Learning Depth-Three Neural Networks in Polynomial Time

Surbhi Goel* and Adam Klivans†

Department of Computer Science, University of Texas at Austin
{surbhi,klivans}@cs.utexas.edu

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Abstract

We give a polynomial-time algorithm for learning neural networks with one hidden layer of sigmoids feeding into any smooth, monotone activation function (e.g., sigmoid or ReLU). We make no assumptions on the structure of the network, and the algorithm succeeds with respect to any distribution on the unit ball in \( n \) dimensions (hidden weight vectors also have unit norm). This is the first assumption-free, provably efficient algorithm for learning neural networks with more than one hidden layer.

Our algorithm—Alphatron—is a simple, iterative update rule that combines isotonic regression with kernel methods. It outputs a hypothesis that yields efficient oracle access to interpretable features. It also suggests a new approach to Boolean function learning via smooth relaxations of hard thresholds, sidestepping traditional hardness results from computational learning theory.

Along these lines, we give improved results for a number of longstanding problems related to Boolean concept learning, unifying a variety of different techniques. For example, we give the first polynomial-time algorithm for learning intersections of halfspaces with a margin (distribution-free) and the first generalization of DNF learning to the setting of probabilistic concepts (queries; uniform distribution). Finally, we give the first provably correct algorithms for common schemes in multiple-instance learning.

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1 Introduction

Giving provably efficient algorithms for learning neural networks is a longstanding and fundamental challenge in the theory of machine learning. Despite the remarkable achievements obtained in practice from applying tools for learning neural networks, surprisingly little is known from a theoretical perspective. In fact, much theoretical work has led to negative results showing that— from a worst-case perspective— even learning the simplest architectures seems computationally intractable [LSSS14, SVWX17]. For example, there are known hardness results for agnostically learning a single halfspace (learning a halfspace with adversarial noise) [KS09, Dan16].

As such, much work has focused on finding algorithms that succeed after making various restrictive assumptions on both the network’s architecture and the underlying marginal distribution. Recent work gives evidence that for gradient-based algorithms these types of assumptions are actually necessary [Sha16]. In this paper, we focus on understanding the frontier of efficient neural network learning: what is the most expressive class of neural networks that can be learned, provably, in polynomial-time without taking any additional assumptions?

1.1 Our Results

We give a simple, iterative algorithm that efficiently learns neural networks with one layer of sigmoids feeding into any smooth, monotone activation function (for example, Sigmoid or ReLU). Both the first hidden layer of sigmoids and the output activation function have corresponding hidden weight vectors. We assume nothing about these weight vectors other than the standard normalization that they have 2-norm equal to one. The algorithm succeeds with respect to any distribution on the unit ball in \( n \) dimensions. This is the first provably efficient, assumption-free result for learning neural networks with more than one hidden layer.

Our algorithm, which we call \textit{Alphatron}, combines the expressive power of kernel methods with an additive update rule inspired by work from isotonic regression. Alphatron also outputs a hypothesis that gives efficient oracle access to interpretable features. That is, if the output activation function is \( u \), Alphatron constructs a hypothesis of the form \( u(f(x)) \) where \( f \) is an implicit encoding of products of features from the instance space, and \( f \) yields an efficient algorithm for random access to the coefficients of these products.

More specifically, we obtain the following new supervised learning results by choosing an appropriate kernel function in conjunction with Alphatron:

- Let \( c(x_1, \ldots, x_n) \) be any feedforward neural network with one hidden layer of sigmoids of size \( k \) feeding into any activation function \( u \) that is monotone and \( L \)-Lipschitz. Given independent draws \( (x, y) \) from \( S^{n-1} \times [0, 1] \) with \( \mathbb{E}[y|x] = c(x) \), we obtain an efficiently computable hypothesis \( u(f(x)) \) such that \( \mathbb{E}[(c(x) - u(f(x)))^2] \leq \epsilon \) with running time and sample complexity \( \text{poly}(n, k, 1/\epsilon, L) \) (the algorithm succeeds with high probability).

- We obtain the first efficient PAC algorithm for learning intersections of polynomially many halfspaces (with a margin) with respect to any distribution on \( S^n \) (prior work due to [KS08] gave a quasipolynomial-time algorithm). We show that this is a special case of a more general class of Boolean learning problems where the goal is to learn Lipschitz-bounded combinations of Boolean functions in the probabilistic concept model due to Kearns and Schapire [KS94]. In this framework, we can learn smooth combinations of halfspaces (with a margin) whose sample complexity is \textit{independent} of the number of halfspaces.
We give the first generalization of well-known results for PAC learning DNF formulas with respect to the uniform distribution (given query access to the unknown DNF) to the setting of probabilistic concepts. Concretely, we give a query algorithm–KMtron– that learns any random variable whose conditional mean is a smooth, monotone combination of functions of bounded $L_1$-norm with respect to the uniform distribution on $\{0,1\}^n$. It is easy to see this captures the function class of polynomial-size DNF formulas.

We give the first provably efficient algorithms for nontrivial schemes in multiple instance learning (MIL). Consider an MIL scheme where a learner is given a set or bag of instances $x_1, \ldots, x_t$, and the learner is told only some function of their labels, namely $u(c(x_1), \ldots, c(x_t))$ for some unknown concept $c$ and combining function $u$. We give the first provably efficient algorithms for correctly labeling future bags even if the instances within each bag are not identically distributed. Our algorithms hold if the underlying concept $c$ is sigmoidal or a halfspace with a margin. If the combining function averages label values (a common case), we obtain bounds that are independent of the bag size.

Almost all of our results holds in the probabilistic concept model of learning due to Kearns and Schapire [KS94] and only require that the conditional mean of the label $y$ given instance $x$ is approximated by bounded-norm elements from a Reproducing Kernel Hilbert Space (RKHS). We learn specifically with respect to square-loss, though this will imply polynomial-time learnability for most commonly studied loss functions.

1.2 Relationship to Traditional Boolean Function Learning

PAC learning simple Boolean concept classes has proved challenging. For example, the best known distribution-free algorithm for learning an intersection of just two halfspaces runs in exponential time in the dimension. For learning intersections of polynomially many halfspaces, there are known hardness results based on cryptographic assumptions [KS09] or the hardness of constraint satisfaction problems [Dan16]. A source of angst in machine learning theory is that these hardness results do not square with recent practical successes for learning expressive function classes.

A key conceptual aspect of this work is to shift from the PAC model to the probabilistic concept model. We hope to revive the probabilistic concept model as a fertile area for constructing supervised learning algorithms, as it can handle both Boolean and real-valued concepts. Additionally, this model has the following interesting benefit that we feel has been overlooked: it allows for Boolean learning problems where an output hypothesis can answer “don’t know” by giving the value $1/2$. As mentioned above, hardness results from computational learning theory indicate that simple Boolean function classes such as intersections of halfspaces can encode pseudorandom outputs. For these classes, PAC learning is hopeless. On the other hand, in the probabilistic concept model, we measure error with respect to square-loss. In this model, for subsets of inputs encoding pseudorandom labels, a hypothesis may simply output $1/2$, which is essentially the optimal strategy.

The models we study in this paper still capture Boolean learning problems. More specifically, let $(x,y)$ be a random draw from a distribution where $y \in \{0,1\}$ with $E[y|x] = c(x)$. If $c$ always outputs 0 or 1, then we are in the typical PAC scenario. On the other hand, $c$ may be a real-valued function. Our approach is to consider Boolean learning problems where the conditional

\footnote{Since we only put a requirement on the conditional mean, this model naturally inherits strong noise-tolerant properties that previous work does not handle.}
mean function is computed by a real-valued neural network. These networks can be viewed as relaxations of Boolean function classes.

For example, one natural relaxation of an AND of \( k \) Boolean inputs would be a piecewise-linear combining function \( u \) that is 0 for all inputs in \( \{0, \ldots, k - 1\} \), equal to 1 on input \( k \), and a line that interpolates between \( u(k - 1) \) and \( u(k) \). Additionally, we could relax any halfspace \( \text{sign}(w \cdot x) \) defined on the unit sphere to \( \sigma(w \cdot x) \) where \( \sigma(z) = \frac{1}{1 + e^{-z}} \), a sigmoid. Although PAC learning an intersection of halfspaces seems out of reach, we can give fully polynomial-time algorithms for learning sums of polynomially many sigmoids feeding into \( u \) as a probabilistic concept.

1.3 Our Approach

The high-level approach is to use algorithms for isotonic regression to learn monotone combinations of functions approximated by elements of a suitable RKHS. Our starting point is the Isotron algorithm, due to Kalai and Sastry [KS09a], and a refinement due to Kakade, Kalai, Kanade and Shamir [KKKS11] called the GLMtron. These algorithms efficiently learn any generalized linear model (GLM): distributions on instance-label pairs \((x, y)\) where the conditional mean of \( y \) given \( x \) is equal to \( u(w \cdot x) \) for some (known) smooth, non-decreasing function \( u \) and unknown weight vector \( w \). Their algorithms are simple and use an iterative update rule to minimize square-loss, a non-convex optimization problem in this setting. Both of their papers remark that their algorithms can be kernelized, but no concrete applications are given.

Around the same time, Shalev-Shwartz, Shamir, and Sridharan [SSSS11] used kernel methods and general solvers for convex programs to give algorithms for learning a halfspace under a distributional assumption corresponding to a margin in the non-realizable setting (agnostic learning). Their kernel was composed by Zhang et al. [ZLJ16] to obtain results for learning sparse neural networks with certain smooth activations, and Goel et al. [GKKT16] used a similar approach in conjunction with general tools from approximation theory to obtain learning results for a large class of nonlinear activations including ReLU and Sigmoid.

1.4 Our Algorithm

We combine the two above approaches into an algorithm called Alphatron that inherits the best properties of both: it is a simple, iterative update rule that does not require regularization, and it learns broad classes of networks whose first layer can be approximated via an appropriate feature expansion into an RKHS. It is crucial that we work in the probabilistic concept model. Even learning a single ReLU in the non-realizable or agnostic setting seems computationally intractable [GKKT16].

