When Can Two Unsupervised Learners Achieve PAC Separation?

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Abstract. In this paper we study a new restriction of the PAC learning framework, in which each label class is handled by an unsupervised learner that aims to fit an appropriate probability distribution to its own data. A hypothesis is derived by choosing, for any unlabeled instance, the label whose distribution assigns it the higher likelihood.
The motivation for the new learning setting is that the general approach of fitting separate distributions to each label class, is often used in practice for classification problems. The set of probability distributions that is obtained is more useful than a collection of decision boundaries. A question that arises, however, is whether it is ever more tractable (in terms of computational complexity or sample-size required) to find a simple decision boundary than to divide the problem up into separate unsupervised learning problems and find appropriate distributions.
Within the framework, we give algorithms for learning various simple geometric concept classes. In the boolean domain we show how to learn parity functions, and functions having a constant upper bound on the number of relevant attributes. These results distinguish the new setting from various other well-known restrictions of PAC-learning. We give an algorithm for learning monomials over input vectors generated by an unknown product distribution. The main open problem is whether monomials (or any other concept class) distinguish learnability in this framework from standard PAC-learnability.

1 Introduction

A standard approach to classification problems (see e.g. Duda and Hart [10]) is the following. For each class, find a *discriminant function* that maps elements of the input domain to real values. These functions can be used to label any input element $\mathbf{x}$ by giving it the class label whose associated discriminant function takes the largest value on $\mathbf{x}$. The discriminant functions are usually estimates of the probability densities of points having some class label, weighted by the class prior (relative frequency of that class label).

In learning theory e.g. PAC learning [2] or more recently support vectors [7] the approach is to find decision boundaries that optimize some performance guarantee. (The guarantee is usually based on observed classification performance in

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conjunction with other features of the boundary such as syntactic or combinatorial complexity, or the number of support vectors and margin of separation.) The general approach clearly requires examples with different labels to be taken in conjunction with each other when finding a decision boundary. By contrast, discriminant functions are constructed from individual label classes in isolation.

There are practical advantages to applying an unsupervised learning method to each label class, and obtaining estimates of the distribution over that label class. In contrast with decision boundaries, we obtain for any input vector $\mathbf{x}$, the values of the probability densities of label classes at $\mathbf{x}$, which provide a conditional distribution over the class label of $\mathbf{x}$. A predicted class label for $\mathbf{x}$ can then take into account variable misclassification penalties, or changes in the assumed class priors. There are of course other ways to obtain such distributions, for example using logistic regression, or more generally (for k-class classification) neural networks with k real-valued outputs re-scaled using the softmax activation function (see Bishop [3] for details). Learning using an unsupervised learner for each class has other advantages over these techniques, notably the first two of the following observations.

1. For applications such as handwritten digit recognition, it is more natural to model the data generation process in terms of 10 separate probability distributions, than as a collection of thresholds between different digits.
2. Label classes can be added without re-training the system. So for example if the euro symbol were added to a character set, then given a good estimate of the probability distribution over images of euro symbols, this can be used in conjunction with pre-existing models for how other symbols are generated.
3. The approach can treat situations where class overlap occurs (as is usually the case in practice). Standard PAC algorithms do not address this problem (although there have been extensions such as "probabilistic concepts" [18] that do so, and of course versions of support vector networks also allow decision boundaries that do not necessarily agree with all observed data).

Another difficulty with decision boundaries arises specifically in the context of multiclass classification. It has been noted [1] that multiclass classifiers are often constructed using multiple 2-class classifiers. How to combine them is a challenging topic that has itself received much recent attention, see for example [13, 1]. In practical studies such as [19] that build a multi-class classifier from a collection of 2-class classifiers, a distinction is made between separating each class from the union of the others (*1-v-r* classifiers, where 1-v-r stands for one-versus-rest) and pairwise separation (*1-v-1* classifiers). Neither is entirely satisfactory – for example it may be possible to perform linear 1-v-1 separation for all pairs of classes, but not linear 1-v-r separation, while a problem with 1-v-1 classification (as studied in [19]) is the difficulty of combining the collection of pairwise classifiers to get an overall classification, in a principled way, for example ensuring that all classes are treated the same way. In [19], the first test for any unlabeled input is to apply the separator that distinguishes 0 from 9. Thus 0 and 9 are being treated differently from other digits (which in turn are also treated differently from each other.)

1.1 Main Research Questions

In view of the advantages we have noted of using unsupervised learners to solve classification problems, we propose to search for a gap between the tractability of classification problems and the tractability of classification problems subject to the restriction that each class be learned with its own unsupervised learner. Does there exist a learning problem for which we can both obtain a positive result for finding a decision boundary, and a negative result for the problem of fitting appropriate probability distributions to the classes so that maximum likelihood gives rise to a decision boundary with the same performance guarantees?

We consider this question in the basic Probably Approximately Correct (PAC) setting of [20, 21], since it is well-understood. In PAC learning, the usual algorithmic challenge is to separate the two classes of examples. It would be remarkable if it turned out that PAC-learnability were equivalent to PAC-learnability using unsupervised learners, in view of the way the PAC criterion seems to lead to a search for class separation. The main drawback of studying PAC-learnability is the loss of realism associated with class separability.

