C_{ij}}) \leftarrow \mathrm{CPLearn}(X_i)$ with $h : X_i \to \{i, j\}$
    $\widehat{C}_i \leftarrow \bigcap_{j \in \mathbf{k} \setminus i} C_{ij}$
    mark all of $\widehat{C}_i$ with label i
    if $X_i \setminus \widehat{C}_i \neq \emptyset$ **then** $\mathrm{KClassLearn}(X_i \setminus \widehat{C}_i, \mathbf{k} \setminus i)$

4 Lower Bounds

This section gives a detailed sketch of the proof of Theorem 4, recalled here for convenience:

Theorem 4. *For all $m \geq 2$, all $k \geq 2$, and all $\gamma \leq m^{-3/2}/16$ there exists a distribution of instances with k classes in $\mathbb{R}^m$ with strong convex hull margin γ where any randomized algorithm using* SEED *and* LABEL *queries that returns $\mathcal{C}$ with probability at least $\frac{1}{2}$ makes at least $\left\lfloor \frac{k}{2} \right\rfloor \frac{m}{24 \log m} \log \frac{1}{2\gamma}$ total queries in expectation.*

We first give the sketch for $k = 2$, and then extend it to $k \geq 2$. For a full proof see Appendix B. **Set-up.** The construction is adapted from Proposition 2 of Thiessen and Gärtner [2021]. Let $e_1, \ldots, e_m$ be the canonical basis of $\mathbb{R}^m$ and let $\ell = \lfloor 1/\sqrt{2\gamma\sqrt{m}} \rfloor$; note that $\gamma \leq \frac{m^{-3/2}}{16}$ and $m \geq 2$ ensure $\ell \geq 4$. Let $p = m - 1$, and for each $i \in [p]$ and $j \in [\ell]$ define $x_i^j = e_i + j \cdot e_m$. Finally, let $X = \{x_i^j : i \in [p], j \in [\ell]\}$ and define the concept class $\mathcal{H} = \left\{ \bigcup_{i \in [p]} \{x_i^1, \ldots, x_i^{\ell_i}\} : (\ell_1, \ldots, \ell_p) \in [\ell]^p \right\}$. Let $\mathcal{C} = (C_1, C_2)$ be any partition of X such that $C_1 \in \mathcal{H}$. One can easily verify that $\mathcal{C}$ has strong convex hull margin $\frac{1}{2\ell^2\sqrt{m}} \geq \gamma$. See Figure 2 for reference.

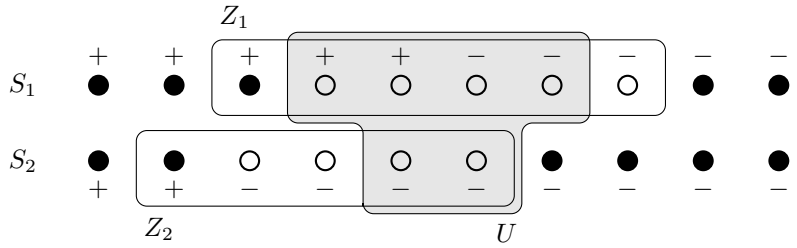

Figure 2: X for $p = 2$ and $\ell = 10$. Filled points represent the agreement region. The maximum point of $S_1 \cap C_1$ (resp. $S_2 \cap C_1$) can be any point in Z_1 (resp. Z_2). U is a possible query.

