Estimating a mixture of two product distributions

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Abstract

We describe an efficient algorithm for estimating a mixture of two product distributions over binary vectors.

1 Introduction

There are two major lines in research in Machine learning, supervised learning and unsupervised learning. Supervised learning has been the more appealing to theoretical analysis, since the goal that it sets is very clear. We have some unknown target function that labels the examples, and we would like to build a good approximation for it. In unsupervised learning the goal is far less clear. We are given examples, but there is no labeling. The vague general goal is to find meaningful structure in the data.

One way to find a structure in the data is to approximate the distribution that generates it. This is the well studied problem of distribution estimation or density estimation. This problem has a well-defined and agreed upon goal and measure of performance. Given a sample generated from some target distribution, the goal is to output a distribution which is close to the target distribution. The most common measures of performance are the likelihood of the data given the model and the Kullback-Leibler (KL) divergence between the model and the true distribution.

Much of the research in distribution estimation is focused on mixture of simple distributions, e.g. mixture of Gaussians. The motivation is that each component in the mixture represents a “cluster” of similar instances.

Given unlabeled data that is generated from this mixture we have two related tasks, one is to estimate the parameters of the mixture distribution, and the other, usually referred to as “clustering”, is to identify each example with the cluster (or clusters) that is most likely to have generated it. Many algorithms for estimating mixture distributions, including our algorithm, work by alternating between the two tasks. Improving the model estimate is used to improve the accuracy of the association of each example with a cluster and improving the accuracy of these associations is used to improve the estimate of the parameters.

In this work our simple distributions are product distribution over binary n-bit vectors. The target distribution is a mixture of two such product distributions. Even this simple case turns out to be quite challenging, especially when we want our algorithm to be efficient for high dimensional data and the distance between the mixture components is small. We design an algorithm that given a large enough sample from the target distribution finds a mixture of two product distributions which are close to the target distribution in terms of the KL-divergence. Our algorithm is efficient both in its sample complexity and its computational complexity.

Our algorithm uses two novel ideas, which might also be useful in other cases. The first idea is to have a held-out set of attributes. We use one set of attributes to split in the sample into two parts, with the goal that the parts be very different from each other in terms of the ratio of instances originating from the two mixture components. If the components are sufficiently far from each other, than each part will contain almost exclusively instances from one component and the problem becomes trivial. However, even if the split is far from perfect we show how to estimate the distribution accurately. To do that we use the held-out attributes. The advantage of using the held-out attributes is that the marginal distribution of these attributes is a mixture of two product distributions for each part of the split sample. This is not the case with the original attributes that were used to
split the sample. The second idea is that of a dimension reduction. We are given data from an n-dimensional space and show how to reduce the n-dimensional search to a one-dimensional search over α line, which greatly reduces the computational complexity.

We do not attempt to give here a comprehensive review on the work on distribution estimation, but rather mention a few results whose main concern (as in this work) is the computational complexity. The work of Kearns et al. [KMR+94] defines the computational setting of learning distributions, and also gives a few examples of distributions which can be learned efficiently. The work of Freund and Ron [FR95] studies a related problem of identifying biased coins from sequences.

There is a vast literature in statistics on distribution estimation in general, and mixture models in particular. There is a necessary and sufficient condition for a mixture to be identifiable [YS98]. Identifiability means that each mixture distribution has a unique representation. Note that identifiability is stronger than learnability, since for learnability it is enough to output some good model, and it might be that the true model is not unique.

We are interested here in the possibility of learning mixtures with similar components in a high dimensional space and with relatively small samples. One source of difficulty in this case is that the difference between the components might be undetectable when considering any small subset of the components. Thus any method that relies on low order statistics, such as the moment method for learning mixture distributions (described, for example, in [TSM85]) will necessarily require very large amounts of data. Another popular method for learning mixtures is EM, and our algorithm can be seen as a version of EM. However, while the analysis of EM usually guarantees only asymptotic convergence, we are interested here in designing an algorithm that can be proven to converge within a single iteration.

The paper is organized as follows. In Section 2 we define our notation and the learning model. In Section 3 we describe the algorithm. We prove its correctness in Section 4.

2 Model and Notation

2.1 Notation

Given a vector x we denote its ith coordinate by x_i. For a set of attributes S ⊆ {1, ..., n}, and a vector q of length n, we denote by q_S a vector that includes only the coordinates in S. The inner product of two n-dimensional vectors a and b, is <a, b> = \sum_{i=1}^{n} a_i b_i. For a set S of attributes then <a, b>_{S} = \sum_{i \in S} a_i b_i. A random set S \subseteq \{1, ..., n\} has Pr[i \in S] = 1/2 independently for each i. The operation round(ρ, q) receives a vector q ∈ [+1, −1]^n and returns a vector q' such that, if q_i < ρ then q'_i = ρ, if q_i > 1 − ρ then q'_i = 1 − ρ, otherwise q'_i = q_i.

2.2 Product distributions

A product distribution over binary vectors in \{-1, +1\}^n is characterized by its expected value q ∈ [-1, 1]^n. A random vector x from the distribution q is generated by independently selecting each coordinate x_i to be 1 with probability (1 + q_i)/2 or x_i = −1 with probability (1 − q_i)/2. It is easy to verify that the expected value of vectors selected in this way is indeed q, a fact which we express as

E_{x \sim q}[x] = q

A mixture of two product distributions is characterized by a triplet (q^{(1)}, q^{(2)}, γ) where q^{(1)}, q^{(2)} ∈ [-1, 1]^n are the component centers and γ ∈ [0, 1/2] is the mixture coefficient. To generate an example x from the mixture distribution, we select the index b to be 1 or 2 with probabilities γ or 1 − γ, respectively, and then generate x according to the product distribution q^{(b)}.