There are not many papers on unsupervised learning in the computational learning theory literature; the topic was introduced in [17], see also [8, 11, 12, 9]. The algorithms we describe here differ substantially from these previous ones (as well as from the algorithms in the much more extensive general literature on unsupervised learning). The reason is that our aim is not really to approximate a distribution over inputs. Rather, it is to construct a discriminant function in such a way that we expect it to work well in conjunction with the corresponding discriminant function constructed on data with the opposite class label.

From a theoretical perspective, we address a natural question in asking how much it hampers learning not to have simultaneous access to examples with different labels. The topic appears to raise new and interesting research problems. The main theoretical question (which we leave open) is of course: are all PAC learnable problems also learnable in this framework, and if not, how does the set of learnable problems compare with other subsets of PAC learnable problems, for example Statistical Query (SQ) learnability [16]. (In the case of SQ learning, we find that parity functions are learnable in this framework but from [16] they are not learnable using SQs.)

1.2 Formalizing the Learning Framework

In PAC learning there is a source of data consisting of instances generated by a probability distribution D over a domain X, labeled using an unknown function $f : X \longrightarrow \{0, 1\}$. Thus f divides members of X into two sets $f^{-1}(0)$ and $f^{-1}(1)$, and the learner's objective is to find good approximations to those sets. As usual we will let ϵ and δ denote the target error and uncertainty respectively.

We use the standard convention of referring to the two classes of inputs associated with the two class labels as the "positive examples" and the "negative examples". Each learner has access to a source of examples having one of the two class labels. More precisely, one learner may (in unit time) draw a sample

from D restricted to the positive examples, and the other may sample from D restricted to the negative examples. This formalism loses any information about the class priors, *i.e.* the relative frequency of positive and negative examples, but PAC learnability is in fact equivalent to PAC learnability where the class priors are concealed from the learner. (Formally, this is the equivalence of the standard PAC framework with the "two-button" version, where the learner has access to a "positive example oracle" and a "negative example oracle" [14]. The two-button version conceals the class priors and only gives the learner access to the distribution as restricted to each class label.)

We assume that neither unsupervised learner knows whether it is receiving the positive or the negative examples. Consequently both learners must apply the same algorithm. Note that for a concept class that is closed under complementation, output labels are of no help to the learners. For a concept class that is not closed under complementation (such as rectangles), observe that it is PAC learnable if and only if its closure under complementation is PAC learnable. Hence any learning algorithm in our framework which required class labels to be provided to each of the two learners, would lack a robustness property that standard PAC algorithms have. That observation also indicates that the main question of distinguishability from standard PAC-learnability is independent of the assumption that class labels (positive/negative) are provided. Note however that for some concept classes (notably monomials, section 3.1) we can (without much difficulty) find algorithms in our setting that use labeled examples, but we have so far not found any algorithm that works with unlabeled examples.

The class label which the pair of learners assign to input x is the one associated with the data sent to the learner that assigned x the higher likelihood. If x is given the same likelihood by both distributions generated by the learners, the tie is broken at random.

1.3 Notation and Terminology

We refer to the unsupervised learners as learners A and B, and we also assume by convention that learner A is the one receiving the positive examples, however as we have noted above, learner A (and likewise B) is not told its identity.

Theorem 1 below justifies the design of algorithms in which instead of insisting that the outputs of the unsupervised learners define probability distributions, we allow unrestricted discriminant functions from domain X to the real numbers $\mathbf{R}$. The comparison of the two values assigned to any $x \in X$ is used to determine the class label that the hypothesis classifier assigns to x. In what follows we refer to the "score" assigned to an input vector $\mathbf{x}$ by an unsupervised learner to mean the value taken by its discriminant function on input $\mathbf{x}$.

We will say that learner A (respectively B) "claims" an input x if it gives x a higher likelihood or score than learner B (respectively A). We say that a learner "rejects" an input if it assigns a likelihood of 0, or alternatively a score of minimal value (it is convenient to use $-\infty$ to denote such a score). Thus if a learner rejects an input, it will be claimed by the other learner provided that the other learner does not also reject that input.

2 General Results

In this section we give some general results about the two unsupervised learners framework. (Then in section 3 we give some algorithms for specific PAC learning problems. The results of section 3 also serve to distinguish our learning setting from other restrictions of the PAC setting in terms of what concept classes may be learned.) We show first that if hypotheses may be any real-valued discriminant functions, then the algorithm may be modified so that the hypotheses are probability distributions, and the separation is still PAC. There is no particular reason to suppose that probability distributions obtained in this way will approximate the underlying distributions generating the instances, according to previously-studied metrics such as variation distance or KL-distance.

Theorem 1. *Let X be a domain of inputs. If there is a PAC algorithm in which each unsupervised learner may assign any real number to an element of X, then there is a PAC algorithm in which the learners must choose numbers that integrate or sum to 1 over the domain (i.e. are a probability distribution).*

Proof. Let $\mathcal{A}$ be an algorithm that returns any discriminant function. So in a problem instance, $\mathcal{A}$ is applied twice, once to A's data and once to B's data, and we obtain functions $f_A : X \longrightarrow \mathbf{R}$ and $f_B : X \longrightarrow \mathbf{R}$. (So for example any $x \in X$ with $f_A(x) > f_B(x)$ would be labeled as positive by the overall hypothesis, under our convention that A receives the positive examples.)