One technical challenge is handling the approximation error induced from embedding into an RKHS. In some sense, we must learn a noisy GLM. For this, we use a learning rate and a slack variable to account for noise and follow the outline of the analysis of GLMtron (or Isotron). The resulting algorithm is similar to performing gradient descent on the support vectors of a target element in an RKHS. Our convergence bounds depend on the resulting choice of kernel, learning rate, and quality of RKHS embedding. We can then leverage several results from approximation theory and obtain general theorems for two different notions of RKHS approximation: 1) the function class can be uniformly approximated by low-norm elements of a suitable RKHS or 2) the function class is separable (similar to the notion of a margin) by low-norm elements of an RKHS.
For generalizing uniform-distribution DNF learning algorithms to the probabilistic concept setting, we re-interpret the KM algorithm for finding large Fourier coefficients \cite{KM93} as a query algorithm that gives accurate estimates of sparse, high-dimensional gradients. For the case of square-loss with respect to the uniform distribution on the hypercube, we can combine these estimates with a projection operator to learn smooth, monotone combinations of $L_1$-bounded functions (it is easy to see that DNF formulas fall into this class).

For Multiple Instance Learning (MIL), we observe that the problem formulation is similar to learning neural networks with two hidden layers. We consider two different types of MIL: deterministic (the Boolean label is a deterministic function of the instance labels) and probabilistic (the Boolean label is a random variable whose mean is a function of the instance labels). We make use of some further kernel tricks, notably the mean-map kernel, to obtain a compositional feature map for taking averages of sets of instances. This allows us to prove efficient run-time and sample complexity bounds that are, in some cases, independent of the bag size.

1.5 Related Work

The literature on provably efficient algorithms for learning neural networks is extensive. In this work we focus on common nonlinear activation functions: sigmoid, ReLU, or threshold. For linear activations, neural networks compute an overall function that is linear and can be learned efficiently using any polynomial-time algorithm for solving linear regression. Livni et al. \cite{LSSS14} observed that neural networks of constant depth with constant degree polynomial activations are equivalent to linear functions in a higher dimensional space (polynomials of degree $d$ are equivalent to linear functions over $n^d$ monomials). It is known, however, that any polynomial that computes or even $\epsilon$-approximates a single ReLU requires degree $\Omega(1/\epsilon)$ \cite{GKKT16}. Thus, linear methods alone do not suffice for obtaining our results.

The vast majority of work on learning neural networks takes strong assumptions on either the underlying marginal distribution, the structure of the network, or both. Works that fall into these categories include \cite{KOS04, KM13, JSA15, SAL14, ZPS17, ZLJ16, DFS16, ZSJ17, GK17}. In terms of assumption-free learning results, Goel et al. \cite{GKKT16} used kernel methods to give an efficient, agnostic learning algorithm for sums of sigmoids (i.e., one hidden layer of sigmoids) with respect to any distribution on the unit ball.

Another line of work related to learning neural networks focuses on when local minima found by gradient descent are actually close to global minima. In order to give polynomial-time guarantees for finding a global minimum, these works require assumptions on the underlying marginal or the structure of the network (or both) \cite{CHM15, Kaw16, BG17, SC16, LY17, Sol17}. All of the problems we consider in this paper are non-convex optimization problems, as it is known that a single sigmoid with respect to square-loss has exponentially many bad local minima \cite{AHW96}.

For classical generalization and VC dimension bounds for learning neural networks we refer the reader to Anthony and Bartlett \cite{AB99} (the networks we consider in this paper over the unit ball have VC dimension $\Omega(nk)$ where $k$ is the number of hidden units in the first layer).

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\cite{AB99} In their setting, even the case of linear activations are interesting as the goal is explicitly recovering the parameters of the hidden units’ weight vectors.
1.6 Organization

In the preliminaries we define the learning models we use and review the core tools we need from kernel methods and approximation theory. We then present our main algorithm, Alphatron, and give a proof of its correctness. We then combine Alphatron with various RKHS embeddings to obtain our most general learning results. Using these general results, we subsequently describe how to obtain all of our applications, including our main results for learning depth-three neural networks.

2 Preliminaries

Notation. Vectors are denoted by bold-face and $|| \cdot ||$ denotes the standard 2-norm of the vector. We denote the space of inputs by $X$ and the space of outputs by $Y$. In our paper, $X$ is usually the unit sphere/ball and $Y$ is $[0, 1]$ or $\{0, 1\}$. Standard scalar (dot) products are denoted by $a \cdot b$ for vectors $a, b \in \mathbb{R}^n$, while inner products in a Reproducing Kernel Hilbert Space (RKHS) are denoted by $\langle a, b \rangle$ for elements $a, b$ in the RKHS. We denote the standard composition of functions $f_1$ and $f_2$ by $f_1 \circ f_2$.

2.0.1 Learning Models

We consider two learning models in our paper, the standard Probably Approximately Correct (PAC) learning model and a relaxation of the standard model, the Probabilistic Concept (p-concept) learning model. For completeness, we define the two models and refer the reader to [Val84, KS90] for a detailed explanation.

Definition 1 (PAC Learning [Val84]). We say that a concept class $C \subseteq \{0, 1\}^X$ is Probably Approximately Correct (PAC) learnable, if there exists an algorithm $A$ such that for every $c \in C, \delta, \epsilon > 0$ and $D$ over $X$, if $A$ is given access to examples drawn from $D$ and labeled according to $c$, $A$ outputs a hypothesis $h : X \rightarrow \{0, 1\}$, such that with probability at least $1 - \delta$,

$$\Pr_{x \sim D}[h(x) \neq c(x)] \leq \epsilon. \quad (1)$$

Furthermore, we say that $C$ is efficiently PAC learnable to error $\epsilon$ if $A$ can output an $h$ satisfying the above with running time and sample complexity polynomial in $n, 1/\epsilon$, and $1/\delta$.

Definition 2 (p-concept Learning [KS90]). We say that a concept class $C \subseteq Y^X$ is Probabilistic Concept (p-concept) learnable, if there exists an algorithm $A$ such that for every $\delta, \epsilon > 0, c \in C$ and distribution $D$ over $X \times Y$ with $\mathbb{E}[y|x] = c(x)$ we have that $A$, given access to examples drawn from $D$, outputs a hypothesis $h : X \rightarrow Y$, such that with probability at least $1 - \delta$,

$$\mathbb{E}_{(x,y) \sim D}[(h(x) - c(x))^2] \leq \epsilon. \quad (2)$$

Furthermore, we say that $C$ is efficiently p-concept learnable to error $\epsilon$ if $A$ can output an $h$ satisfying the above with running time and sample complexity polynomial in $n, 1/\epsilon$, and $1/\delta$.

Here we focus on square loss for p-concept since an efficient algorithm for square-loss implies efficient algorithms of various other standard losses.
2.0.2 Generalization Bounds

The following standard generalization bound based on Rademacher complexity is useful for our analysis. For a background on Rademacher complexity, we refer the reader to [BM02].

**Theorem 1 (BM02).** Let $D$ be a distribution over $X \times Y$ and let $L : Y' \times Y$ (where $Y \subseteq Y' \subseteq \mathbb{R}$) be a $b$-bounded loss function that is $L$-Lipschitz in its first argument. Let $F \subseteq (Y')^X$ and for any $f \in F$, let $L(f; D) := \mathbb{E}_{(x,y) \sim D}[L(f(x),y)]$ and $\hat{L}(f; S) := \frac{1}{m} \sum_{i=1}^{m} L(f(x_i),y_i)$, where $S = ((x_1,y_1),\ldots,(x_m,y_m)) \sim D^m$. Then for any $\delta > 0$, with probability at least $1 - \delta$ (over the random sample draw for $S$), simultaneously for all $f \in F$, the following is true:

$$|L(f; D) - \hat{L}(f; S)| \leq 4 \cdot L \cdot \mathcal{R}_m(F) + 2 \cdot b \cdot \sqrt{\frac{\log(1/\delta)}{2m}}$$

where $\mathcal{R}_m(F)$ is the Rademacher complexity of the function class $F$.

For a linear concept class, the Rademacher complexity can be bounded as follows.

**Theorem 2 (KST09).** Let $X$ be a subset of a Hilbert space equipped with inner product $\langle \cdot, \cdot \rangle$ such that for each $x \in X$, $\langle x, x \rangle \leq X^2$, and let $W = \{x \mapsto \langle x, w \rangle \mid \langle w, w \rangle \leq W^2\}$ be a class of linear functions. Then it holds that

$$\mathcal{R}_m(W) \leq X \cdot W \cdot \sqrt{\frac{1}{m}}.$$ 

The following result is useful for bounding the Rademacher complexity of a smooth function of a concept class.

**Theorem 3 (BM02 LT91).** Let $\phi : \mathbb{R} \to \mathbb{R}$ be $L_\phi$-Lipschitz and suppose that $\phi(0) = 0$. Let $Y \subseteq \mathbb{R}$, and for a function $f \in Y^X$. Finally, for $F \subseteq Y^X$, let $\phi \circ F = \{\phi \circ f : f \in F\}$. It holds that $\mathcal{R}_m(\phi \circ F) \leq 2 \cdot L_\phi \cdot \mathcal{R}_m(F)$.

2.1 Kernel Methods

We assume the reader has a basic working knowledge of kernel methods (for a good resource on kernel methods in machine learning we refer the reader to [SS02]). We denote a kernel function by $K(x,x') = \langle \psi(x), \psi(x') \rangle$ where $\psi$ is the associated feature map and $\mathcal{H}$ is the corresponding reproducing kernel Hilbert space (RKHS).

Here we define two kernels and a few of their properties that we will use for our analysis. First, we define a variant of the polynomial kernel, the multinomial kernel due to Goel et al. [GKKT16]:

**Definition 3 (Multinomial Kernel [GKKT16]).** Define $\psi_d : \mathbb{R}^n \to \mathbb{R}^{N_d}$, where $N_d = 1 + n + \cdots + n^d$, indexed by tuples $(k_1,\ldots,k_j) \in [n]^j$ for each $j \in \{0,1,\ldots,d\}$, where the entry of $\psi_d(x)$ corresponding to tuple $(k_1,\ldots,k_j)$ equals $x_{k_1} \cdots x_{k_j}$. (When $j = 0$ we have an empty tuple and the corresponding entry is 1.) Define kernel $\mathcal{M}K_d$ as follows:

$$\mathcal{M}K_d(x,x') = \langle \psi_d(x), \psi_d(x') \rangle = \sum_{j=0}^{d} (x \cdot x')^j.$$ 

Also define $\mathcal{H}_{\mathcal{M}K_d}$ to be the corresponding RKHS.
It is easy to see that the multinomial kernel is efficiently computable. A multivariate polynomial $p$ of degree $d$ can be represented as an element $v \in H_{MK_d}$. Also, every $v \in H_{MK_d}$ can be interpreted as a multivariate polynomial of degree $d$ such that

$$p(x) = \langle v, \psi_d(x) \rangle = \sum_{(i_1, \ldots, i_n) \in \{0, \ldots, d\}^n} \beta(i_1, \ldots, i_n)x_1^{i_1} \cdots x_n^{i_n}.$$  

where coefficient $\beta(i_1, \ldots, i_n)$ is as follows,

$$\beta(i_1, \ldots, i_n) = \sum_{k_1, \ldots, k_j \in [n]^j} v(k_1, \ldots, k_j).$$

Here, $v(\cdot)$ is used to index the corresponding entry in $v$.