2.3 Learning Algorithm

A learning algorithm A samples examples from a mixture distribution (q^{(1)}, q^{(2)}, γ). It outputs a mixture model (q^{(1)}, q^{(2)}, g), such that the KL-divergence between the models is small, where The KL-divergence between two distributions P and Q is KL(Q || P) = E_{Q}[log(Q/P)]

Formally, an algorithm A is a learning algorithm for mixture of two product distributions if after sampling m examples it outputs a model (q^{(1)}, q^{(2)}, g), such that with probability 1 − δ,

KL[(q^{(1)}, q^{(2)}, γ) || (q^{(1)}, q^{(2)}, g)] ≤ ε.

Algorithm A is an efficient algorithm if it runs in time polynomial in 1/ε, log(1/δ) and n.

3 The Algorithm

3.1 Overview

Consider the centers q^{(1)} and q^{(2)} as points in an n-dimensional space. The crux of our algorithm is to reconstruct the line that connects q^{(1)} to q^{(2)}. In order to reconstruct a line we need only two points. The average value of the mixture (q^{(1)}, q^{(2)}, γ) is one point on the line. Our main aim is to find another point on this line. Once we have this second point we can reconstruct the line and perform a brute-force search on it.

Given access to a mixture distribution with the same centers and different mixture coefficient, i.e., (q^{(1)}, q^{(2)}, μ), it is easy to construct the second point. Simply take the average of the distribution. Here is how we find such a distribution.

We identify a subset of the examples such that the fraction of examples from q^{(1)} is μ ≠ γ. The problem is
that after the split the attributes in the examples from \( q_{(a)} \) are not independent. This is where we use the idea of a held-out set of attributes. We ignore the held-out set of attributes during the splitting process. After the split, the distribution on the held-out attributes is a mixture of the two product distributions with a different mixture coefficient. Thus we can compute the average of the new mixture and use it as the second point to define the line.

Since we are not given the averages exactly, our algorithm has to be numerically stable. For this reason we need that \( |\gamma - \mu| \) is non-negligible.

To complete the algorithm we search on this line for the optimal pair of centers to maximize the likelihood of the data. The main feature of this algorithm is that it reduced an \( n \)-dimensional search into a one dimensional search.

### 3.2 Description of the algorithm

The following is a high level sketch of the algorithm. (The detailed algorithm is described in Figure 1.) The main procedure (MAIN) receives as input a sample \( T \) of size \( m \) and outputs a model for the distribution. It works in the following way. First it computes the average of the entire sample and computes the likelihood it generated the sample \( T \). Then it chooses a random set \( S \) (which is used to partition the coordinates) and calls the procedure \( \text{Estimate}\_\text{SET} \) once with inputs \( S \) and \( T \) and once with inputs \( S \) and \( T \). We would like a split \( S \) to be such, that the difference between the centers would be significant both in coordinates in \( S \) and in \( T \). (In Section 4.1 we show that with probability \( 1/2 \) we have a good split.) The procedure \( \text{Estimate}\_\text{SET} \) outputs a model for each call, and we combine the two models, for \( S \) and \( T \) to get a global model, and test its likelihood. The output of MAIN is the model with the highest likelihood.

The procedure \( \text{Estimate}\_\text{SET} \) receives the sets \( S \) and \( T \) as input, and outputs a model for the distribution restricted to \( S \). Its operation consists of the following steps.

1. Choose a random vector \( x^* \) from the sample \( T \) of size \( m \). (Each \( x \in T \) has probability \( 1/m \).) We like \( x^* \) to have the property, that when restricted to \( S \), examples from different centers have different expected value of inner product with \( x^* \). (In Section 4.3 we lower bound this probability.)

2. Given \( x^* \) we compute a threshold \( \hat{\theta} \) and split \( T \) to \( T^{(\ge)} \), which includes all the examples for which the inner product is more than \( \hat{\theta} \) and \( T^{(\le)} \) which includes the remaining examples. We set \( \hat{\theta} \) to the average value of the inner product of \( x^* \) with \( y \in T \), i.e., \((1/m)\sum_{y \in T} <x^*, y> \geq S \). (In Section 4.3 we shows that the fraction of examples in \( T^{(\le)} \) from any of the two centers is different than \( \gamma \) and \( 1 - \gamma \).

3. Compute the average of examples in \( T \) on \( S \) (denoted by \( \hat{q}_{(a)} \)) and the average of \( T^{(\le)} \) on \( S \) (denoted by \( \hat{q}_{(a)} \)). (In Section 4.4 we show that there is a non-negligible distance between the two vectors.)

4. We connect \( q_{(a)} \) and \( q_{(a)} \) to a line, and define on it points with a spacing of \( \lambda \), where \( \lambda = \hat{q}_{(a)} - \hat{q}_{(a)} \) and \( \lambda \) is a parameter. We also discretize the value of \( \gamma \) with a spacing parameter \( \lambda \gamma \). Given any pair of discretized points \( p_1 \) and \( p_2 \) on the line and any discretized value \( g \) for the mixture coefficient, we compute the likelihood that the model \( \langle p_1, p_2, g \rangle \) generated \( T \). The model with the maximum likelihood is our estimator of the target mixture distribution on \( S \). The number of models we consider is at most \((\beta/\lambda)^2(1/\lambda \gamma)\), where \( \beta = 2/\max_j \{\lambda j\} \). (In Section 4.5 we show that there is a model which we consider and is near the target model. In Section 4.6 we show that it has a small KL divergence to the true model.)

### 4 Proof of learnability

In this section we show that our algorithms learns efficiently a mixture of two product distributions. As a part of the proofs we show how to determine the parameters of the algorithm.

#### 4.1 Splitting the attributes

Given two vectors \( q^{(1)}, q^{(2)} \in [-1, 1]^n \), we assume that the distance between them is non-negligible, i.e., \( \|q^{(1)} - q^{(2)}\|_2 \) is large. We like to show that with non-negligible probability, if we choose a random set \( S \), then both \( \sum_{i \in S} (q_i^{(1)} - q_i^{(2)})^2 \) and \( \sum_{i \notin S} (q_i^{(1)} - q_i^{(2)})^2 \) are not negligible.