Our approach is to re-scale any function returned by the algorithm so that the outcome of any comparison is preserved, but the new functions sum or integrate to 1. In a case where, for example, $\sum_{x \in X} f_A(x) = 1$ and $\sum_{x \in X} f_B(x) = 2$, this initially appears problematic: f_B has to be scaled down, but then the new values of f_B may become less than f_A. Note however that we can modify f_A by choosing an arbitrary $\hat{x}$ in A's data, and adding 1 to $f_A(\hat{x})$. This can only improve the resulting classifier (it may cause $\hat{x}$ to be claimed by A where previously it was claimed by B). Now the new f_A together with f_B can both be rescaled down by a factor of 2, and comparisons are clearly preserved.

Making the above idea general, suppose that algorithm $\mathcal{A}$ takes a sample of data S and returns a function $f : X \longrightarrow \mathbf{R}$. Modify $\mathcal{A}$ as follows. Define $g(x) = e^{f(x)}/(1 + e^{f(x)})$, so the range of g is $(0, 1)$. Let $P(X)$ be a probability distribution over X that does not vanish anywhere. Let $s = \sum_{x \in X} g(x)P(x)$, or $\int_{x \in X} g(x)P(x)dx$ for continuous X. s is well-defined and lies in the range $(0, 1)$. Now for a discrete domain X, the probability distribution returned by the modified $\mathcal{A}$ is $D'(x) = g(x)P(x)$ for all $x \in X$ except for some arbitrary $\hat{x} \in S$, where $D'(\hat{x}) = g(x)P(x) + 1 - s$. For a continuous domain the probability distribution is the mixture of the continuous density $D'(x) = g(x)P(x)$ with coefficient s and a point probability mass located at some $\hat{x} \in S$ with probability $1 - s$. ♢

In view of the above result, we subsequently give algorithms for hypotheses that may output unrestricted real numbers. The next two results about PAC-learning with two unsupervised learners provide some further information about

how it compares with other variants of PAC-learning in terms of which concept classes become learnable. First, note that the framework can be extended to a misclassification noise situation by letting each learner have examples that are (correctly or incorrectly) assigned the class label associated with that learner.

Theorem 2. *Any concept class that is PAC-learnable in the presence of uniform misclassification noise can be learned by two unsupervised learners in the presence of uniform misclassification noise if the input distribution is known to both learners.*

Proof. Let D be the known distribution over the input domain X. Let $\mathcal{C}$ be a concept class that is PAC-learnable with uniform misclassification noise. We may assume that $\mathcal{C}$ is closed under complementation (we have noted that if it is not closed under complementation we can take it closure under complementation which should still be PAC learnable).

Each learner takes a set of N examples, where N is chosen such that a standard PAC algorithm would have error bound ϵ^2. Let D^+ (resp. D^-) be the probability that an example generated by D belongs to target T (resp. $X \setminus T$). Let ν be the noise rate. With probability $\frac{(1-\nu)D^+}{(1-\nu)D^+ + \nu D^-}$ an example received by A belongs to target T; meanwhile with probability $\frac{(1-\nu)D^-}{(1-\nu)D^- + \nu D^+}$ an example received by B comes from $X \setminus T$.

Each learner labels all its examples as positive, and then generates a set of N examples from D, each of which is labeled positive with some probability $p < \frac{1}{2}$, otherwise negative. For learner A, the union of these two sets consists of a set of examples from a new probability distribution D', labeled by the same target concept T. It may be verified that the examples from T have misclassification noise with noise rate

$$\frac{(1-p)(D^+(1-\nu) + D^-\nu)}{(1-p)(D^+(1-\nu) + D^-\nu) + 1 - \nu}$$

and the examples from $X \setminus T$ have misclassification noise with noise rate

$$\frac{\nu + p(D^+(1-\nu) + D^-\nu)}{\nu + (D^+(1-\nu) + D^-\nu)}.$$

It may be verified from these expressions that there is a unique value of p in the range $[0, \frac{1}{2}]$ for which these two noise rates are equal, and for that value of p they are both strictly less than $\frac{1}{2}$.

Hence for some value of p we obtain data with uniform misclassification noise. An appropriate p can be found by trying all values $p = r\epsilon$ for $r = 0, \ldots, 1/2\epsilon$, and checking whether the hypothesis obtained (using a standard noise-tolerant PAC algorithm) is consistent with uniform misclassification noise.

The same reasoning applies to learner B using $X \setminus T$ as the target concept.

Let H be the set of examples labeled positive by the resulting hypothesis. Each learner assigns discriminant function values as follows. If the observed value

of $D'(H)$ is at least $1-\epsilon$, use a value of $\frac{1}{2}$ for all elements of X. Otherwise use a value of 1 for elements of H and a value of 0 for elements of $X \setminus H$.

Let D'_A and D'_B be the D''s for learners A and B.

$D(T)$ is the probability that a random example from D belongs to T. Assuming $D(T) < 1-\epsilon$, we can say that error $O(\epsilon^2)$ with respect to D'_A implies error $O(\epsilon)$ with respect to D. If alternatively $D(T) \geq 1-\epsilon/2$, the hypothesis H found by A will have a probability $D'(H) > 1-\epsilon$ as observed on the data. A learner finding such a hypothesis then gives all examples a score of $\frac{1}{2}$, allowing B's scores to determine the overall classification. A similar argument applies for low values of $D(T)$, *i.e.* $\leq \epsilon/2$, (where we expect B to assign scores of $\frac{1}{2}$). $\Diamond$

It is probably not the case that noise-free distribution-specific learnability with two unsupervised learners is actually equivalent to standard PAC-learnability with uniform misclassification noise. This is because, given the Noisy Parity Assumption (that it is hard to PAC-learn parity functions in the presence of random misclassification noise given the uniform distribution over input vectors), noise-free distribution-specific learning with two unsupervised learners is tractable (see corollary 2) in a situation where the uniform misclassification noise situation is intractable.