The following lemma is due to [GKKT16], following an argument of Shalev-Shwartz et al. [SSSS11]:

**Lemma 1.** Let $p(t) = \sum_{i=0}^{d} \beta_it^i$ be a given univariate polynomial with $\sum_{i=1}^{d} \beta_i^2 \leq B^2$. For $w$ such that $\|w\| \leq 1$, the polynomial $p(w \cdot x)$ equals $\langle p_w, \psi(x) \rangle$ for some $p_w \in H_{MK_d}$ with $\|p_w\| \leq B$.

**Remark.** Observe that we can normalize the multinomial feature map such that $\forall x \in X, MK_d(x, x) \leq 1$ for bounded space $X$. More formally, $\max_{x \in X} MK_d(x, x) = \max_{x \in X} \sum_{i=0}^{d} ||x||^2 \leq \sum_{j=0}^{d} X_j^2$ where $X = \max_{x \in X} ||x||$, hence we can normalize using this value. Subsequently, in the above, $\|p_w\|$ will need to be multiplied by the same value. For $X = S^{n-1}$, the scaling factor is $d + 1$ [GKKT16]. Throughout the paper, we will assume the kernel to be normalized as discussed.

For our results on Multiple Instance Learning, we make use of the following known kernel defined over sets of vectors:

**Definition 4** (Mean Map Kernel [SGSS07]). Let $X^*$ denote the Kleene closure of $X$.

The mean map kernel $K_{mean} : X^* \times X^* \to \mathbb{R}$ of kernel $K : X \times X \to \mathbb{R}$ with feature vector $\psi : X \to Z$ is defined as,

$$K_{mean}(S, T) = \frac{1}{|S||T|} \sum_{s \in S, t \in T} K(s, t).$$

The feature map $\psi_{mean} : X^* \to Z$ corresponding to this kernel is given by

$$\psi_{mean}(S) = \frac{1}{|S|} \sum_{s \in S} \psi(s).$$

Also define $H_{mean}$ to be the corresponding RKHS.

**Fact.** If $\forall x, x' \in X, K(x, x') \leq M$ then $\forall S, S' \in X^*, K_{mean}(S, S') \leq M$.

### 2.2 Approximation Theory

We will make use of a variety of tools from approximation theory to obtain specific embeddings of function classes into a RKHS. The following lemma for approximating the Boolean sign function was given by [Dan15].
Lemma 2. Let $a, \gamma, \tau > 0$. There exists a polynomial $p$ of degree $O\left(\frac{1}{\gamma} \cdot \log \left(\frac{1}{\tau}\right)\right)$ such that

- For $x \in [-a, a]$, $|p(x)| < 1 + \tau$.
- For $x \in [-a, a] \setminus [-\gamma \cdot a, \gamma \cdot a]$, $|p(x) - \text{sign}(x)| < \tau$.

The above lemma assumes $\text{sign}$ takes on values $\{\pm 1\}$, but a simple linear transformation also works for $\{0, 1\}$.

A halfspace is a Boolean function $h : \mathbb{R}^n \to \{0, 1\}$ defined by a vector $w \in \mathbb{R}^n$ and threshold $\theta$, given input $x \in \mathbb{R}^n$, $h(x) = \text{sign}(w \cdot x + \theta)$ where $\text{sign}(a)$ is 0 if $a < 0$ else 1. Given $\mathcal{X} \subseteq \mathbb{R}^n$ and halfspace $h$ over $\mathbb{R}^n$, $h$ is said to have margin $\rho$ with respect to $\mathcal{X}$ if $\rho = \min\{|z - y| : z \in \mathcal{X}, y \in \mathbb{R}^n, h(z) \neq h(y)\}/\max\{|z| : z \in \mathcal{X}\}$. Let $h_w(x)$ for $i \in [t]$ with $|w_i| \leq 1$ be the $t$ halfspaces, and $f_{\text{AND}} = \text{AND}(h_{w_1}, \ldots, h_{w_t}(x))$ equals the intersection. The following lemma due to Klivans and Servedio [KS08] gives a construction of a polynomial whose sign always equals an intersection of halfspaces with a margin. We give the proof as it is useful for a subsequent lemma.

Lemma 3. For $\rho > 0$, there exists a polynomial $P_{\text{AND}}$ of degree $O(\sqrt{1/\rho \log t})$ such that, if each of the $t$ halfspaces has margin $\rho$ on $\mathcal{X} \subseteq \mathbb{S}^{n-1}$, then $\forall x \in \mathcal{X}$, $P_{\text{AND}}(x) \geq 1/2$ if $f_{\text{AND}}(x) = 1$ and $P_{\text{AND}}(x) \leq -1/2$ if $f_{\text{AND}}(x) = 0$. Constructively, $P_{\text{AND}}$ is as follows,

$$P_{\text{AND}}(x) = t + \frac{1}{2} - \sum_{i=1}^t p(w_i \cdot x)$$

where $p(a) = T_r(1 - a)^{\lceil \log 2t \rceil}$ for $r = \lceil \sqrt{1/\rho} \rceil$ and $T_r$ is the $r$th Chebyshev polynomial of the first kind.

Proof. We have $\forall i, \rho \leq |w_1 \cdot x| \leq 1$. From the properties of Chebyshev polynomials, we know that $|T_r(1 - a)| \leq 1$ for $a \in [0, 1]$ and $T_r(1 - a) \geq 2$ for $a \leq \rho$. Hence,

- If $f_{\text{AND}}(x) = 1$, for each $i$, $\rho \leq w_i \cdot x \leq 1$ hence $|p(w_1 \cdot x)| \leq 1$, implying $P_{\text{AND}}(x) \geq t + 1/2 - t = 1/2$.
- If $f_{\text{AND}}(x) = 0$, then there exists $i$ such that $-1 \leq w_i \cdot x \leq \rho$, thus $p(w_i \cdot x) \geq 2^{\lceil \log 2t \rceil} \geq 2t$. Also observe that $\forall i, p(w_i \cdot x) \geq -1$. This implies $P_{\text{AND}}(x) \leq t + 1/2 - 2t + t - 1 \leq -1/2$. \hfill \square

We extend the above lemma to give a threshold function for $\text{OR}^3$ of a fixed halfspace with margin over a set of vectors. Let $h_w(x) = \text{sign}(w \cdot x)$ be a halfspace with $||w||_2 \leq 1$ and $f_{\text{OR}}(S) = \text{OR}(h_w(s_1), \ldots, h_w(s_t))$ represent the conjunction over any set $S = \{s_1, \ldots, s_t\}$ of vectors. Let $\mathcal{X} \subseteq \mathbb{S}^{n-1}$ over which the halfspace has margin.

Lemma 4. For $\rho, N > 0$, there exists a function $P_{\text{OR}}$ such that, if the halfspace $h$ has margin $\rho$ on $\mathcal{X} \subseteq \mathbb{S}^{n-1}$, then for all sets $S \subseteq \mathcal{X}^*$ such that $|S| \leq N$, $P_{\text{OR}}(S) \geq 1/2$ if $f_{\text{OR}}(S) = 1$ and $P_{\text{OR}}(S) \leq -1/2$ if $f_{\text{OR}}(S) = 0$. Constructively, $P_{\text{OR}}$ is as follows,

$$P_{\text{OR}}(S) = -\frac{1}{2} - N + \frac{N}{|S|} \sum_{s \in S} p(w \cdot s)$$

where $p(a) = T_r(1 + a)^{\lceil \log 2N \rceil}$ for $r = \lceil \sqrt{1/\rho} \rceil$ and $T_r$ is the $r$th Chebyshev polynomial of the first kind.

\text{\textsuperscript{3}}A similar construction would hold for AND, with $P_{\text{AND}}(S) = \frac{1}{2} + N - \frac{N}{|S|} \sum_{s \in S} p(w \cdot s)$. }

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Proof. Similar to the previous proof, we have \( \forall x \in \mathcal{X}, \rho \leq |w \cdot x| \leq 1 \). From the properties of Chebyshev polynomials, we know that \( |T_r(1 + a)| \leq 1 \) for \( a \in [-1, 0] \) and \( T_r(1 + a) \geq 2 \) for \( a \geq \rho \). Hence,

- If \( f_{OR}(S) = 0 \), for each \( s \in S, -1 \leq w \cdot s \leq -\rho \) hence \( |p(w \cdot s)| \leq 1 \), implying \( P_{OR}(S) \leq -1/2 - N + N = -1/2 \).

- If \( f_{OR}(S) = 1 \), then there exists \( s \in S \) such that \( \rho \leq w \cdot s \leq 1 \), thus \( p(w \cdot s) \geq 2^{[\log 2N]} \geq 2N \). Also observe that \( \forall s \in S, p(w \cdot s) \geq -1 \). This implies \( P_{OR}(S) \geq -1/2 - N + 2N - N + 1 \geq 1/2 \) since \( N \geq |S| \).

Finally we state the following lemmas that bound the sum of squares of coefficients of a univariate polynomial:

**Lemma 5** \( ([\text{She12}]) \). Let \( p(t) = \sum_{d=0}^{d} \beta_i t_i \) be a univariate polynomial of degree \( d \). Let \( M \) be such that \( \max_{t \in [-1,1]} |p(t)| \leq M \). Then \( \sum_{i=0}^{d} \beta_i^2 \leq (d + 1) \cdot (4e)^d \cdot M^2 \).

**Lemma 6.** \( ([\text{KS08}]) \) Let \( p(t) = \sum_{i=0}^{d} \beta_i t_i \) be a univariate polynomial of degree \( d \) such that \( |\beta_i| \leq M \) for all \( i \in [d] \). For any \( r \in \mathbb{Z}^+ \) consider \( p^r(t) = \left( \sum_{i=0}^{d} \beta_i t_i \right)^r = \sum_{i=0}^{dr} \eta_i t_i \) then, \( \sum_{i=0}^{dr} \eta_i^2 \leq (Md)^{2r} \).