**Lemma 4.1** Let \( a_1, \ldots, a_n \) be a set of non-negative real numbers whose maximal value is \( a_{\text{max}} \) and whose sum is \( L \). Let \( S \) be a random subset of \( \{1, \ldots, n\} \) which includes each element with probability \( 1/2 \). Then with probability at least \( 1/2 \), we have both \( \sum_{i \in S} a_i \geq (L - a_{\text{max}})/4 \) and \( \sum_{i \notin S} a_i \geq (L - a_{\text{max}})/4 \).

**Proof:** There is a set \( T \subset \{1, \ldots, n\} \) such that \( |(\sum_{i \in T} a_i) - (\sum_{i \notin T} a_i)| \leq a_{\text{max}} \). Let \( \sum_{i \in T} a_i = L_1 \). For any subset \( S_1 \subset T \) either \( \sum_{i \in S_1} a_i \geq L_1/2 \) or \( \sum_{i \in T - S_1} a_i \geq L_1/2 \). Similarly, let \( \sum_{i \in S_2} a_i = L_2 \). For any subset \( S_2 \subset T \) either \( \sum_{i \in S_2} a_i \geq L_2/2 \) or \( \sum_{i \in T - S_2} a_i \geq L_2/2 \).

Choosing a random set of coordinates \( S \) by picking each coordinate independently at random is equivalent
to choosing $S_1$ at random from $T$, $S_2$ from $\hat{T}$ and then choosing with probability $1/4$ one of the four combinations: $S_1 \cup S_2$, $S_1 \cup S_3$, $S_2 \cup S_3$, and $S_1 \cup S_3$. Therefore, the probability that the larger sum in $S_1$ is matched with the smaller sum in $S_2$ is $1/2$. This guarantees that the elements in $S$ have a sum of at least $L_1/2$ and the elements in $\hat{S}$ have a sum of at least $L_2/2$. Since $L_1 + L_2 = L$ and $|L_1 - L_2| \leq \epsilon_{\text{max}}$, the lemma follows. □

To apply this lemma to our problem we define the distance between two centers, $d$, to be

$$d = \frac{\|q(1) - q(2)\|_2 - \max\{(q(1) - q(2))^2\}}{4}.$$ 

Setting $\epsilon_{\text{th}} = (q(1) - q(2))^2$ we get the following corollary from Lemma 4.1.

**Corollary 4.2** Let $q(1)$, $q(2)$ be any two vectors in $[+1, -1]^n$. With probability at least $1/2$, a random set of coordinates $S$ has the property that both $\|q(s) - q(s')\|_2 \geq d$ and $\|q(\hat{s}) - q(\hat{s}')\|_2 \geq d$.

### 4.2 Finding a Split

Let us review how we find a split: (1) we choose a random vector $x^*$ from our sample, and a threshold $\hat{\theta}$. (2) For each $y \in T$ we compute $<x^*, y > s$. (3) If $<x^*, y > s$ is larger than $\hat{\theta}$ then $y$ belongs to $T(>)$ and otherwise $y$ belongs to $T(<)$. Our main aim will be to show that the fraction of elements from $q(1)$ in $T(\leq)$ is significantly different from $\gamma$.

We start by showing that there exists some $\theta$ for which the behavior of the two centers is different. Assume that $x$ is distributed according to $q(1)$ and $y$ is distributed according to $q(2)$. Then,

$$E_{x \sim q(1), y \sim q(2)}[<x, y > s] = E_{x \sim q(1), y \sim q(2)}[<x, y > s]$$

In the case that $y$ is chosen from $q(1)$, we have

$$E_{x \sim q(1), y \sim q(1)}[<x, y > s] = E_{x \sim q(1), y \sim q(1)}[<x, y > s]$$

We hope that there is a significant difference between the two expectations, so that it will influence the split. However, the difference in the expectation is $<q(1), (q(1) - q(2)) > s$, which might be zero. (Recall that we have no assumption on the norm of $q(1)$ and $q(2)$.)

We show that the difference can not be zero both in the case that $x$ is chosen from $q(1)$ and from $q(2)$. Let,

$$\text{diff}(x) = E_{y \sim q(1)}[<x, y^{(1)} > s] - E_{y \sim q(2)}[<x, y^{(2)} > s]$$

We have that,

$$E_{x \sim q(1)}[\text{diff}(x)] + E_{x \sim q(0)}[\text{diff}(x)] = <q(1), q(1) - q(2) > s + <q(2), q(2) - q(1) > s = \|q(1) - q(2)\|_2$$

This implies immediately the following lemma.

**Lemma 4.3** Either $E_{x \sim q(1)}[\text{diff}(x)] \geq d/2$ or $E_{x \sim q(2)}[\text{diff}(x)] \geq d/2$.

We say that a vector $x \in \{-1, +1\}^n$ is good if $\text{diff}(x) \geq d/4$. The next lemma gives a lower bound on the probability of choosing a good vector.

**Lemma 4.4** Let $x$ be generated by $(q(1), q(2), \gamma)$. The probability that $x$ is good is at least $p = \gamma \min\{d/32, 1/2\}$.

**Proof:** Without loss of generality assume that $E_{x \sim q(1)}[\text{diff}(x)] = \eta \geq d/2$. The probability that $x$ is generated from $q(1)$ is at least $\gamma$. Assume that $x$ is generated by $q(1)$.

By definition, $\text{diff}(x) = \sum_{y \in T} X_y(q_y^{(1)} - q_y^{(2)})$, where $X_y$ is $+1$ with probability $(q_y^{(1)}/2)$ and otherwise $-1$.

We can now apply a Chernoff bound on $\text{diff}(x)$,

$$P[|\text{diff}(x) - \eta| > \eta/2] \leq e^{-\eta/8} \leq e^{-d/16}.$$

For $d \geq 16$ this probability is less than $1/2$. For $d < 16$ this probability is less than $1 - d/32$. This implies that the probability that $\text{diff}(x) \geq d/2$ is at least $\min\{1/2, d/32\}$. □

We expect that, with high probability, that a large fraction of the examples in $T$ are good.

**Corollary 4.5** For $m > (8/p) \log(1/\delta)$, with probability $1 - \delta$, at least $pm/2$ of the points in $T$ are good.