The following result is a sufficient condition for learning with unsupervised learners:

Theorem 3. *If a concept class is closed under complementation and learnable from positive examples only, then it is learnable with two unsupervised learners.*

Proof. Let $X = X_A \cup X_B$ be the partition of the domain X where X_A is the set of positive examples and X_B the negative examples. Closure under complementation implies that X_B as well as X_A is a member of the concept class.

Both learners apply an algorithm that learns from positive examples only. Consequently A's hypothesis must be a subset of X_A and B's hypothesis must be a subset of X_B. A and B use discriminant functions f_A and f_B that are the indicator functions of their hypotheses. As a result, if f_A and f_B both have error at most ϵ, then A and B correctly claim all but a fraction ϵ of examples from X_A and X_B respectively. $\Diamond$

As a consequence we have

Corollary 1. *Boolean functions over a constant number of variables are learnable using unsupervised learners.*

Proof. The class of functions is clearly closed under complementation.

To learn the class from positive examples, suppose k is the number of variables in the target formula. Given a set S of boolean vectors that constitutes the observed data (assumed to be positive examples), label a new vector $\mathbf{v}$ as positive if and only if for each set of k attributes in $\mathbf{v}$, there is a member of S that agrees with $\mathbf{v}$ on those attributes.

It can be readily verified that for constant k, the time and sample complexity of the above rule is polynomial in the total number of variables. $\Diamond$

The following result distinguishes our learning setting from learnability with uniform misclassification noise, or learnability with a restricted focus of attention. A *parity function* [15] has an associated subset of the variables, and an associated "target parity" (even or odd), and evaluates to 1 provided that the parity of the number of "true" elements of that subset agrees with the target parity, otherwise the function evaluates to 0.

Corollary 2. *The class of parity functions is learnable by unsupervised learners.*

Proof. Once again it is clear that the class is closed under complementation.

To learn a parity function from positive examples only, then similar to the algorithm of [15], each unsupervised learner finds the affine subspace of $GF(2)^n$ spanned by its examples, and assigns a score of 1 to elements of that subspace and a score of 0 to all elements of the domain. ◊

3 Examples of Concrete Learning Problems

The algorithms in this section give an idea of the new technical challenges, and also distinguish the learning setting from various others. We have already distinguished the learning setting from learnability with uniform misclassification noise or learnability with a restricted focus of attention, and the result of section 3.2 distinguishes it from learnability with one-sided error or learnability from positive or negative examples only.

3.1 Monomials

Recall that a monomial is a boolean function consisting of the conjunction of a set of literals (where a literal is either a boolean attribute or its negation). Despite the simplicity of this class of functions, we have not resolved its learnability in the two unsupervised learners framework, even for monotone (*i.e.* negation-free) monomials. If the unsupervised learners are told which of them has the positive and which the negative examples, then the problem does have a simple solution (a property of any class of functions that is learnable from either positive examples only or else negative examples only). The "negative" unsupervised learner assigns a score of $\frac{1}{2}$ to all boolean vectors. The "positive" unsupervised learner uses its data to find a PAC hypothesis, and assigns a score of 1 to examples satisfying that hypothesis, and 0 to other examples.

Discussion of the Distribution-independent Learning Problem. Given a monomial f, let $pos(f)$ denote its satisfying assignments. The problem that arises when the unsupervised learners are not told which one is receiving the positive examples, is that the distribution over the negative examples could in fact produce boolean vectors that satisfy some monomial m that differs from target monomial t, but if $D(pos(m) \cap pos(t)) > \epsilon$ this may give excessive error. This problem can of course be handled in the special case where the monomial is over a constant number k of literals, and corollary 1 applies.

Learnability of Monomials over Vectors of Attributes Generated by a Product Distribution. In view of the importance of the concept class of monomials, we consider whether they are learnable given that the input distribution D belongs to a given class of probability distributions. This situation is intermediate between knowing D exactly (in which case by theorem 2 the problem would be solved since monomials are learnable in the presence of uniform misclassification noise) and the distribution-independent setting. We assume now that the class priors are known approximately, since we no longer have the equivalence of the one-button and two-button versions of PAC learnability. Formally, assume each learner can sample from D, but if the example drawn belongs to the other learner's class then the learner is told only that the example belonged to the other class, and no other information about it. Hence each learner has an "observed class prior", the observed probability that examples belong to one's own class.

Suppose that D is known to be a product distribution. Let $x_1, \ldots, x_n$ be the boolean attributes in examples. Let d_i, $i = 1, \ldots, n$, be the probability that the i-th attribute equals 1. For attribute x_i for which one of the literals x_i or $\overline{x_i}$ is in the target monomial t (we assume that they are not both in t), let p_i be the probability that the literal is satisfied, so $p_i = d_i$ for an un-negated literal, otherwise $p_i = 1 - d_i$.

We say that attribute x_i is "useful" if x_i or $\overline{x_i}$ is in t, and also $p_i \in [\epsilon, 1-\epsilon/n]$. Note that if $p_i < \epsilon$ then the probability that any example is positive is also $< \epsilon$, and if $p_i > 1 - \epsilon/n$ then only a very small fraction of examples can be negative due to their value of x_i.

The Algorithm.