**Proof.** We have \( p^r(t) = \sum_{i_1,\ldots,i_r \in [d]} \beta_{i_1} \cdots \beta_{i_r} t_{i_1+i_2+\cdots+i_r} \). It follows that \( \left( \sum_{i=0}^{d} \beta_i t_i \right)^r = \sum_{i=0}^{dr} \eta_i t_i \) is bounded above by

\[
\left( \sum_{i_1,\ldots,i_r \in [d]} |\beta_{i_1} \cdots \beta_{i_r}| \right)^2 \leq M^{2r} \left( \sum_{i_1,\ldots,i_r \in [d]} 1 \right)^2 = (Md)^{2r}.
\]

\( \square \)

### 3 The Alphatron Algorithm

Here we present our main algorithm Alphatron (Algorithm 1) and a proof of its correctness. In the next section we will use this algorithm to obtain our most general learning results.

Define \( v^t = \sum_{i=1}^{m} \alpha_i^t \psi(x_i) \) implying \( h^t(x) = u(v^t, \psi(x)) \). Let \( \epsilon(h) = \mathbb{E}_{x,y}[h(x) - \mathbb{E}[y|x]^2] \) and \( err(h) = \mathbb{E}_{x,y}[(h(x) - y)^2] \). It is easy to see that \( \epsilon(h) = err(h) - err(\mathbb{E}[y|x]) \). Let \( \hat{\epsilon}, \hat{err} \) be the empirical versions of the same.

The following theorem generalizes Theorem 1 of \( ([\text{KKS11}]) \) to the bounded noise setting in a high dimensional feature space. We follow the same outline, and their theorem can be recovered by setting \( \psi(x) = x \) and \( \xi \) as the zero function.

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Algorithm 1: Alphatron

Input : data \((x_i, y_i)_{i=1}^m \in \mathbb{R}^n \times [0,1]\), non-decreasing \(L\)-Lipschitz function \(u : \mathbb{R} \rightarrow [0,1]\), kernel function \(\mathcal{K}\) corresponding to feature map \(\psi\), learning rate \(\lambda > 0\), number of iterations \(T\), held-out data of size \(N \langle a_j, b_j \rangle_{j=1}^N \in \mathbb{R}^n \times [0,1]\)

1. \(\alpha^1 := 0 \in \mathbb{R}^m\)
2. for \(t = 1, \ldots, T\) do
3. \(\quad h^t(x) := u(\sum_{i=1}^m \alpha^t_i \mathcal{K}(x, x_i)) \text{ for } i = 1, 2, \ldots, m\) do
4. \(\quad \alpha^{t+1}_i := \alpha^t_i + \frac{\lambda}{m} (y_i - h^t(x_i))\)
5. end
6. end

Output: \(h^r\) where \(r = \arg \min_{t \in \{1, \ldots, T\}} \sum_{j=1}^N (h^t(a_j) - b_j)^2\)

Theorem 4. Let \(\mathcal{K}\) be a kernel function corresponding to feature map \(\psi\) such that for all \(x \in \mathcal{X}\), \(|\psi(x)| \leq 1\). Consider samples \((x_i, y_i)_{i=1}^m\) drawn iid from distribution \(\mathcal{D}\) on \(\mathcal{X} \times [0,1]\) such that \(E[y|x] = u(\langle v, \psi(x) \rangle + \xi(x))\) where \(u : \mathbb{R} \rightarrow [0,1]\) is a known \(L\)-Lipschitz non-decreasing function, \(\xi : \mathbb{R}^n \rightarrow [-\epsilon_0, \epsilon_0]\) for some \(\epsilon_0 \in (0,1)\) and \(|\psi| \leq B\). Then for \(\delta \in (0,1)\), with probability \(1 - \delta\), Alphatron with \(\lambda = 1/L, T = CBL\sqrt{m/\log(1/\delta)}\) and \(N = C'm\log(T/\delta)\) for large enough constants \(C, C' > 0\) outputs a hypothesis \(h\) such that,

\[
\varepsilon(h) \leq O \left( L\epsilon_0 + BL\sqrt{\log(1/\delta)/m} \right).
\]

Proof. Let \(\Delta = \frac{1}{m}\sum_{i=1}^m (y_i - u(\langle v, \psi(x_i) \rangle + \xi(x_i)))\psi(x_i)\) and \(\Delta^t = \frac{1}{m}\sum_{i=1}^m (y_i - u(\langle v^t, \psi(x_i) \rangle))\psi(x_i)\). We will first prove the following lemma and subsequently use it to prove the theorem.

Lemma 7. At iteration \(t\) in Alphatron, suppose \(|v^t - v| \leq B\) for \(B > 1\), then if \(|\Delta| \leq \eta < 1\), then

\[
|v^t - v|^2 - |v^{t+1} - v|^2 \geq \lambda \left( \frac{2}{L} - \lambda \right) \varepsilon(h^t) - 2\epsilon_0 - 2B\eta - \lambda\eta^2 - 2\lambda\eta.
\]

Proof. Expanding the left hand side of the equation above, we have

\[
|v^t - v|^2 - |v^{t+1} - v|^2 = 2\lambda \langle v - v^t, \Delta^t \rangle - \lambda^2 |\Delta^t|^2
\]

\[
= 2\lambda \langle v - v^t, \Delta^t - \Delta \rangle + 2\lambda \langle v - v^t, \Delta \rangle - \lambda^2 |\Delta^t|^2
\]

\[
\geq 2\lambda \frac{m}{m} \sum_{i=1}^m (u(\langle v, \psi(x_i) \rangle + \xi(x_i)) - u(\langle v^t, \psi(x_i) \rangle)) v - v^t, \psi(x_i)) - 2\lambda B |\Delta| - \lambda^2 |\Delta^t|^2
\]

\[
= 2\lambda \frac{m}{m} \sum_{i=1}^m (u(\langle v, \psi(x_i) \rangle + \xi(x_i)) - u(\langle v^t, \psi(x_i) \rangle)) (\langle v, \psi(x_i) \rangle + \xi(x_i) - \langle v^t, \psi(x_i) \rangle)
\]

\footnote{We present the algorithm and subsequent results for non-decreasing function \(u\). Non-increasing functions can also be handled by negating the update term, i.e., \(\alpha^{t+1}_i := \alpha^t_i - \frac{\lambda}{m} (y_i - h^t(x_i))\).}

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that for all
Here (13) follows by expanding the square and (12) follows by applying Jensen’s inequality to show
ables with norm bounded by
and, (8) follows from
Now using the previous lemma with
We now bound
By definition we have that
(9) follows from observing that the first term equals
and subsequently using the fact that
since the range of
and vectors
m
and using the assumption
We now bound \(|\Delta^t|\) as follows.

\[
||\Delta^t||^2 = \left|\frac{1}{m} \sum_{i=1}^{m} (y_i - u(\langle v, \psi(x_i) \rangle + \xi(x_i)) + u(\langle v, \psi(x_i) \rangle + \xi(x_i)) - u(\langle v^t, \psi(x_i) \rangle))\psi(x_i)\right|^2
\]

\[
\leq ||\Delta||^2 + \left|\frac{1}{m} \sum_{i=1}^{m} (u(\langle v, \psi(x_i) \rangle + \xi(x_i)) - u(\langle v^t, \psi(x_i) \rangle))\psi(x_i)\right|^2
\]

\[
+ 2||\Delta|| \left|\frac{1}{m} \sum_{i=1}^{m} (u(\langle v, \psi(x_i) \rangle + \xi(x_i)) - u(\langle v^t, \psi(x_i) \rangle))\psi(x_i)\right|
\]

\[
\leq \eta^2 + \tilde{\epsilon}(h^t) + 2\eta
\]

Here (13) follows by expanding the square and (12) follows by applying Jensen’s inequality to show that for all \(a, b \in \mathbb{R}^m\) and vectors \(v_i\) for \(i \in \{1, \cdots , m\}\), \(\left|\frac{1}{m} \sum_{i=1}^{m} (a_i - b_i)v_i\right|^2 \leq \frac{1}{m} \sum_{i=1}^{m} (a_i - b_i)^2||v_i||^2\) and subsequently using the fact that \(||\psi(x_i)|| \leq 1\). Combining (9) and (12) gives us the result.

By definition we have that \((y_i - u(\langle v, \psi(x_i) \rangle + \xi(x_i)))\psi(x_i)\) are zero mean iid random variables with norm bounded by 1. Using Hoeffding’s inequality (and the fact that that the \(x_i\)'s are independent draws), with probability \(1 - \delta\) we have

\[
||\Delta|| = \left|\frac{1}{m} \sum_{i=1}^{m} (y_i - u(\langle v, \psi(x_i) \rangle + \xi(x_i)))\psi(x_i)\right| \leq \frac{1}{\sqrt{m}} \left(1 + \sqrt{2\log(1/\delta)}\right).
\]

Now using the previous lemma with \(\lambda = 1/L\) and \(\eta = \frac{1}{\sqrt{m}} \left(1 + \sqrt{2\log(1/\delta)}\right)\), we have

\[
||v^t - v||^2 - ||v^{t+1} - v||^2 \geq \frac{1}{L} \left(\frac{\tilde{\epsilon}(h^t)}{L} - 2\epsilon_0 - 2B\eta - \frac{\eta^2}{L} - \frac{2\eta}{L}\right).
\]

Thus, for each iteration \(t\) of Alphatron, one of the following two cases needs to be satisfied,
Case 1: \(|v^t - v|^2 - |v^{t+1} - v|^2 \geq \frac{Bn}{L}|

Case 2: \(\hat{\varepsilon}(h^t) \leq 3LB\eta + 2L\epsilon_0 + \eta^2 + 2\eta = O\left(L\epsilon_0 + BL\sqrt{\frac{\log(1/\delta)}{m}}\right)\) (assuming that \(B > \eta\) and \(L > 1\))

Let \(t\) be the first iteration where Case 2 holds. We need to show that such an iteration exists. Assume the contradictory, that is, Case 2 fails for each iteration. Since \(|v^0 - v|^2 \leq B^2\), however, in at most \(\frac{BL}{\eta}\) iterations Case 1 will be violated and Case 2 will have to be true. If \(\frac{BL}{\eta} \leq T\) then \(t\) exists such that

\[\hat{\varepsilon}(h^t) \leq O\left(L\epsilon_0 + BL\sqrt{\frac{\log(1/\delta)}{m}}\right).

We need to bound \(\varepsilon(h)\) in terms of \(\hat{\varepsilon}(h)\). Define \(\mathcal{F} = \{x \rightarrow u(\langle z, \psi(x)\rangle) : |z| \leq 2B\}\), and \(\mathcal{Z} = \{x \rightarrow f(x) - u(\langle v, \psi(x)\rangle + \xi(x)) : f \in \mathcal{F}\}\). Using Theorem 2 and 3 we have \(\mathcal{R}_m(\mathcal{F}) = O(BL\sqrt{1/m})\).