The above corollary guarantees that with high probability we have a sample such that the fraction of good points is at least $p/2$.

### 4.3 Choosing the threshold $\hat{\theta}$

The next step is to choose the threshold parameter $\hat{\theta}$. Given $x$ let $\theta(x) = E[<x, y > s]$, where $y$ is distributed according to the mixture distribution $(q(1), q(2), \gamma)$. By definition,

$$\theta(x) = \gamma E_{y \sim q(1)}[<x, y^{(1)} > s] + (1 - \gamma) E_{y \sim q(2)}[<x, y^{(2)} > s].$$

Let

$$R(x, \theta) = \min\{|E_{y \sim q(1)}[<x, y^{(1)} > s] - \theta|, |\theta - E_{y \sim q(2)}[<x, y^{(2)} > s]|\}.$$

Note that, $R(x, \theta(x)) \geq \gamma \text{diff}(x)$. This implies that $x$ is good if $x$ is good then $R(x, \theta(x)) \geq \gamma d/4$. Let,

$$\hat{\theta}(x) = \frac{1}{m} \sum_{y \in T} <x, y > s.$$

The following lemma (whose proof is in the Appendix) bounds the error in $\hat{\theta} = \theta(x^*)$. 


Lemma 4.6 With probability $1 - \delta$ we have that for each $x \in T$, $|\hat{\theta}(x) - \theta(x)| \leq \gamma d^2 / \delta$, given that $m > c(n/(\gamma^2 d^2)) \log(1/\delta)$, for some constant $c$.

Note that if $|\hat{\theta}(x^*) - \theta(x^*)| \leq \gamma d^2 / \delta$ and $x^*$ is good then $|R(x^*, \hat{\theta})| \geq \gamma d / \delta$. (Recall that $\hat{\theta} = \hat{\theta}(x^*)$.)

4.4 Properties of the split

Let $R = R(x^*, \hat{\theta})$. We assume, without loss of generality, that $E_{y \sim q_1}[<x^*, y > s] > \hat{\theta} + R$ and $E_{y \sim q_0}[<x^*, y > s] < \hat{\theta} - R$. We are interested in computing the probabilities:

$$\mu(b) = \Pr_{y \sim q(b)}[<x^*, y > s > \hat{\theta}],$$

for $b \in \{1, 2\}$. The probability that a vector $x$ was generated from the component $q^{(1)}$, given that $<x^*, y > s > \hat{\theta}$ is $\mu = \mu^{(1)} / (\gamma^{(1)} + (1 - \gamma)\mu^{(2)})$. We would like to show that $|\mu - \gamma|$ is large.

The simple case is if $d = \Omega(\sqrt{n \log n})$. This implies that $R = \Omega(\sqrt{n \log n})$. In such a case we have that $\mu^{(1)} \approx 1$, and thus we have a perfect split, and we are done. The more challenging case is when $d$ is small, and thus $R$ is small, and this is the case we address here. (The proof is given in the Appendix.)

Lemma 4.7 Fix $x$ and let $Q = (q^{(1)}, q^{(2)}, \gamma)$ be a model of mixture of two product distributions, such that $\sum_{j \in \{1, 2\}} q_j^{(b)} \in [-1 + \alpha, 1 - \alpha]$, for some constant $\alpha$ and $b \in \{1, 2\}$. Let $Q'$ be the distribution $Q$ restricted to vectors $y$ such that $<x, y > s > \hat{\theta}(x)$.

Then $Q'$ is a mixture distribution $(q^{(1)}, q^{(2)}, \gamma)$ and $|\mu - \gamma| > c_0 R(x, \hat{\theta}(x)) \gamma / \sqrt{n}$, for some constant $c_0$.

Now we like to say that if $x^*$ is good, a similar claim holds for it. Recall that $T^{(\leq)} = \{y \in T : <x, y > s \leq \hat{\theta}\}$. For the analysis we need to split the set $T$ to a part generated by $q^{(1)}$ and a part generated by $q^{(2)}$. Clearly we do not have this split in the algorithm, but we use it only for the analysis. Let $T^{(b)}$ include the examples in $T$ generated using $q^{(b)}$, for $b \in \{1, 2\}$. Let,

$$\mu^{(b)} = \frac{|T^{(b)} \cap T^{(\leq)}|}{|T^{(\leq)}|}.$$

Using a standard Chernoff bound we have the following lemma.

Lemma 4.8 For $m > 16 \lambda^{-2} \log(2/\delta)$, with probability $1 - \delta/2$, we have that $|\mu^{(b)} - \mu^{(b)}| \leq \lambda / 4$.

4.5 Choosing the candidate models

Up to now we have computed some split using part of the attributes, i.e. $S$. Now we will use the other part, $\tilde{S}$, of the attributes to find candidate centers. We would like to show that we can find two centers which are very near the true centers, and thus would be a good approximation. From now on we will consider only the second part of the attributes, $\tilde{S}$.

Let $q^{(a)}_s = \gamma q^{(1)}_s + (1 - \gamma)q^{(2)}_s$. Then $q^{(1)}_s = q^{(a)}_s + (1 - \gamma)\Delta$ and $q^{(2)}_s = q^{(a)}_s - \gamma \Delta$, where $\Delta = q^{(1)}_s - q^{(2)}_s$.

Using our sample we compute an estimate of $q^{(a)}_s$, which is $q^{(a)}_s = \frac{1}{m} \sum_{y \in T} y \tilde{s}$. Let $\epsilon_s = q^{(a)}_s - q^{(a)}_s$.

Now assume that we are given another sample of the data distributed according to a different set of mixture coefficients. This is the effect that we get by using our split, we sample form $q^{(1)}_s$ with probability $\mu$ (rather than $\gamma$). Let $q^{(a)}_s = \mu q^{(1)}_s + (1 - \mu)q^{(2)}_s$. Similarly $q^{(a)}_s$ is the observed average, i.e. $\frac{1}{|T^{(\leq,s)}|} \sum_{y \in T^{(\leq,s)}} y \tilde{s}$ and $\epsilon_s$ is the error. We have,

$$\Delta = q^{(a)}_s - q^{(a)}_s$$

We can estimate the direction of $\Delta$ using $\hat{\Delta} = q^{(a)}_s - q^{(a)}_s$, but since we do not know either $\gamma$ or $\mu$ we can not approximate $\Delta$ directly. The following lemma bound the errors in the estimations.