We use the fact that for D a product distribution, D restricted to the positive examples of a monomial is also a product distribution. We apply a test (step 3 of the algorithm) to see whether the observed data appears to come from a product distribution. The test identifies negative data when there is more than one useful attribute. The discriminant function (computed in step 4) also handles the case when at most one attribute is useful.

1. Draw a sample S of size $O((n/\epsilon)^3 \log(\frac{1}{\delta}))$.
2. If the observed class prior of the examples is $\leq \epsilon/2$, reject all examples. Otherwise do the following.
3. (product distribution test) For each literal l that is satisfied by at least a fraction ϵ/n of elements of S, let S_l denote elements of S which satisfy l, and for each literal $l' \neq l$ check whether the fraction of examples satisfying l' differs by at least ϵ/n^2 from the fraction of examples belonging to S_l that satisfy l'. If any such l' exists, the test "fails" and we assume that the negative examples are being seen, and give all examples a score of $1/2$. Otherwise (the test is "passed") proceed to step 4:
4. Let L be the set of literals satisfied by *all* elements of S.
   (a) If an example satisfies all the literals in L *and* fails to satisfy all literals that are satisfied by a fraction $< \epsilon/2n$ of elements of S, give that example a score of 1.

(b) Otherwise, if the example still satisfies L, assign a score of $1/2$.
(c) Otherwise assign a score of 0.

Note: step 3 is a test with "one-sided error" in the sense that we may reasonably expect all product distributions to pass the test, but there exist distributions other than product distributions that may also pass. However, we show below that when a product distribution restricted to the negative data of a monomial passes the test, then (with probability $\geq 1-\delta$) there is at most one useful attribute.

Proving That the Algorithm is PAC. There must be at least one useful attribute in order for the frequency of both positive and negative examples to exceed ϵ. We consider two cases: first when there is only one useful attribute, second, when there is more than one.
Case 1: In this case, we expect the distributions over both the positive and negative examples to be close to product distributions, so that the test of step 3 of the algorithm will be passed in both A's case and B's case. Learner A (with probability $1-O(\delta)$) gives a score of 1 to examples that satisfy the useful literal l, with the exception of a small fraction of them due to the additional requirement in step 4a. Meanwhile, learner B assigns a score of $\leq \frac{1}{2}$ to all examples satisfying l, since l is not satisfied by any of B's data. Hence learner A claims all but a fraction $< \epsilon/2$ of the positive data. By a similar argument, learner B claims all but a fraction $< \epsilon/2$ of the negative data.
Case 2: When there are two useful attributes, the positive examples are still generated by a product distribution, so A's data pass the test of step 3. Meanwhile, with probability $> 1-\delta$, B's data fail this test, since when we choose literal l in target t that happens to be useful, and remove elements of S which satisfy l, then the conditional probability that any other useful literal is satisfied, changes by $> \epsilon/n^2$. (A Chernoff bound analysis assures that the change will be detected with probability $1-\delta/2$.) All examples are then given scores of $1/2$, and this allows A to claim positives and leave B the negatives.

3.2 Unions of Intervals

Let the domain be the real numbers $\mathbf{R}$, and assume that the target concept is a union of k intervals in $\mathbf{R}$. We show that this concept class is learnable by two unsupervised learners. This result shows that learnability with two unsupervised learners is distinct from learnability from positive examples only, or from negative examples only.

Each learner does the following. Let S be the set of real values that constitutes its data. Define discriminant function f as

$$f(r) = -\Big(\min_{s\in S, s>r}(s) - \max_{s\in S, s<r}(s)\Big) \text{ if } r \notin S$$

$$f(r) = 1 \text{ if } r \in S.$$

This choice of discriminant function ensures that when A's and B's scores are combined, the set of all points that are claimed by A consists of a union of at most k intervals, and this set contains A's data but not B's data. Hence we have a consistent hypothesis of V-C dimension no more than the target concept, so this method is PAC (with runtime polynomial in k, ϵ^{-1} and δ^{-1}). Note that the value of k needs to be prior knowledge for the purpose of identifying a sufficient sample size. This is in contrast with PAC learning in the standard setting, where an appropriate sample size can be identified using the standard on-line approach of comparing the number of examples seen so far with the complexity of the simplest consistent classifier, and continuing until the ratio is large enough.

3.3 Rectangles in the Plane with Bounded Aspect Ratio

Let α denote the length of the target rectangle divided by the width, and we give a PAC-learning algorithm that is polynomial in α as well as the standard PAC parameters. We do not have a PAC algorithm that works without the bound on the aspect ratio. A notable feature of this learning problem is that it seems to require quite a complex method, despite the simplicity of the concept class. Extensions are discussed in the next section.

The general idea is that each learner partitions the domain into rectangles containing equal numbers of its data points, and given a query point $\mathbf{q}$, compares the coordinates of $\mathbf{q}$ with other points in the partition element within which $\mathbf{q}$ falls. A high score is given when there exist points in that partition element with similar coordinate values.

The Algorithm. Each learner does the following.