By definition of Rademacher complexity, we have

\[
\mathcal{R}_m(\mathcal{Z}) = \mathbb{E}_{\mathcal{X}, \sigma_i} \left[ \sup_{z \in \mathcal{Z}} \left( \frac{2}{m} \sum_{i=1}^{m} \sigma_i z(x_i) \right) \right]
= \mathbb{E}_{\mathcal{X}, \sigma_i} \left[ \sup_{f \in \mathcal{F}} \left( \frac{2}{m} \sum_{i=1}^{m} \sigma_i (f(x_i) - u(\langle v, \psi(x_i)\rangle + \xi(x_i))) \right) \right]
= \mathbb{E}_{\mathcal{X}, \sigma_i} \left[ \sup_{f \in \mathcal{F}} \left( \frac{2}{m} \sum_{i=1}^{m} \sigma_i f(x_i) \right) \right] - \mathbb{E}_{\mathcal{X}} \left[ \frac{2}{m} \sum_{i=1}^{m} \mathbb{E}_{\sigma_i} [\sigma_i] u(\langle v, \psi(x_i)\rangle + \xi(x_i)) \right]
= \mathcal{R}_m(\mathcal{F})
\]

Here, \(\sigma_i \in \{\pm 1\}\) are iid Rademacher variables hence \(\forall i, E[\sigma_i] = 0\) and \(x_i\) are drawn iid from \(\mathcal{D}\).

Recall that \(h(x) = u(\langle v^T, \psi(x)\rangle)\) is an element of \(\mathcal{U}\) as \(|v^T - v|^2 \leq B^2\) (case 1 is satisfied in iteration \(t-1\)) and \(|v| \leq B\). A direct application of Theorem 1 on \(\mathcal{Z}\) with loss function \(\mathcal{L}(a, \cdot) = a^2\), gives us the following bound on \(\varepsilon(h^t)\) with probability \(1 - \delta\),

\[\varepsilon(h^t) \leq \hat{\varepsilon}(h) + O\left(BL\sqrt{\frac{1}{m}} + \sqrt{\frac{\log(1/\delta)}{m}}\right) = O\left(L\epsilon_0 + BL\sqrt{\frac{\log(1/\delta)}{m}}\right).

The last step is to show that we can indeed find a hypothesis satisfying the above guarantee. Since for all \(h\), \(\varepsilon(h)\) is up to constants equal to \(err(h)\) we can do so by choosing the hypothesis with the minimum \(err\) using a fresh sample set of size \(O(\log(T/\delta)/\epsilon^2) \leq N\). This holds as given the sample size, by Chernoff bound using the fact that \(\hat{\varepsilon}(h^t)\) is bounded in \([0, 1]\), each \(h^t\) for \(t \leq T\) will have empirical error within \(\epsilon\) of the true error with probability \(1 - \delta/T\) and hence all will simultaneously satisfy this probability \(1 - \delta\),

\[\varepsilon(h) \leq O\left(\epsilon + L\epsilon_0 + BL\sqrt{\frac{\log(1/\delta)}{m}}\right).
\]

Setting \(\epsilon = 1/\sqrt{m}\) will give us the required bound. \(\square\)

Alphetron runs in time \(\text{poly}(n, m, \log(1/\delta), t_K)\) where \(t_K\) is the time required to compute the kernel function \(K\).
4 Some General Theorems Involving Alphatron

In this section we use Alphatron to give our most general learnability results for the p-concept model and PAC learning setting. We then state several applications in the next section. Here we show that if a function can be uniformly approximated by an element of an appropriate RKHS then it is p-concept learnable. Similarly, if a function is separable by an element in an appropriate RKHS then it is PAC learnable. We assume that the kernel function is efficiently computable, that is, computable in polynomial time in the input dimension. Formally, we define approximation and separation as follows:

Definition 5 ((ε, B)-approximation). Let f be a function mapping domain X to X. Let K be a kernel function with corresponding RKHS H and feature vector ψ. We say f is (ε, B)-approximated by K if for all x ∈ X, |f(x) − ⟨v, ψ(x)⟩| ≤ ε for some v ∈ H such that ||v|| ≤ B.

Definition 6 (B-separation). Let f be a boolean function mapping domain X to {0, 1}. Let K be a kernel function with corresponding RKHS H and feature vector ψ. We say f is B-separated by K if for all x ∈ X, if f(x) = 1 then ⟨v, ψ(x)⟩ ≥ 1/2 and if f(x) = 0 then ⟨v, ψ(x)⟩ ≤ −1/2 for some v ∈ K such that ||v|| ≤ B.

Combining Alphatron and the approximation (separation) guarantees, we have the following general learning results:

Theorem 5. Consider distribution D on X × [0, 1] such that E[y|x] = u(f(x)) where u is a known L-Lipschitz non-decreasing function and f is (ε, B)-approximated by some kernel function K such that K(x, x′) ≤ 1. Then for δ ∈ (0, 1), there exists an algorithm that draws m iid samples from D and outputs a hypothesis h such that with probability 1 − δ, ε(h) ≤ O(Lε) for m ≥ (BL/ε)2 · log(1/δ) in time poly(n, B, L, 1/ε, log(1/δ)) where n is the dimension of X.

Proof. Let H be the RKHS corresponding to K and ψ be the feature vector. Since f is (ε, B)-approximated by kernel function K, we have ∀ x, |f(x) − ⟨v, ψ(x)⟩| ≤ ε for ||v|| ≤ B. This implies that f(x) = ⟨v, ψ(x)⟩ + ξ(x) for some function ξ : X → [−ε, ε]. Thus E[y|x] = u(f(x)) = u(⟨v, ψ(x)⟩ + ξ(x)). Applying Theorem 4 we have that Alphatron outputs a hypothesis h such that

ε(h) ≤ CL 2(ε + (BL/ε)2 · log(1/δ))

for some constants C > 0. Also Alphatron requires at most O(BL√m/ log(1/δ)) iterations. Setting m = (BL/ε)2 · log(1/δ) gives us the required result.

Theorem 6. Consider a sample of size m > 0 drawn from distribution D over X and labeled by Boolean function f. Assume f is B-separated by some kernel function K such that K(x, x′) ≤ 1. Then there exists an algorithm that outputs a hypothesis h such that with probability 1 − δ, Prx∼D[h(x) = f(x)] ≤ ε for m ≥ C (B/ε)2 · log(1/δ) for sufficiently large constant C > 0 in time poly(n, B, 1/ε, log(1/δ)) where n is the dimension of X.

Proof. Let v be the vector that B-separates f and P(x) = ⟨v, ψ(x)⟩. Consider u as follows:

u(a) = \begin{cases} 
0 & a ≤ −1/2 \\
1/2 & −1/2 < a < 1/2 \\
1 & a ≥ 1/2 
\end{cases}

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Note that $u$ is monotone and 1-Lipschitz. Observe that,

- If $f(x) = 1$ then $u(P(x)) = 1$ since $P(x) \geq 1/2$.
- If $f(x) = 0$ then $u(P(x)) = 0$ since $P(x) \leq -1/2$.

From above, we can see that the samples drawn from the distribution satisfy $\Pr_\text{x} \left| \text{inequality} \right.$, we have $\Pr_\text{x} x$, two hidden layers (depth-3) with one unit in hidden layer 2 and $C >$ sufficiently large constant $C > 0$ to obtain output hypothesis $h'$ with $\epsilon(h') \leq \epsilon$ (with probability $1 - \delta$).

Recall that $h'$ may be real-valued as Alphatron learns with square loss. Let us define $h(x)$ to equal 1 if $h'(x) \geq 1/2$ and 0 otherwise. We will show that $\Pr_\text{x}[h(x) \neq f(x)] \leq O(\epsilon)$. Using Markov’s inequality, we have $\Pr_\text{x}[(h'(x) - u(P(x)))^2 \geq 1/4] \leq 4\epsilon$. For $x$, suppose $(h'(x) - u(P(x)))^2 < 1/4 \implies |h'(x) - u(P(x))| < 1/2$. Since $u(P(x)) = f(x) \in \{0, 1\}$ then clearly $h(x) = f(x)$. Thus, $\Pr_\text{x}[h(x) \neq f(x)] \leq 4\epsilon$. Scaling $\epsilon$ appropriately, we get the required result. ∎

## 5 Main Applications

The general framework of the previous section can be used to give new learning results for well studied problems. In this section we give polynomial time learnability results for depth-three neural networks with sigmoidal activations in the p-concept model. We follow this by showing how to obtain the first polynomial-time algorithms PAC learning a polynomial number of intersections/majorities of halfspaces with a margin.

### 5.1 Learning Depth-3 Neural Networks

Following standard convention (see for example [SS16]), we define a neural network with one hidden layer (depth-2) with $k$ units as follows:

$$N_2 : x \to \sum_{i=1}^{k} b_i \sigma(a_i \cdot x)$$

for $x \in \mathbb{R}^n$, $a_i \in \mathbb{S}^{n-1}$ for $i \in \{1, \ldots, k\}$, $b \in \mathbb{S}^{k-1}$. We subsequently define a neural network with two hidden layers (depth-3) with one unit in hidden layer 2 and $k$ units in hidden layer 1 as:

$$N_3 : x \to \sigma'(N_1(x)) = \sigma' \left( \sum_{i=1}^{k} b_i \sigma(a_i \cdot x) \right)$$

for $x \in \mathbb{R}^n$, $a_i \in \mathbb{S}^{n-1}$ for $i \in \{1, \ldots, k\}$, $b \in \mathbb{S}^{k-1}$ and $\sigma, \sigma' : \mathbb{R} \to \mathbb{R}$.

[GKKT16] showed that activation functions sigmoid: $\sigma_{\text{sig}}(a) = \frac{1}{1+e^{-a}}$ and ReLU: $\sigma_{\text{relu}}(a) = \max(0,a)$ can be $(\epsilon,B)$-approximated by the multinomial kernel for $B$ dependent on $\epsilon$, more formally they showed the following:

**Lemma 8** (Approximating a Single Hidden Unit). *We have,

1. **Sigmoid**: For all $a \in \mathbb{S}^{n-1}$ there exists a corresponding $v \in \mathcal{H}_{\mathcal{MK}_d}$ for $d = O(\log(1/\epsilon))$, such that

$$\forall x \in \mathbb{S}^{n-1}, |\sigma_{\text{sig}}(a \cdot x) - \langle v, \psi(x) \rangle| \leq \epsilon.$$

Further, $\|v\| \leq (1/\epsilon)^{O(1)}$. This implies that $\sigma_{\text{sig}}$ is $(\epsilon,(1/\epsilon)^{O(1)})$-approximated by $\mathcal{MK}_d$. 