Lemma 4.9 For $m > 16 \lambda^{-2} \log(4n/\delta)$, with probability $1 - \delta$, we have that $\|q^{(a)}_s - q^{(a)}_s\|_\infty \leq \lambda$ and $\|q^{(a)}_s - q^{(a)}_s\|_\infty \leq \lambda$.

Proof: For each attribute, with probability $1 - \delta / 4n$, the error is at most $\lambda$. This immediately implies that with probability $1 - \delta / 4$ the error in all the estimations is at most $\lambda$, i.e., $\|q^{(a)}_s - q^{(a)}_s\|_\infty \leq \lambda$.

Proving the bound of $\|q^{(a)}_s - q^{(a)}_s\|_\infty \leq \lambda$ is slightly more delicate, since the split is define only after we have the sample. First we argue that our sample has (approximately) the correct ratio of the split. By Lemma 4.8, $|\hat{\mu} - \mu| < \lambda / 4$, with probability $1 - \delta/2$. Using a Chernoff bound, the average in $T^{(b)} \cap T^{(\leq,s)}$ differs from $q^{(1)}$ by at most $\lambda / 4$, with probability at most $1 - \delta/2$. The total error is at most $3\lambda / 4 < \lambda$.

We use $q^{(a)}_s$ and $q^{(a)}_s$ to create a line, and then discretize the line with a small spacing. The following lemma bound the distance of the “true” centers to the discrete points on this line.

Lemma 4.10 With probability $1 - \delta$, for $b \in \{1, 2\}$, there exists an integer $j_b$, such that,

$$\|q^{(b)}_s - \hat{\theta}^{(b)} - j_b \lambda(q^{(a)}_s - q^{(a)}_s))\|_\infty < \frac{6 \lambda}{|\gamma - \mu|}$$
4.6 Maximum Likelihood

In this section we show that the maximum likelihood would give us a good approximation of the target distribution.

**Lemma 4.11** Let $Q$ be any distribution. Let $P = (p^{(1)}, p^{(2)}, \gamma')$ be a model of mixture of two product distributions, such that $p_j^{(j)} \in [p, 1 - \rho]$. With probability $1 - \delta$, we have,

$$|E_{x \sim Q}[\log P(x)] - \frac{1}{m} \sum_{y \in T} -\log P(y)| \leq n \log(1/\rho) \sqrt{\frac{\log(1/\delta)}{m}},$$

where $y \in T$ are i.i.d. sample from $Q$.

**Proof:** For any $y$ we have $-\log P(y) < n \log(1/\rho)$. The lemma follows from a Chernoff bound. □

The above lemma states that we have a good estimate of the log-loss of a distribution (and therefore of the KL divergence). We need to show that if we have a model which is near the true model then its log-loss is small. (The proof is found in the Appendix.)

**Lemma 4.12** Let $Q = (q^{(1)}, q^{(2)}, \gamma)$ be a model of mixture of two product distributions. Let $P = (p^{(1)}, p^{(2)}, \gamma')$ be a model of mixture of two product distributions. Also, $|\gamma - \gamma'| < \lambda_\gamma$ and $p_j^{(j)} \in [\rho, 1 - \rho]$. Then,

$$KL(Q || P) = E_Q[\log(Q(x)/P(x))] \leq \gamma \frac{||p^{(1)} - q^{(1)}||^2}{2p(1 - p)} + (1 - \gamma) \frac{||p^{(2)} - q^{(2)}||^2}{2p(1 - p)} + \lambda_\gamma n \log(1/\rho) \frac{n}{m}$$

The following corollary would be later used to show that if $d$ is small we can approximate the mixture by a single product distribution.

**Corollary 4.13** Let $Q = (q^{(1)}, q^{(2)}, \gamma)$ be a model of mixture of two product distributions and let $q^{(a)} = \gamma q^{(1)} + (1 - \gamma)q^{(2)}$, and $q_j^{(b)} \in [\rho, 1 - \rho]$, for $b \in \{1, 2\}$. Then,

$$KL(Q || q^{(a)}) = E_Q[\log(Q(x)/q^{(a)}(x))] \leq \frac{||q^{(1)} - q^{(2)}||^2}{2p(1 - p)} \max\{\frac{\lambda q_j^{(1)} - q_j^{(2)}}{2p(1 - p)}\}$$

4.7 Putting it all together

We now group all the pieces to prove the correctness of our algorithm.

**Theorem 4.14** Our algorithm, given access to examples from $(q^{(1),}, q^{(2),}, \gamma)$, with probability $1 - \delta$, outputs a model $(q^{(1),}, q^{(2),}, g)$ such that,

$$KL[(q^{(1),}, q^{(2),}, \gamma)][(q^{(1),}, q^{(2),}, g)] \leq \epsilon$$

and the running time and the sample size of our algorithm is bounded by $\text{poly}(n, \epsilon, \log(1/\delta))$ assuming that $q_j^{(b)} \in [\alpha, 1 - \alpha]$ for $b \in \{1, 2\}$ and for some constant $\alpha$.

**Proof:** The proof is done in the following steps. First we show (under some “optimistic” assumptions) that one of the models that we will consider is near to the true model, and thus our output model has a small KL divergence. Second we show that with high probability, in some iteration, all our “optimistic” assumptions hold. Third, we compute the sample size. Fourth, we compute the running time. Finally, we discuss the case where $d$ is very small.

We start by showing that, with high probability, one of the models that we consider has a small KL divergence. Since we are approximating well the log-loss it implies that the model with the lowest log-loss has also the smallest KL divergence.