1. Generate a sample of size $N = \Theta(\alpha \log(\delta^{-1})/\epsilon^9)$.
2. Build a partition P of the domain $\mathbf{R}^2$ as follows:
   (a) Partition the domain into $1/\epsilon^2$ pieces using lines normal to the y-axis, such that each piece contains the same number of data points.[1]
   (b) Partition each element of the above partition into $1/\epsilon^2$ pieces using lines normal to the x-axis, such that each piece contains the same number of data points.
3. For query point $\mathbf{q} \in \mathbf{R}^2$ the score assigned to $\mathbf{q}$ is computed as follows.
   (a) Let $P_{\mathbf{q}} \in P$ be the rectangle in P containing $\mathbf{q}$.
   (b) Let $S(P_{\mathbf{q}})$ be the sample points that lie inside $P_{\mathbf{q}}$.
   (So $|S(P_{\mathbf{q}})| = \Theta(\alpha \log(\delta^{-1})/\epsilon^5)$)
   (c) Sort $S(P_{\mathbf{q}}) \cup \{\mathbf{q}\}$ by x-coordinate. If $\mathbf{q}$ is among the first $(\frac{1}{\epsilon})^{-1}$ elements or among the last $(\frac{1}{\epsilon})^{-1}$ elements, then reject $\mathbf{q}$, *i.e.* assign $\mathbf{q}$ a score of $-\infty$ and terminate.
   (d) If $\mathbf{q}$ was not rejected, define the x-cost of $\mathbf{q}$ to be the difference between the x-coordinates of the two neighbors of $\mathbf{q}$.
   (e) Sort $S(P_{\mathbf{q}}) \cup \{\mathbf{q}\}$ by y-coordinate. If $\mathbf{q}$ is among the first $(\frac{1}{\epsilon})^{-1}$ elements or among the last $(\frac{1}{\epsilon})^{-1}$ elements, then reject $\mathbf{q}$.

[1] Throughout we ignore rounding error in situations where for example an equal partition is impossible; such rounding will only change quantities by a constant.

(f) If $\mathbf{q}$ was not rejected, define the y-cost of $\mathbf{q}$ to be the difference between the y-coordinates of the two neighbors of $\mathbf{q}$.
(g) Finally, the score assigned to $\mathbf{q}$ is the negation of the sum of the x-cost and y-cost.

Proving That the Algorithm is PAC. Let P_A be the partition constructed by A and let P_B be the partition constructed by B. Let μ_A (respectively μ_B) be the measure on $\mathbf{R}^2$ induced by the input distribution D restricted to target T (respectively T', the complement of T) and re-normalised, so that we have $\mu_A(\mathbf{R}^2) = \mu_B(\mathbf{R}^2) = 1$. So, given region $R \subseteq \mathbf{R}^2$, $\mu_A(R)$ is the probability that a random input x lies within R conditioned on x being an element of T. Let $\hat{\mu}_A$ and $\hat{\mu}_B$ denote the measures μ_A and μ_B as observed by A and B respectively on the random examples used in the algorithm. The well-known V-C theory of [4] says that for a concept class $\mathcal{C}$ of V-C dimension v, given a sample of size[2] $O(v \log(\delta^{-1}\epsilon^{-1})/\epsilon)$, we have that with probability $1-\delta$,

$$|\hat{\mu}(C) - \mu(C)| \leq \epsilon \text{ for all } C \in \mathcal{C}$$

where μ is a probability measure and $\hat{\mu}$ is the measure as observed on the sample. Noting that axis-aligned rectangles in $\mathbf{R}^2$ have V-C dimension 4, we deduce that if learners A and B draw samples of size $O(\log(\delta^{-1}\epsilon^{-1})/\epsilon)$, then with probability $1-\delta$,

$$|\hat{\mu}_A(R) - \mu_A(R)| \leq \epsilon \text{ and}$$

$$|\hat{\mu}_B(R) - \mu_B(R)| \leq \epsilon, \text{ for all rectangles } R.$$

The following fact emerges automatically from the V-C bounds:

Remark 1. N is chosen such that if learners A and B use samples of size N, then with probability $1 - O(\delta)$ we have that for all rectangles R:

$$|\hat{\mu}_A(R) - \mu_A(R)| \leq \epsilon^9$$

$$|\hat{\mu}_B(R) - \mu_B(R)| \leq \epsilon^9.$$

From the construction of partition P we note:

Remark 2. P_A and P_B are each of size $(1/\epsilon)^4$, and each element of P_A (respectively P_B) contains $\Theta(\alpha \log(\delta^{-1})(1/\epsilon)^5)$ of A's (respectively B's) data points.

From remark 2, given rectangle $R \in P_A$, $\hat{\mu}_A(R) = \epsilon^4$, and consequently $|\mu_A(R) - \epsilon^4| \leq \epsilon^9$ with high probability, using remark 1. Clearly all rectangles in P_A intersect target rectangle T (similarly members of P_B intersect T'). Now consider the potential problem of rectangles in P_B that contain positive examples. We continue by upper-bounding the number of those rectangles, and

[2] This is weaker than the known bound — we are using a weak bound to simplify the presentation.

upper-bounding the amount of damage each one can do (due to claiming data examples that should be claimed by A).

Let $P_A^* \subseteq P_A$ be elements of P_A which intersect T' (so are not proper subsets of T). Similarly let P_B^* denote elements of P_B which intersect T. We show that the number of elements of P_A^* and P_B^* is substantially smaller than the cardinalities of P_A and P_B.

Remark 3. Any axis-aligned line cuts $(\frac{1}{\epsilon})^2$ elements of P_A and similarly $(\frac{1}{\epsilon})^2$ elements of P_B.

Corollary 3. *The boundary of T intersects at most $O((\frac{1}{\epsilon})^2)$ elements of P_A and similarly at most $O((\frac{1}{\epsilon})^2)$ elements of P_B.*

In particular, it intersects at most $4.(\frac{1}{\epsilon})^2$ elements of either partition.