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2. ReLU: For all \( a \in \mathbb{S}^{n-1} \) there exists a corresponding \( v \in \mathcal{H}_{MK_d} \) for \( d = O(1/\epsilon) \), such that
\[
\forall x \in \mathbb{S}^{n-1}, |\sigma_{\text{relu}}(a \cdot x) - \langle v, \psi(x) \rangle| \leq \epsilon.
\]

Further, \( \|v\| \leq 2^{O(1/\epsilon)} \). This implies that \( \sigma_{\text{relu}} \) is \( (\epsilon, 2^{O(1/\epsilon)}) \)-approximated by \( MK_d \).

The following lemma extends the approximation guarantees to linear combinations of function classes.

**Lemma 9.** If for all \( i \in [k] \), \( f_i \) is \( (\epsilon, B) \)-approximated in kernel \( K \), then \( \sum_{i=1}^{k} a_i f_i(x) \) for \( a \in \mathbb{R}^k \) such that \( \|a\|_1 \leq W \) is \( (\epsilon W, WB) \)-approximated in kernel \( K \).

**Proof.** We have for each \( i \in [k] \), \( \forall x \in \mathcal{X} \), \( |f_i(x) - \langle v_i, \psi(x) \rangle| \leq \epsilon \) for some \( v_i \in \mathcal{H} \) such that \( \|v_i\| \leq B \). Consider \( v = \sum_{i=1}^{k} a_i v_i \). We have \( \forall x \in \mathcal{X}, \)
\[
\left| \sum_{i=1}^{k} a_i f_i(x) - \langle v, \psi(x) \rangle \right| = \left| \sum_{i=1}^{k} a_i (f_i(x) - \langle v_i, \psi(x) \rangle) \right| \leq \sum_{i=1}^{k} |a_i||f_i(x) - \langle v_i, \psi(x) \rangle| \leq \epsilon \|a\|_1 = \epsilon W.
\]

Also \( \|v\| = \left\| \sum_{i=1}^{k} a_i v_i \right\| \leq \sum_{i=1}^{k} |a_i||v_i| \leq WB \). Thus \( v \) satisfies the required approximation. \( \Box \)

The following theorem is our main result for learning classes of depth-three neural networks in polynomial time:

**Theorem 7.** Consider samples \((x_i, y_i)_{i=1}^{m}\) drawn iid from distribution \( D \) on \( \mathbb{S}^{n-1} \times [0, 1] \) such that 
\( E[y|x] = N_3(x) \) with \( \sigma' : \mathbb{R} \to [0, 1] \) is a known \( L \)-Lipschitz non-decreasing function and \( \sigma = \sigma_{\text{sig}} \) is the sigmoid function. There exists an algorithm that outputs a hypothesis \( h \) such that, with probability \( 1 - \delta \),
\[
\mathbb{E}_{x,y \sim D} \left[ (h(x) - N_3(x))^2 \right] \leq \epsilon
\]
for \( m = \left( \frac{kL}{\epsilon} \right)^{O(1)} \cdot \log(1/\delta) \). The algorithm runs in time polynomial in \( m \) and \( n \).

**Proof.** Combining Lemmas 8 and 9 we have that \( N_2 \) for activation function \( \sigma_{\text{sig}} \) is \( (\epsilon_0 \sqrt{k}, (\sqrt{k}/\epsilon_0)^C) \)-approximated by some kernel \( MK_d \) with \( d = O(\log(1/\epsilon_0)) \) and sufficiently large constant \( C > 0 \). Thus by Theorem 5 we have that there exists an algorithm that outputs a hypothesis \( h \) such that, with probability \( 1 - \delta \),
\[
\mathbb{E}_{x,y \sim D}(h(x) - N_3(x))^2 \leq C'L \left( \epsilon_0 \sqrt{k} + \left( \frac{\sqrt{k}}{\epsilon_0} \right)^C \sqrt{\frac{\log(1/\delta)}{m}} \right)
\]
for some constants \( C' > 0 \). Setting \( \epsilon_0 = \frac{\epsilon}{2kC'L} \) and \( m = \left( \frac{2kC'L}{\epsilon} \right)^{2C} \cdot \left( \frac{4\log(1/\delta)}{\epsilon^2} \right) \) gives us the required result (the claimed bounds on running time also follow directly from Theorem 5). \( \Box \)

We also obtain results for networks of ReLUs, but the dependence on the number of hidden units, \( \epsilon \), and \( L \) are exponential (the algorithm still runs in polynomial-time in the dimension):
Theorem 8. Consider samples \((x_i, y_i)_{i=1}^m\) drawn iid from distribution \(\mathcal{D}\) on \(\mathbb{S}^{n-1} \times [0,1]\) such that \(E[y|x] = \mathcal{N}_\beta(x)\) with \(\beta : \mathbb{R} \rightarrow [0,1]\) is a known \(L\)-Lipschitz non-decreasing function and \(\beta = \sigma_{\text{relu}}\) is the ReLU function. There exists an algorithm that outputs a hypothesis \(h\) such that with probability \(1 - \delta\),

\[
E_{x,y \sim \mathcal{D}} \left[ (h(x) - \mathcal{N}_\beta(x))^2 \right] \leq \epsilon
\]

for \(m = 2^{O(kL/\epsilon)} \cdot \log(1/\delta)\). The algorithm runs in time polynomial in \(m\) and \(n\).

Although our algorithm does not recover the parameters of the network, it still outputs a hypothesis with interpretable features. More specifically, our learning algorithm outputs the hidden layer as a multivariate polynomial. Given inputs \(x_1, \ldots, x_m\), the hypothesis output by our algorithm Alphatron is of the form \(h(x) = u(\sum_{i=1}^m \alpha_i^* M k_d(x, x_i)) = u(\langle v, \psi_d(x) \rangle)\) where \(v = \sum_{i=1}^m \alpha_i^* \psi_d(x_i)\) and \(d\) is dependent on required approximation. As seen in the preliminaries, \(\langle v, \psi_d(x) \rangle\) can be expressed as a polynomial and the coefficients can be computed as follows,

\[
\beta(i_1, \ldots, i_n) = \sum_{i=1}^m \alpha_i^* \left( \sum_{k_1, \ldots, k_j \in [n]^j \atop j \in \{0, \ldots, d\}} (x_{i_1})_{k_1} \cdots (x_{i_j})_{k_j} \right) = \sum_{i=1}^m \alpha_i^* C(i_1, \ldots, i_n)(x_{i_1})_{i_1} \cdots (x_{i_n})_{i_n}.
\]

Here, we follow the notation from [GKKT16]; \(M\) maps ordered tuple \((k_1, \ldots, k_j) \in [n]^j\) for \(j \in [d]\) to tuple \((i_1, \ldots, i_n) \in \{0, \ldots, d\}^n\) such that \(x_{k_1} \cdots x_{k_j} = x_{i_1}^{i_1} \cdots x_{i_n}^{i_n}\) and \(C\) maps ordered tuple \((i_1, \ldots, i_n) \in \{0, \ldots, d\}^n\) to the number of different orderings of the \(i_j\)’s for \(j \in \{0, \ldots, n\}\). The function \(C\) can be computed from the multinomial theorem (cf. [Wik16]). Thus, the coefficients of the polynomial can be efficiently indexed. Informally, each coefficient can be interpreted as the correlation between the target function and the product of features appearing in the coefficient’s monomial.

5.2 Learning Smooth Functions of Halfspaces with a Margin

In this section we consider the problem of learning a smooth combining function \(u\) of \(k\) halfspaces with a margin \(\rho\). We assume that all examples lie on the unit ball \(\mathbb{S}^{n-1}\) and that for each weight vector \(w\), \(|w| = 1\). For simplicity we also assume each halfspace is origin-centered, i.e. \(\theta = 0\) (though our techniques easily handle the case of nonzero \(\theta\)).

Theorem 9. Consider samples \((x_i, y_i)_{i=1}^n\) drawn iid from distribution \(\mathcal{D}\) on \(\mathbb{S}^{n-1} \times [0,1]\) such that \(E[y|x] = u\left(\sum_{i=1}^t a_i h_i(x)\right)\) where \(u : \mathbb{R}^n \rightarrow [0,1]\) is a \(L\)-Lipschitz non-decreasing function, \(h_i\) are origin-centered halfspaces with margin \(\rho\) on \(\mathcal{X}\) and \(|a|_1 = A\). There exists an algorithm that outputs a hypothesis \(h\) such that with probability \(1 - \delta\),

\[
E_{x,y \sim \mathcal{D}} \left[ \left( h(x) - u\left(\sum_{i=1}^t a_i h_i(x)\right) \right)^2 \right] \leq \epsilon
\]

for \(m = (\frac{L A}{\epsilon})^{O(1/\rho)} \log(1/\delta)\). The algorithm runs in time polynomial in \(m\) and \(n\).
Proof. We use Lemma 2 to show the existence of polynomial \( p \) of degree \( d = O \left( \frac{1}{\rho} \cdot \log \left( \frac{1}{\epsilon_0} \right) \right) \) such that for \( a \in [-1, 1] \), \( |p(a)| < 1 + \epsilon_0 \) and for \( a \in [-1, 1 \parallel [-\rho, \rho], \ |p(a) - \text{sign}(a)| < \epsilon_0 \).

Since for each \( i, \rho \leq |w_i \cdot x| \leq 1 \), we have \( |p(w_i \cdot x) - \text{sign}(w_i \cdot x)| \leq \epsilon_0 \) such that \( p \) is bounded in \( [-1, 1] \) by \( 1 + \epsilon_0 \). From Lemma 9 and 10 we have that for each \( i \), \( p(w_i \cdot x) = \langle v_i, \psi_d(x) \rangle \) such that \( \|v_i\| = \left( \frac{1}{\epsilon_0} \right)^{O(1/\rho)} \) where \( \psi_d \) is the feature vector corresponding to the multinomial kernel of degree \( d \). Using Lemma 9 we have that \( \sum_{i=1}^{t} a_i h_i(x) \) is \( \left( \epsilon_0 A, A \left( \frac{1}{\epsilon_0} \right)^{O(1/\rho)} \right) \)-approximated by \( MK_d \).