Let us make the assumption that $S$ is good, $x^*$ is good, and $R(x^*, \hat{\theta}(x^*)) \geq \gamma d/8$. By Lemma 4.10, with probability $1 - \delta$, for $b \in \{1, 2\}$, there is an integer $j_b$ such that

$$||q_j^{(b)} - (q^{(a)} + j_b \lambda(q_j^{(a)} - q_j^{(b)}))||_\infty < \frac{6 \lambda}{\gamma - \mu} < \frac{\epsilon d \sqrt{n} \lambda}{\gamma^2 d}$$

where the last inequality is by Lemma 4.7. Let $q^{(b, e)}$ be the vectors associated with $j_b$, $b \in \{1, 2\}$.

Consider the model $(q_j^{(1, e)}, q_j^{(2, e)}, \gamma')$, where $\gamma' = \lambda_\gamma \gamma / \lambda_\gamma$. Now by Lemma 4.12 the KL divergence between those two models is bounded by,

$$\lambda_\gamma n \log(1/\rho) + \frac{n \lambda^2}{\rho(1 - \rho) d^2 \gamma^4}$$

For

$$\lambda_\gamma < \frac{\epsilon}{n \log(1/\rho)} \text{ and } \lambda < \frac{\epsilon d \gamma^2 \sqrt{\rho(1 - \rho)}}{n}$$

the model $(q_j^{(1, e)}, q_j^{(2, e)}, \gamma')$ has KL divergence is at most $2\epsilon$.

By Lemma 4.11 we have that the errors in our estimation of the log-loss is at most $\epsilon$. This implies that the observer error of $(q_j^{(1, e)}, q_j^{(2, e)}, \gamma')$ is at most $3\epsilon$. Therefore the model with the lowest observed log-loss would have KL divergence of at most $4\epsilon$. 
The next step is to show that with high probability all our assumptions hold. First we show the probability that $S$ is good. Consider the procedure $\textsc{Main}$. The probability that we choose a good $S$ is at least $1/2$ each time in the loop, by Corollary 4.2. Therefore with probability $1 - \delta$ some set $S$ we choose is good.

For each set $S$, in procedure $\textsc{EstimateSET}$ runs $N$ times. The probability that $x^*$ is good is, by Lemma 4.4 and Corollary 4.5, at least $p/2 = \gamma \min\{d/64, 1/4\}$. Given that $x^*$ is good, by Lemma 4.6, the probability that $R(x^*, \theta(x)) \geq \gamma d/8$ is at least $1 - \delta$. Therefore, for $N = (\max\{128/d, 8\}) \log(2/\delta)$ the probability of success is at least $1 - \delta/2$. This completes the correctness.

The running time is bounded by,

$$O(\log(1/\delta)N m(\beta/\lambda)^2 (1/\lambda_1 \ln) = \text{poly}(\log(1/\delta), n, \epsilon).$$

The only parameter we still need to bound is $\beta = 2/\max\{\Delta_i\}$. For $\Delta = q^{(1)} - q^{(2)}, ||\Delta||_\infty > d^{1/2}n^2/n$. This implies that $\beta > 2n/d^{1/2}\gamma^2$. By our assumption that $q^{(2)}(a) \in [\alpha, 1 - \alpha]$, we can set $\rho = \alpha$, which is a constant.

The sample size required is,

$$\max\left\{ \frac{\log(1/\delta)}{\beta}, \frac{n}{\gamma d^2 \log(1/\delta)}, \frac{n^2 \gamma^2}{\epsilon^2 d^2 (1 - \rho)}, \frac{n^2 \gamma^2}{\epsilon^2 (\log(1/\rho)(\log w/\delta))} \right\} = \text{poly}(\log(1/\delta), n, \epsilon),$$

where $w$ is the number of models we generate and test, which is at most $(\beta/\lambda)^2 \lambda_1$. Note that (ignoring logarithmic factors) the behavior is $n^2/\epsilon^2$, which is a result of the accuracy requirement on the log-loss.

Both the sample size and the running time are inversely proportional to $d$, which is a problem if $d$ is very small. We can replace in the bounds $d$ by $\max\{d, \epsilon(1 - \rho)/4\}$, which solves the problem for small values of $d$. This is done by showing that if $d$ is very small we can approximate the mixture distribution by a single product distribution. If $d < c\epsilon(1 - \rho)/4$ then by Corollary 4.13,

$$KL(q^{(1)}, q^{(2), \gamma} || q^{(a)} \leq \frac{4d}{\rho(1 - \rho)} \leq \epsilon$$

where $q^{(a)} = \gamma q^{(1)} + (1 - \gamma) q^{(2)}$. Since we test $q^{(a)}$ in $\textsc{Main}$ the model we output has an observed KL divergence of at most $2\epsilon$, and thus a true KL divergence of at most $3\epsilon$. □

5 Conclusion

In this paper we focused on a very specific case: a mixture of two product distributions over binary vectors. We have given a polynomial time algorithm that computes a mixture distribution which is close to the target distribution, from which we are sampling.

There are many extensions which would be very interesting to pursue. One extension is to the case that the distributions are not over binary vectors but over the real valued vectors. For example, in each center each attribute is distributed according to a Gaussian distribution and the covariance matrix is diagonal. In such a case it seems that our techniques would be able to learn the mixture distribution.

A more challenging extension is to consider a mixture of three or more distribution. In this case one needs first to quantify when the mixture is non-redundant. Namely, when can the target mixture be well approximated by fewer centers. In the case of two centers this is easily captured by the distance between the centers. However when we are considering more centers the problem becomes non-trivial. Upcoming work by Dasgupta [Das] uses random projections of the data in a different and novel way in order to learn a mixture of an arbitrary number of Gaussians.

On a different front, recent work by Qiang Li [Li99] proves convergence rates on a greedy approach to learning mixture distributions. However, this work falls short of providing an efficient algorithm because it is unknown how to perform the greedy step in polynomial time with respect to the number of dimensions.