So partition P_B has $(\frac{1}{\epsilon})^4$ elements each containing $(\frac{1}{\epsilon})^5$ data points, and only $O((\frac{1}{\epsilon})^2)$ of them intersect T. Now we consider how an element $R \in P_B$ could intersect T. We divide the kinds of overlap into

1. An edge overlap, where one edge and no vertices of T are overlapped by R.
2. A two-edge overlap, where 2 opposite edges and no corner of T are overlapped by R.
3. Any overlap where R contains a corner of T.

We treat these as separate cases. Note that since there are ≤ 4 overlaps of type 3 we may obtain relatively high bounds on the error they introduce, by comparison with the edge and two-edge overlaps, of which there may be up to $(\frac{1}{\epsilon})^2$. Throughout we use the following notation. Let $\mathbf{x}$ be a point in target rectangle T which is being assigned scores using A's and B's partitions. Let $\mathbf{x} \in$ rectangle $R_A \in P_A$ and $\mathbf{x} \in R_B \in P_B$, so that R_A intersects T.

Case 1: (edge overlap) R_B has an edge overlap with T. Consider steps 3c and 3e of the algorithm. When $\mathbf{x}$ is being compared with the points in R_B it will have either an x-coordinate or a y-coordinate which is maximal or minimal for data points observed in R_B. One of these steps of the algorithm will cause B to reject $\mathbf{x}$. But $\mathbf{x}$ will only have a probability $O(\epsilon^5)$ of having a maximal or minimal coordinate value amongst points in R_A (since R_A contains $(\frac{1}{\epsilon})^5$ data points and $\mathbf{x}$ is generated by the same distribution that generated those data points).

Case 2: (two-edge overlap) There are at most $(\frac{1}{\epsilon})^2$ two-edge overlaps possible. Suppose that in fact R_B overlaps the top and bottom edges of T (the following argument will apply also to the other sub-case). Hence all the two-edge overlaps do in fact overlap the top and bottom edges of T. Let x_T and y_T denote the lengths of T as measured in the x and y directions, so we have $x_T/y_T \in [1/\alpha, \alpha]$. Then the y-cost of R_B is at least y_T. Meanwhile, all but a fraction ϵ of boxes in P_A will give a y-cost of $\leq \epsilon \cdot y_T$. Also, all but a fraction ϵ of boxes in P_A will have x-costs at most $\epsilon \cdot x_T$. Using our aspect ratio assumption, this is at most $\epsilon\alpha y_T$. Hence, for points in all but a fraction ϵ of boxes in P_A, the y-cost will dominate, and the score assigned by B will exceed A's score.

Case 3: (corner overlap) Suppose R_B overlaps a corner of T. We show that R_B introduces error $O(\epsilon)$, and since there are at most 4 such rectangles, this case

is then satisfactory. For R_B to introduce error $> \epsilon$, it must overlap a fraction $\Omega(\epsilon)$ of rectangles in P_A, hence $> (\frac{1}{\epsilon})^3$ rectangles in P_A. In this situation, R_B contains $\Omega((\frac{1}{\epsilon})^3)$ recangles in P_A in its interior. On average, both the x and y coordinates of sample points in these interior rectangles will be $\Omega(\frac{1}{\epsilon})$ closer to each other than the points in R_B. This means that only an ϵ-fraction of points in these elements of P_A will have coordinates closer to points in R_B, than to some other point in the same element of P_A. Hence all but an ϵ-fraction of these points will be claimed by A.

Discussion, possible extensions. Obviously we would like to know whether it is possible to have PAC learnability without the restriction on the aspect ratio of the target rectangle. The restriction is arguably benign from a practical point of view. Alternatively, various reasonable "well-behavedness" restrictions on the input distribution would probably allow the removal of the aspect ratio restriction, and also allow simpler algorithms.

The extension of this result to unions of k rectangles in the plane is fairly straightforward, assuming that the aspect ratio restriction is that both the target region and its complement are expressible as a union of k rectangles all with bound α on the aspect ratio. The general idea being used is likely to be extendable to any constant dimension, but then the case analysis (on the different ways that a partition element may intersect the region with the opposite class label) may need to be extended. If so it should generalize to unions of boxes[3] in fixed dimension (as studied in [6] in the setting of query learning, a generalization is studied in [5] in PAC learning). Finally, if boxes are PAC learnable with two unsupervised learners in time polynomial in the dimension, then this would imply learnability of monomials, considered previously.

3.4 Linear Separators in the Plane

Given a set S of points in the plane, it would be valid for an unsupervised learner to use a probability distribution whose domain is the convex hull[4] of S, *provided that only a "small" fraction of elements of S are actually vertices of that convex hull.* For a general PAC algorithm we have to be able to handle the case when the convex hull has most or all of the points at its vertices, as can be expected to happen for an input distribution whose domain is the boundary of a circle, for example. Our general approach is to start out by computing the convex hull P and give maximal score to points inside P (which are guaranteed to have the same class label as the observed data). Then give an intermediate score to points in a polygon Q containing P, where Q has fewer edges. We argue that the way Q is chosen ensures that most points in Q are indeed claimed by the learner.

[3] A *box* means the intersection of a set of halfspaces whose bounding hyperplanes are axis-aligned, *i.e.* each hyperplane is normal to one of the axes.