Query bound. Let $V_0 = \{(C_1, C_2) : C_1 \in \mathcal{H}\}$. This is the initial version space. We let the target concept $\mathcal{C} = (C_1, C_2)$ be drawn uniformly at random from V_0. Note that for $k = 2$, any lower bound on the number of SEED queries alone, also holds for any combination of SEED and LABEL queries, as $\mathrm{LABEL}(x)$ can be simulated by $\mathrm{SEED}(x, 1)$. Thus, without loss of generality, we can assume that the algorithm is only using SEED queries. For all $t = 0, 1, \ldots$, we denote by V_t the version space after the first t SEED queries made by the algorithm. Now fix any $t \geq 1$ and let $\mathrm{SEED}(U, y)$ be the t-th such query. Without loss of generality we assume $y = 1$; a symmetric argument applies to $y = 2$. If $U \cap C_1$ contains a point x whose label can be inferred from the first $t - 1$ queries, then we return x. Therefore we can continue under the assumption that U does not contain any such point (doing otherwise cannot reduce the probability that the algorithm learns nothing). The oracle answers so to maximize $\frac{|V_t|}{|V_{t-1}|}$, as described below.

For each $i \in [p]$ let $S_i = \{x_i^j : j \in [\ell]\}$. We consider S_i as sorted by the index j. Let Z_i be the subset of S_i in the disagreement region of V_{t-1} together with the point in S_i preceding this region; observe that this point always exists, as $x_i^1 \in C_1$ is in the agreement region. Note that Z_i is necessarily an interval of S_i. We let $U_i = Z_i \cap U$ for each $i \in [p]$ and $P(U) = \{i \in [p] : U_i \neq \emptyset\}$. For every $i \in P(U)$, we let α_i be the fraction of points of Z_i that precede the first point in U_i. Let $x_i^* = \arg\max\{j : x_i^j \in S_i \cap C_1\}$. Observe that $|V_{t-1}| = \prod_{i\in[p]} |Z_i|$.Indeed, x_i^* is uniformly distributed over Z_i; either x_i^* is a point in the disagreement region of S_i, or the disagreement region of S_i is fully contained in C_2 and x_i^* is the point preceding the disagreement region of S_i.

Now we show that $\mathbb{E}[|V_{t-1}|/|V_t|] \leq m$. Let $\mathcal{E}$ be the event that $\textsc{seed}(U, 1) = \textsc{nil}$. Write:

$$\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\right] = \Pr(\mathcal{E})\,\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\,\middle|\,\mathcal{E}\right] + \Pr(\overline{\mathcal{E}})\,\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\,\middle|\,\overline{\mathcal{E}}\right] \tag{1}$$

We bound each one of the two terms in the right-hand side.

For the first term, note that $\mathcal{E}$ holds if and only if $U_i \cap C_1 = \emptyset$ for all $i \in P(U)$. Since x_i^* is uniformly distributed over Z_i, for all $i \in P(U)$ we have $\Pr(C_1 \cap U_i = \emptyset) = \alpha_i$, and since the distributions of those points are independent, then $\Pr(\mathcal{E}) = \prod_{i\in P(U)} \alpha_i$. If $\Pr(\mathcal{E}) > 0$ and $\mathcal{E}$ holds, then x_i^* is uniformly distributed over the first $\alpha_i|Z_i|$ points of Z_i, as the rest of Z_i belongs to C_2. This holds independently for all i, thus:

$$|V_t| = \left(\prod_{i\in P(U)} \alpha_i|Z_i|\right)\left(\prod_{i\in[p]\setminus P(U)} |Z_i|\right) = \left(\prod_{i\in P(U)} \alpha_i\right)\left(\prod_{i\in[p]} |Z_i|\right) = |V_{t-1}| \prod_{i\in P(U)} \alpha_i \tag{2}$$

It follows that $\Pr(\mathcal{E})\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\,\middle|\,\mathcal{E}\right] \leq 1$.