Subsequently, applying Theorem 3 we get that there exists an algorithm that outputs a hypothesis \( h \) such that with probability \( 1 - \delta \),

\[
\varepsilon(h) \leq CLA \left( \epsilon_0 + \left( \frac{1}{\epsilon_0} \right)^{C'/\rho} \cdot \sqrt{\frac{\log(1/\delta)}{m}} \right)
\]

for some constants \( C, C' > 0 \). Setting \( \epsilon_0 = \frac{\epsilon}{2CL\lambda} \) and \( m = \left( \frac{2CL\lambda}{\epsilon} \right)^{2C'/\rho} \cdot \left( \frac{4\log(1/\delta)}{\epsilon^2} \right) \) to gives us the required result. \qed

Remark. If \( \mathbb{E}[y|x] = u \left( \frac{1}{t} \sum_{i=1}^{t} h_i(x) \right) \), that is, a function of the fraction of true halfspaces, then the run-time is independent of the number of halfspaces \( t \). This holds since \( A = 1 \) in this case.

5.3 PAC Learning Intersection/Majority of Halfspaces with a Margin

Consider \( t \)-halfspaces \( \{h_1, \ldots, h_t\} \). An intersection of these \( t \)-halfspaces is given by \( f_{\text{AND}}(x) = \bigwedge_{i=1}^{t} h_i(x) \). A majority of \( t \)-halfspaces is given by \( f_{\text{maj}}(x) = \text{sign} \left( \sum_{i=1}^{t} h_i(x) - t/2 \right) \).

The following lemmas show that there exists kernels that separate intersection/majority of halfspaces.

Lemma 10. Intersection of \( t \)-halfspaces on \( \mathbb{S}^{n-1} \) is \( B \)-separated by a kernel \( K \) such that \( \forall x \in \mathcal{H}, K(x, x) \leq 1 \) with \( B = t^{O(\sqrt{1/\rho})} \).

Proof. Consider \( P_{\text{AND}} \) given by Lemma 8 for given \( \rho \). We know that \( \forall x \in \mathbb{S}^{n-1}, P_{\text{AND}}(x) \geq 1/2 \) if \( f_{\text{AND}}(x) = 1 \) and \( P_{\text{AND}}(x) \leq -1/2 \) if \( f_{\text{AND}}(x) = 0 \). We know that each coefficient of \( T_r(a) \) is bounded by \( 2^r \). It is easy to see that each coefficient of \( T_r(1-a) \) is bounded by \( 2^{O(r)} \). Using Lemma 8 the sum of squares of the coefficients of \( p(a) \) are bounded by \( 2^{O(r[\log 2r])} = t^{O(r)} \). Now using Lemma 11 we know that \( p(w_i \cdot x) = \langle v_i, \psi_d(x) \rangle \) for the feature vector \( \psi_d \) of the multinomial kernel with \( d = r[\log 2r] \). such that \( \|v_i\| \leq t^{O(r)} \). Thus, \( P_{\text{AND}}(x) = \langle v, \psi_d(x) \rangle \) (adjusting the constant term corresponding to the 1 entry in the feature vector) such that \( \|v\| \leq t^{O(r)} \). We can assume that \( \|\psi(x)\| \leq 1 \) by scaling the weight vector appropriately as before. Thus, \( f_{\text{AND}} \) is \( t^{O(r)} \)-separated by kernel \( MK_d \). \qed

Lemma 11. Majority of \( t \)-halfspaces on \( \mathbb{S}^{n-1} \) is \( B \)-separated by a kernel \( K \) such that \( \forall x \in \mathcal{H}, K(x, x) \leq 1 \) with \( B = t^{O(1/\rho)} \).

Proof. We use Lemma 2 to show the existence of polynomial \( p \) of degree \( d = O \left( \frac{1}{\rho} \cdot \log t \right) \) such that for \( a \in [-1, 1], \ |p(a)| < 1 + 1/2t \) and for \( a \in [-1, 1 \parallel [-\rho, \rho], \ |p(a) - \text{sign}(a)| < 1/2t \). Consider

\[
P_{\text{maj}}(x) = \sum_{i=1}^{t} p(w_i \cdot x) - \frac{t}{2}
\]
Since for each \( h_i, \rho \leq |w_i \cdot x| \leq 1 \), we have \( |p(w_i \cdot x) - \text{sign}(w_i \cdot x)| \leq 1/2t \). Thus if \( f_{\text{maj}}(x) = 1 \) then \( P_{\text{maj}}(x) \geq \sum_{i=1}^t h_i(x) - t/2 - 1/2 \geq 1/2 \). Similarly if \( f_{\text{maj}}(x) = 0 \) then \( P_{\text{maj}}(x) \leq -1/2 \).

From Lemma 5 and 1 we have that for each \( i, p(w_i \cdot x) = \langle v_i, \psi(x) \rangle \) such that \( ||v_i|| = t^{O(1/\rho)} \) where \( \psi \) is the feature vector corresponding to the multinomial kernel of degree \( d \). Thus, \( P_{\text{maj}}(x) = \langle v, \psi(x) \rangle \) (adjusting the constant term corresponding to the 1 entry in the feature vector) such that \( ||v|| = t^{O(1/\rho)} \). We can assume that \( ||\psi(x)|| \leq 1 \) by scaling the weight vector appropriately as before. Thus, \( f_{\text{maj}} \) is \( t^{O(1/\rho)} \)-approximated by kernel \( K \).

Applying Theorem 6 to the above lemmas, we obtain the following results for PAC learning:

**Corollary 1.** There exists an algorithm that PAC learns any intersection of \( t \)-halfspaces with margin \( \rho > 0 \) on \( \mathbb{S}^n \) in time \( t^{O(\sqrt{1/\rho}) \cdot \text{poly}(n, 1/\epsilon, \log(1/\delta))} \).

This result improves the previous best bound by [KS08] that had running time roughly \( n \cdot (\log t)^{O(\sqrt{1/\rho} \log t)} \). For constant \( \rho \), our algorithm is the first that has running time polynomial in the number of halfspaces.

**Corollary 2.** There exists an algorithm that PAC learns any majority of \( t \)-halfspaces with margin \( \rho > 0 \) on \( \mathbb{S}^n \) in time \( t^{O(1/\rho)} \cdot \text{poly}(n, 1/\epsilon, \log(1/\delta)) \).

### 6 The KMtron Algorithm

In this section, we propose an algorithm, KMtron, which combines isotonic regression with the KM algorithm [KM93] for finding large Fourier coefficients of a function (given query access to the function). In some sense, the KM algorithm takes the place of the “kernel trick” used by Alphatron to provide an estimate for the update step in isotonic regression. Viewed this way, the KM algorithm can be re-interpreted as a query-algorithm for giving estimates of the gradient of square-loss with respect to the uniform distribution on Boolean inputs.

The main application of KMtron is a generalization of celebrated results for PAC learning DNF formulas [Jac97] to the setting of probabilistic concepts. That is, we can efficiently learn any conditional mean that is a smooth, monotone combination of \( L_1 \)-bounded functions.

**Notation.** We follow the notation of [GKK08]. For any function \( P : \{-1,1\}^n \to \mathbb{R} \), we denote the Fourier coefficients by \( \hat{P}(S) \) for all \( S \subseteq [n] \). The support of \( P \), i.e., the number of non-zero Fourier coefficients, is denoted by \( \text{supp}(P) \). The norms of the coefficient vectors are defined as \( L_p(P) = \left( \sum_S |\hat{P}(S)|^p \right)^{1/p} \) for \( p \geq 1 \) and \( L_\infty(P) = \max_S |\hat{P}(S)| \). Similarly, the norm of the function \( P \) are defined as \( ||P||_p = \mathbb{E}_{x \in \{-1,1\}^n} [\sum_S |P(x)|^p]^{1/p} \) for \( p \geq 1 \). Also, the inner product \( P \cdot Q = \mathbb{E}_{x \in \{-1,1\}^n} [P(x)Q(x)] \).

**KM Algorithm.** The KM algorithm learns sparse approximations to boolean functions given query access to the underlying function. The following lemmas about the KM algorithm are important to our analysis.

**Lemma 12 ([KM93]).** Given an oracle for \( P : \{-1,1\}^n \to \mathbb{R} \), \( \text{KM}(P, \theta) \) returns \( Q : \{-1,1\}^n \to \mathbb{R} \) with \( |\text{supp}(Q)| \leq O(L_2(P)^2 \theta^{-2}) \) and \( L_\infty(P - Q) \leq \theta \). The running time is \( \text{poly}(n, \theta^{-1}, L_2(P)) \).
Lemma 13 ([KM93]). If $P$ has $L_1(P) \leq k$, then $\text{KM} \left( P, \frac{\epsilon}{3k} \right)$ returns $Q$ s.t. $\|P - Q\|_2 \leq \epsilon$.

Projection Operator. The projection operator $\text{proj}_K(P)$ for $P : \{-1, 1\}^n \to \mathbb{R}$ maps $P$ to the closest $Q$ in convex set $K = \{ Q : \{-1, 1\}^n \to \mathbb{R} \mid L_1(Q) \leq k \}$, i.e., $\text{proj}_K(P) = \arg\min_{Q \in K} \|Q - P\|_2$. [GKK08] show that $\text{proj}_K$ is simple and easy to compute for sparse polynomials. We use the following lemmas by [GKK08] about the projection operator in our analysis.

Lemma 14 ([GKK08]). Let $P, P'$ be such that $L_\infty(P - P') \leq \epsilon$. Then $L_\infty(\text{proj}_K(P) - \text{proj}_K(P')) \leq 2\epsilon$.

Lemma 15 ([GKK08]). Let $P, P'$ be such that $L_\infty(P - P') \leq \epsilon$. Then $\|\text{proj}_K(P) - \text{proj}_K(P')\|_2 \leq 2\sqrt{\epsilon k}$.

KMtron. The algorithm KMtron is as follows:

**Algorithm 2: KMtron**

| Input | Function $u : \mathbb{R} \to [0, 1]$ non-decreasing and $L$-Lipschitz, query access to $u \circ P$ for some function $P : \{-1, 1\}^n \to \mathbb{R}$, learning rate $\lambda \in (0, 1]$, number of iterations $T$, error parameter $\theta$ |
|-------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1     | $P_0 = 0$                                                                                                                                  |
| 2     | for $t = 1, \ldots, T$ do                                                                                                                  |
| 3     | $P'_t := P_{t-1} + \lambda \text{KM}(u \circ P - u \circ P_{t-1}, \theta)$                                                                  |
| 4     | $P_t = \text{KM}(\text{proj}_K(P'_t), \theta)$                                                                                           |
| 5     | end                                                                                                                                     |
| Output| Return $u \circ P_t$ where $P_t$ is the best over $t = 1, \ldots, T$                                                                     |

To efficiently run KMtron, we require efficient query access to $u \circ P - u \circ P_{t-1}$. Since $P_{t-1}$ is stored as a sparse polynomial, and we are given query access for $u \circ P$, we can efficiently compute $u(P(x)) - u(P_{t-1}(x))$ for any $x$. We can extend the algorithm to handle distribution queries (p-concept), i.e., for any $x$ of our choosing we obtain a sample of $y$ where $\mathbb{E}[y|x] = u(P(x))$. [GKK08] (c.f. Appendix A.1) observed that using distribution queries instead of function queries to the conditional mean is equivalent as long as the number of queries is polynomial.