[4] The *convex hull* of a finite set S of points is the smallest convex polygon (more generally, polytope) that contains S. Clearly all the vertices of the convex hull of S are members of S.

The Algorithm. The general idea is to choose a discriminant function in such a way that we can show that the boundary between the classes is piecewise linear with $O(\sqrt{N})$ pieces, where N is sample size. This sublinear growth ensures a PAC guarantee, since we have an "Occam" hypothesis — the V-C dimension of piecewise linear separators in the plane with $O(\sqrt{N})$ pieces is itself $O(\sqrt{N})$.

1. Draw a sample S of size $N = \Theta(\log(\delta^{-2}\epsilon^{-2})/\epsilon^2)$.
2. Let polygon P be the convex hull of S.
3. Let Q be a polygon having $\leq 2 + \sqrt{N}$ edges such that
   (a) Every edge of Q contains an edge of P
   (b) Adjacent edges of Q contain edges of P that are $\leq \sqrt{N}$ apart in the adjacency sequence of P's edges.
4. Define discriminant function h as follows.
   (a) For points in P use a score of 1.
   (b) For each region contained between P and 2 adjacent edges of Q, give points in that region a score of the negation of the area of that region.
   (c) Reject all other points (not in Q).

Regarding step 3: Q can be found in polynomial time; we allow Q to have $2 + \sqrt{N}$ edges since P may have 2 acute vertices that force pairs of adjacent edges of Q to contain adjacent edges of P.

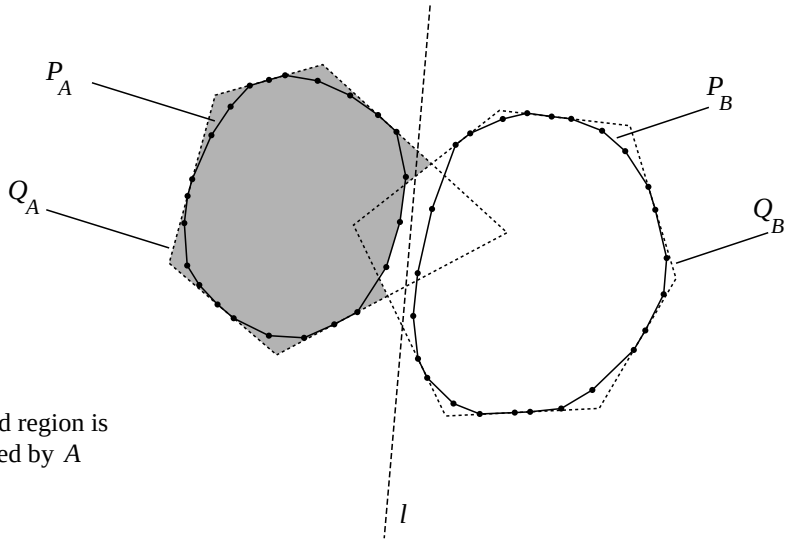

figure 1

Proving That the Algorithm is PAC. Figure 1 illustrates the construction. Let P_A and P_B be the convex hulls initially found by learners A and B respectively. They define subsets of the regions claimed by A and B respectively. Let Q_A and Q_B be the polygons Q constructed by A and B respectively. Let l be a line separating P_A and P_B. Observe that Q_A and Q_B respectively can each only have at most two edges that cross l, and at most one vertex on the opposite side of l from P_A and P_B respectively, using the fact that each edge of Q_A contains an edge of P_A, and similarly for Q_B and P_B.

Hence only one of the regions enclosed between P_A and two adjacent edges of Q_A can cross line l, and potentially be used to claim part of the interior of Q_B. If this region contains more than one of the similar regions in Q_B, then it will not in fact claim those regions of Q_B, since the score assigned to its interior will be lower. Omitting the details, it is not hard to show using these observations that the region claimed by A is enclosed by a polygon with $O(\sqrt{N})$ edges, and similarly for B. N was chosen such that the V-C bound of section 3.3 ensures PAC-ness with parameters ϵ and δ.

4 Conclusion and Open Problems

The standard requirement of PAC learning that algorithms must work for any input distribution D, appears to give rise to very novel algorithmic challenges, even for fairly elementary computational learning problems. At the same time however, the resulting algorithms do not appear to be applicable to the sort of class overlap situations that motivated the learning setting. Probably it will be necessary to model learning situations with an additional assumption that D should belong to some given class of distributions, as we did in section 3.1. Our formalisation of this learning setting will hopefully provide insights into what assumptions need to be made about the distribution of inputs, in order for standard practical methods of unsupervised learning to be applied.

The main open question is whether there is a PAC-learnable concept class that is not PAC-learnable in the two unsupervised learners framework. It would be remarkable if the two learning frameworks were equivalent, in view of the way the PAC criterion seems to impose a discipline of class separation on algorithms. Regarding specific concept classes, the most interesting one to get an answer for seems to be the class of monomials, a special case of nearly all boolean concept classes studied in the literature. It may be possible to extend the approach in section 3.1 to the assumption that D is a mixture of two product distributions, a class of distributions shown to be learnable in [8, 11].

Related open questions are: does there exist such a concept class for computationally unbounded learners (where the only issue is sufficiency of information contained in a polynomial-size sample). Also, can it be shown that *proper* PAC-learnability holds for some concept class but not in the two unsupervised learners version. (So, we have given algorithms for various learning problems that are known to be properly PAC-learnable, but the hypotheses we construct do not generally belong to the concept classes.)

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