References


[YS86] S. J. Yakowitz and J. D. Spragins. On the
A Proofs

Proof of Lemma 4.6: We can think of the sum $\sum_{y \in T} < x, y >$ as being generated in the following fashion. In each of $m$ independent trials we choose $b$ to be 1 or 2 with probabilities $\gamma$ or $1 - \gamma$, respectively. Example $y$ generated according to $q^{(b)}$ are in $T^{(b)}$. Let $m_b$ be the size of $T^{(b)}$. We rewrite $\hat{\theta}(x)$ as follows,

$$
\hat{\theta}(x) = \frac{m_1}{m} \left[ \frac{1}{m_1} \sum_{y \in T^{(1)}} < x, y > + \frac{1}{m_2} \sum_{y \in T^{(2)}} < x, y > \right] + \frac{m_2}{m} \left[ \frac{1}{m_2} \sum_{y \in T^{(2)}} < x, y > \right]
$$

Recall that $\theta(x)$ is,

$$
\theta(x) = \gamma E_{y^{(1)} \sim q^{(1)}} [ < x, y^{(1)} > ] + (1 - \gamma) E_{y^{(2)} \sim q^{(2)}} [ < x, y^{(2)} > ].
$$

With probability $1 - \delta$ we have that $|\gamma - \frac{m_1}{m}| \leq \sqrt{\frac{\log(1/\delta)}{m}} = \epsilon_1$. Now bound the deviation in the estimation for each center,

$$
\left| \frac{1}{m_b} \sum_{y \in T^{(b)}} < x, y > s - E_{y^{(b)} \sim q^{(b)}} [ < x, y^{(b)} > s ] \right| 
\leq \sqrt{\frac{n \log(1/\delta)}{m_b}} = \epsilon_b.
$$

We can bound the total deviation by

$$
\frac{m_1 \epsilon_1}{m} + \frac{m_2 \epsilon_2}{m} + \epsilon_1 \text{diff}(x) = \sqrt{\frac{m_1 n \log(1/\delta)}{m}} + \sqrt{\frac{m_2 n \log(1/\delta)}{m}} + \frac{\log(1/\delta)}{m} \text{diff}(x) < \frac{\gamma \text{diff}(x)}{2}
$$

for $m > c(n \log(1/\delta))/(\gamma^2 d^2)$. \hfill \epf

Proof of Lemma 4.7: We are interested in bounding first $\mu^{(b)}$, for $b \in \{1, 2\}$. Recall that $< x^*, y^b > s = \sum_{j \in S} x^*_j y^b_j$. The problem is that the expectation of $y^b_j$ is $q^{(b)}_j$, and is different for different $j$. The following lemma by Hoeffding [Hoe56] reduces this case to the case where all the $y^b_j$ are i.i.d.

**Lemma A.1** Let $X_i$ be $n$ binary random variables which are independent. Let $\mu = E[\sum_{i=1}^{n} X_i]$. For an integer $k \leq \mu - 1$,

$$
Pr[\sum_{i=1}^{n} X_i \leq k] \leq Pr[\sum_{i=1}^{n} Y_i \leq k]
$$

where $Y_i$ are i.i.d binary random variables with $E[Y_i] = \mu/n$.

This enables us to reduce our case, with $y^b_j$ of different distributions, to a simple case where we have $z^b_j$ i.i.d., and the expectation of $z^b_j$ is $\eta^{(b)} = \sum_{j \in S} q^{(b)}_j / n$, for $b \in \{1, 2\}$. We now like to bound, $Pr[\sum_{j \in S} x^*_j z^b_j > \hat{\theta}]$.

Since the $z^b_j$ are i.i.d. random variables, the median is exactly (up to rounding) the expected value. Therefore,

$$
Pr[\sum_{j \in S} x^*_j \geq \hat{\theta} + R] \geq 1/2
$$

Similarly,

$$
Pr[\sum_{j \in S} x^*_j \geq \hat{\theta} - R] \leq 1/2
$$

Also, for some constant $c_1$, for $R < c_1 \sqrt{n}$,

$$
Pr[\sum_{j \in S} x^*_j \geq (\hat{\theta} + R)] \geq c_2 \frac{R}{\sqrt{n}}
$$

for some constant $c_2$. This implies,

$$
Pr[\sum_{j \in S} x^*_j \geq \hat{\theta}] \geq 1/2 + c_2 \frac{R}{\sqrt{n}}
$$

Therefore,

$$
\mu^{(1)} = Pr_{y \sim q^{(1)}} [ < x, y > s \geq \hat{\theta}] \geq Pr[\sum_{j \in S} x^*_j \geq \hat{\theta}] \geq 1/2 + c_2 \frac{R}{\sqrt{n}}
$$

Similarly,

$$
\mu^{(2)} = Pr_{y \sim q^{(2)}} [ < x, y > s \geq \hat{\theta}] \leq Pr[\sum_{j \in S} x^*_j \leq \hat{\theta}] \leq 1 - Pr[\sum_{j \in S} x^*_j < \hat{\theta}] \leq 1/2.
$$
This implies that,
\[
\mu - \gamma = \frac{\gamma \mu^{(1)}}{\gamma \mu^{(1)} + (1 - \gamma) \mu^{(2)}} - \gamma
\]
\[
= \gamma (1 - \gamma) \frac{\mu^{(1)} - \mu^{(2)}}{\gamma \mu^{(1)} + (1 - \gamma) \mu^{(2)}}
\]
\[
\geq \frac{\gamma R}{\sqrt{n}}
\]
which completes the proof. \( \square \)

**Proof of Lemma 4.10:** We do the proof for \( b = 1 \), the case of \( b = 2 \) is similar. Recall that \( q_s^{(1)} = q_s^{(a)} + (1 - \gamma) \Delta \). Let \( \Delta' = (q_s^{(a)} - q_s^{(a)})/(\gamma - \mu) \). Note that, \( \Delta' = \Delta + \frac{\Delta}{\gamma - \mu} \). The approximation error is,
\[
\|((q_s^{(a)} + (1 - \gamma) \Delta) - (q_s^{(a)} - j_1 \lambda (\gamma - \mu) \Delta'))\|_\infty.
\]
We can bound the error by,
\[
\|q_s^{(a)} - \hat{q}_s^{(a)}\|_\infty + |j_1 \lambda (\gamma - \mu) - (1 - \gamma)||\Delta||_\infty
\]
+\( ||\Delta - \Delta'||_\infty \)

Lemma 4.9 bounds the first term by \( \lambda \). The discretization error in \( |j_1 \lambda (\gamma - \mu) - (1 - \gamma)||\Delta||_\infty \) is bounded by \( \lambda \).