Let us turn to the second term. If $\mathcal{E}$ does not hold, then $\textsc{seed}(U, 1)$ returns the smallest point $x \in U_i$ for any $i \in P(U)$ such that $C_1 \cap U_i \neq \emptyset$ (note that necessarily $x \in C_1$). For any fixed $i \in P(U)$, the probability of returning the smallest point of U_i is bounded by $\Pr(C_1 \cap U_i \neq \emptyset)$, which is $1 - \alpha_i$; and if this is the case, then we have $|V_t| = (1 - \alpha_i)|V_{t-1}|$. By summing over all $i \in P(U)$, this yields:

$$\Pr(\overline{\mathcal{E}})\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\,\middle|\,\overline{\mathcal{E}}\right] \leq \sum_{i\in P(U)} (1-\alpha_i)\frac{1}{(1-\alpha_i)} = |P(U)| \leq p = m - 1 \tag{3}$$

So the two terms of (1) are bounded by respectively 1 and $m - 1$; we conclude that $\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\right] \leq m$.

Next, fix any $\bar{t} \geq 1$. By the concavity of $\log$ and by Jensen's inequality:

$$\mathbb{E}\left[\log\frac{|V_0|}{|V_{\bar{t}}|}\right] = \mathbb{E}\left[\sum_{t=1}^{\bar{t}} \log\frac{|V_{t-1}|}{|V_t|}\right] = \sum_{t=1}^{\bar{t}} \mathbb{E}\left[\log\frac{|V_{t-1}|}{|V_t|}\right] \leq \sum_{t=1}^{\bar{t}} \log\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\right] \tag{4}$$

Since $\mathbb{E}\left[\frac{|V_{t-1}|}{|V_t|}\right] \leq m$, the right-hand side is at most $\bar{t}\log m$. Now, since $|V_0| = \ell^p = \ell^{m-1}$, by Markov's inequality, and since $(m-1)\log\ell - \log 2 \geq \frac{(m-1)\log\ell}{2} \geq \frac{m\log\ell}{4}$:

$$\Pr(|V_{\bar{t}}| \leq 2) = \Pr\left(\log\frac{|V_0|}{|V_{\bar{t}}|} \geq (m-1)\log\ell - \log 2\right) \leq \frac{4\,\mathbb{E}\left[\log\frac{|V_0|}{|V_{\bar{t}}|}\right]}{m\log\ell} \leq \frac{4\,\bar{t}\log m}{m\log\ell} \tag{5}$$

Now let T be the random variable counting the number of queries spent by the algorithm, and let V_T be the version space at return time. Since $\mathcal{C}$ is uniform over V_T and $\mathcal{C}$ is returned with probability at least $\frac{1}{2}$, then $\Pr(|V_T| \leq 2) \geq \frac{1}{2}$. By (5) and linearity of expectation,

$$\frac{1}{2} \leq \Pr(|V_T| \leq 2) \leq \sum_{\bar{t}\geq 0} \Pr(T = \bar{t}) \cdot \frac{4\bar{t}\log m}{m\log\ell} = \mathbb{E}[T]\frac{4\log m}{m\log\ell} \tag{6}$$

Therefore $\mathbb{E}[T] \geq \frac{m\log\ell}{8\log m}$. Now, since $\ell \geq 4$ then $\ell \geq \frac{4}{5\sqrt{2\gamma\sqrt{m}}}$, which since $m \leq (16\gamma)^{-2/3}$ yields, after calculations, $\ell \geq \sqrt[3]{1/\gamma} \cdot \frac{4^{4/3}}{5\sqrt{2}} > 0.89\sqrt[3]{1/\gamma}$. This shows that $E[T] > \frac{m\log\frac{1}{2\gamma}}{24\log m}$, which concludes the proof for $k = 2$.

Extension to k $\geq$ 2. For each $s \in \left\lfloor\frac{k}{2}\right\rfloor$ and each pair of classes C_{2s-1}, C_{2s}, use the construction above shifted along the m-th dimension by $(s-1)\ell$. One can easily verify that learning $\mathcal{C}$ is as hard as learning $\left\lfloor\frac{k}{2}\right\rfloor$ independent binary classifiers, for each of which the bound above holds.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] We clearly state the assumptions under which our results hold.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] This is a purely theoretical work with no direct societal impact, neither positive nor negative.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [N/A]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A]
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