We can bound \( ||\Delta||_\infty \) by \( 2/(\gamma - \mu) \). Finally, \( ||\Delta - \Delta'||_\infty \), using Lemma 4.9, is bounded by \( 2\lambda/|\gamma - \mu| \). \( \square \)

**Proof of Lemma 4.12:** Using a general lemma (see [CT91]) we have that
\[
KL(\gamma q^{(1)} + (1 - \gamma) q^{(2)} || p^{(1)} + (1 - \gamma) p^{(2)})
\]
\[
\leq \gamma KL(q^{(1)} || p^{(1)}) + (1 - \gamma) KL(q^{(2)} || p^{(2)}).
\]
We are interested in computing,
\[
KL(\gamma q^{(1)} + (1 - \gamma) q^{(2)} || p^{(1)} + (1 - \gamma') p^{(2)}).
\]
Assume that \( \gamma \leq \gamma' \). (The case \( \gamma > \gamma' \) would be similar.)
Rewrite the KL divergence as,
\[
KL(\gamma q^{(1)} + (1 - \gamma) q^{(2)} || p^{(1)} + (1 - \gamma') p^{(2)}) = \gamma (p^{(1)} + (1 - \gamma))(\frac{\gamma' - \gamma}{1 - \gamma} p^{(1)} + \frac{1 - \gamma'}{1 - \gamma} p^{(2)})
\]
We can bound this KL divergence by,
\[
\gamma KL(q^{(1)} || p^{(1)}) + (1 - \gamma) KL(q^{(2)} || p^{(2)}) + (\gamma' - \gamma) KL(q^{(2)} || p^{(1)})
\]
Computing \( KL(q^{(b)} || p^{(b)}) \), \( b \in \{1, 2\} \), is rather simple, since we have a product distribution.
\[
KL(q^{(b)} || p^{(b)}) = \sum_{i=1}^n KL(q_i^{(b)} || p_i^{(b)}) \leq \frac{\|p^{(b)} - q^{(b)}\|^2}{2p(1 - p)}
\]
Finally, since \( p_i^{(b)} \in [p, 1 - p] \), we can bound \( (\gamma' - \gamma) KL(q^{(2)} || p^{(1)}) \) by \( \lambda_n \log(1/p) \). \( \square \)
Procedure MAIN

**Input:** A training set $T = \{x_1, \ldots, x_m\}$ where $x_i \in \{-1, +1\}^n$.

Compute the likelihood that the model $q^{(a)}$ generated $T$, where $q^{(a)}_S = \frac{1}{m} \sum_{y_j \in T} (y_j)_S$.

**Repeat for** $i = 1, 2, \ldots, \log(2/\delta)$

1. Choose a set $S$ by including each index $1 \leq i \leq n$ in $S$ with probability $1/2$. Let $\bar{S}$ be the complement of $S$.
2. Call `ESTIMATE_SET(T, S)` and `ESTIMATE_SET(T, \bar{S})`. Let $(q^{(1, S)}, q^{(2, S)}, g_1)$ and $(q^{(1, \bar{S})}, q^{(2, \bar{S})}, g_2)$ be the outputs.
3. Create eight models, $(q^{(b_1, S)}, q^{(b_2, S)}, \bar{q}^{(b_1, S)}, q^{(b_2, \bar{S})}, g_{b_1})$, where $b_1, b_2, b_3 \in \{1, 2\}$, and $\bar{b} = 3 - b$.
4. Compute the likelihood that each model generated the sample $T$.

**Output:** The model with the maximum likelihood to generate $T$.

Figure 1: The algorithm for learning a mixture of two product distributions

Procedure ESTIMATE_SET

**Input:** A training set $T = \{x_1, \ldots, x_m\}$ where $x_i \in \{-1, +1\}^n$, and a set $S \subseteq \{1, \ldots, n\}$.

**Repeat for** $i = 1, 2, \ldots, N$

1. Select a vector $x^*$ uniformly at random from the training set $T$.
2. Set a threshold $\tilde{\theta} = \frac{1}{m} \sum_{y_j \in T} < x^*, y >_S$.
3. Split the training set $T$ into two parts:
   $$T^{(\leq)} = \{ y \in T : < y, x >_S \leq \tilde{\theta} \}, \quad T^{(>)} = \{ y \in T : < y, x >_S > \tilde{\theta} \}$$
4. Calculate the average of each subset on the remaining coordinates:
   $$q^{(a)}_S = \frac{1}{|T^{(\leq)}|} \sum_{y_j \in T^{(\leq)}} (y_j)_S, \quad q^{(a)}_{\bar{S}} = \frac{1}{m} \sum_{y_j \in T} (y_j)_S.$$
5. Let $\hat{\Delta} = q^{(a)}_S - q^{(a)}_{\bar{S}}$, and $\beta = 2/\max_j \{\hat{\Delta}_j\}$. Let $F$ include the points $q^{(\leq)}_j + j \lambda \hat{\Delta}$ for integer $j$, $-\beta/\lambda \leq j \leq \beta/\lambda$. Let $\Gamma$ include the numbers $i \lambda$ for $0 \leq i \leq 1/\lambda$.
6. For each pair $p^{(1)}$ and $p^{(2)}$ in $F$ and $g$ in $\Gamma$ compute the likelihood that the model $(\rho, p^{(1)}), (\rho, p^{(2)}), g$ generated $T$.

**Output:** the model with the highest likelihood.

Figure 2: The procedure `ESTIMATE_SET`. The parameters $\lambda$, $\lambda$, and $N$ are determined in the proofs.