The following theorem proves the correctness of KMtron.

**Theorem 10.** For any non-decreasing $L$-Lipschitz $u : \mathbb{R} \to [0, 1]$ and function $P : \{-1, 1\}^n \to \mathbb{R}$ such that $L_1(P) \leq k$, given query access to $u \circ P$, KMtron run with $\lambda = \frac{\epsilon}{2\sqrt{T}}$, $T = \frac{2k^2L^2}{\epsilon^2}$ and $\theta \leq \frac{C'}{\epsilon k}$ for sufficiently small constant $C' > 0$ and outputs $P^*$ such that $\mathbb{E}_{x \in \{-1, 1\}^n}[(u(P(x)) - u(P^*(x)))^2] \leq \epsilon$. The runtime of KMtron is $\text{poly}(n, k, L, 1/\epsilon)$.

**Proof.** Let $\epsilon(h) = \mathbb{E}_{x \in \{-1, 1\}^n}[(u(P(x)) - u(h(x)))^2] = \|u \circ P - u \circ h\|_2^2$. Similar to Alphatron, we will show that with each iteration $t$ we will move closer to the true solution as long as $\epsilon(P_t)$ is large.

**Lemma 16.** For a suitable choice of $\theta$, $\|P_t - P\|_2^2 - \|P_{t+1} - P\|_2^2 \geq \frac{2\lambda}{T}(\epsilon(P_t) - L\lambda)$.

**Proof.** Let us define the following polynomials for $t \leq T$, $Q'_t = P_{t-1} + \lambda (u \circ P - u \circ P_{t-1})$ and $Q_t = \text{proj}_K(Q'_t)$. For all $t \leq T$,

$$P'_t - Q'_t = (P_{t-1} + \lambda \text{KM}(u \circ P - u \circ P_{t-1}, \theta)) - (P_{t-1} + \lambda (u \circ P - u \circ P_{t-1}))$$

$$= \lambda (\text{KM}(u \circ P - u \circ P_{t-1}, \theta) - (u \circ P - u \circ P_{t-1})).$$
From Lemma \[12\] \(L_\infty(KM(u \circ P - u \circ P_{t-1}, \theta) - (u \circ P - u \circ P_{t-1})) \leq \theta\) implying \(L_\infty(P_t' - Q_t') \leq \lambda \theta \leq \theta\) since \(\lambda \leq 1\).

Using Lemma \[15\] we have \(||\text{proj}_K(P_t') - \text{proj}_K(Q_t')||_2 \leq 2\sqrt{\theta k}||\). Since \(P_t = KM(\text{proj}_K(P_t'), \theta)\) and \(L_1(\text{proj}_K(P_t')) \leq k\), using Lemma \[13\] \(||P_t - \text{proj}_K(P_t')||_2 \leq \sqrt{2\theta k}||\). Using Triangle inequality, we get,

\[||P_t - Q_t||_2 \leq ||P_t - \text{proj}_K(P_t')||_2 + ||\text{proj}_K(P_t') - \text{proj}_K(Q_t')||_2 \leq 4\sqrt{\theta k}||\]

Observe that \(||Q_t - P||_2 \leq L_2(Q_t - P) \leq L_1(Q_t - P) \leq L_1(Q_t) + L_1(P) \leq 2k\). Combining these two observations, we have

\[||P_t - P||_2^2 \leq (||P_t - Q_t||_2 + ||Q_t - P||_2)^2 \leq ||Q_t - P||_2^2 + 16\sqrt{\theta k} + 16\theta k \leq ||Q_t - P||_2^2 + Ck\sqrt{\theta k}||\]

for large enough constant \(C > 0\). Therefore,

\[\text{}\begin{align*}
||P_t - P||_2^2 - ||P_{t+1} - P||_2^2 &\geq ||P_t - P||_2^2 - ||Q_{t+1} - P||_2^2 - Ck\sqrt{\theta k} \\
&\geq ||P_t - P||_2^2 - ||Q_{t+1} - P||_2^2 - Ck\sqrt{\theta k} \\
&= ||P_t - P||_2^2 - ||P_t - P + \lambda(u \circ P - u \circ P_1)||_2^2 - Ck\sqrt{\theta k} \\
&= -2\lambda(u \circ P - u \circ P_1) \cdot (P_t - P) - \lambda^2||u \circ P - u \circ P_1||_2^2 - Ck\sqrt{\theta k} \\
&\geq \frac{2\lambda}{L} \cdot \varepsilon(P_t) - \lambda^2 - Ck\sqrt{\theta k}.
\end{align*}\]

Here, \[13\] follows from the triangle inequality and \[5\], \[14\] follows from projecting to a convex set reducing the distance to points in the convex set, \[16\] follows from \(u\) being monotone, \(L\)-Lipschitz with output bounded in \([0, 1]\). Setting \(\theta\) such that \(Ck\sqrt{\theta k} \leq \lambda^2\) gives the required result. \(\square\)

As long as \(\varepsilon(P_t) \geq 2L\lambda\), we have \(||P_t - P||_2^2 - ||P_{t+1} - P||_2^2 \geq 2\lambda^2\). Since \(||P_0 - P||_2^2 = ||P||_2^2 \leq L_1(P)^2 \leq k^2\), after \(T = \frac{L^2}{k^2}\), there must be some \(r \leq T\) such that \(||P_t - P||_2^2 \geq 2\lambda^2\) does not hold, at this iteration, \(\varepsilon(P_t) \leq 2L\lambda = \epsilon\) for \(\lambda = \frac{\epsilon}{2L}\). The last step of choosing the best \(P_t\) would give us the required hypothesis (similar to Alphatron). Observe that each iteration of KMtron runs in time \(\text{poly}(n, k, L, 1/\epsilon)\) (Lemma \[12\]) and KMtron is run for \(\text{poly}(k, L, 1/\epsilon)\) iterations giving us the required runtime. \(\square\)

**Corollary 3.** Let \(P_i\) be such that \(L_1(P_i) \leq k\) for \(i \in [s]\). If we have query access to \(y\) for all \(x\) such that \(\mathbb{E}[y|x] = u\left(\frac{1}{s} \sum_{i=1}^{s} P_i\right)\) for non-decreasing \(L\)-Lipschitz \(u\), then using the above, we can learn the conditional mean function in time \(\text{poly}(n, k, L, 1/\epsilon)\).

Observe that the complexity bounds are independent of the number of terms. This follows from the fact that \(L_1\left(\frac{1}{s} \sum_{i=1}^{s} P_i\right) \leq k\). This leads to the following new learning result for DNF formulas: fix a DNF \(f\) and let \(\text{frac}(f(x))\) denote the fraction of terms of \(f\) satisfied by \(x\). Fix monotone, \(L\)-Lipschitz function \(u\). For uniformly chosen input \(x\), label \(y\) is equal to 1 with probability \(u(\text{frac}(f(x)))\). Then in time polynomial in \(n, 1/\epsilon\), and \(L\), KMtron outputs a hypothesis \(h\) such that \(\mathbb{E}[(h(x) - u(\text{frac}(f(x))))^2] \leq \epsilon\) (recall \(L_1(\text{AND}) = 1\)). Note that the running time has no dependence on the number of terms.

As an easy corollary, we also obtain a simple (no Boosting required) polynomial time query-algorithm for learning DNFs under the uniform distribution\(^5\).

\(^5\)Feldman [Fel12] was the first to obtain a query-algorithm for PAC learning DNF formulas with respect to the uniform distribution that did not require a Boosting algorithm.
Corollary 4. Let \( f \) be a DNF formula from \( \{-1,1\}^n \to \{0,1\} \) with \( s \) terms. Then \( f \) is PAC learnable under the uniform distribution using membership queries in time \( \text{poly}(n,s, 1/\epsilon) \).

Proof. Let \( \{T_i\}_{i=1}^s \) be the ANDs corresponding to each term of the DNF. Let \( T = \sum_{i=1}^{s} T_i \). By definition of \( f \), if \( f(x) = 1 \) then \( T(x) \geq 1 \) and if \( f(x) = 0 \) then \( T(x) = 0 \). Observe that \( L_1(T) \leq \sum_{i=1}^{s} L_1(T_i) \leq s \) using the well known fact that AND has \( L_1 \) bounded by 1.

Consider the following \( u \),

\[
    u(a) = \begin{cases} 
    0 & a \leq 0 \\
    a & 0 < a < 1 \\
    1 & a \geq 1 
\end{cases}
\]

Observe that \( u \) is 1-Lipschitz. It is easy to see that \( f(x) = u(T(x)) \) on \( \{-1,1\}^n \). Hence, given query access to \( f \) is the same as query access to \( u \circ T \) over \( \{-1,1\}^n \).

Since \( L_1(T) \) is bounded, we can apply Theorem 10 for the given \( u \). We get that in time \( \text{poly}(n,s, 1/\epsilon) \), KMtron outputs a polynomial \( P \) such that \( \mathbb{E}_{x \in \{-1,1\}^n}[(u(T(x)) - u(P(x)))^2] \leq \epsilon \).

Following the proof of Theorem 6 we can move from square-loss to zero-one loss and show that \( \Pr_{x \in \{-1,1\}^n}[f(x) \neq \text{sign}(u(P(x)))] \leq 4\epsilon \). Scaling \( \epsilon \) appropriately, we obtain the required result. \( \square \)

7 Multiple Instance Learning

Multiple Instance Learning (MIL) is a generalization of supervised classification in which a label is assigned to a bag, that is, a set of instances, instead of an individual instance [DLLP97]. The bag label is induced by the labels of the instances in it. The goal we focus on in this work is to label future bags of instances correctly, with high probability. We refer the reader to [Amo13, HVB+16] for an in-depth study of MIL. In this section we apply the previously developed ideas to MIL and give the first provable learning results for concrete schemes that do not rely on unproven assumptions.

Comparison to Previous Work. Under the standard MI assumption, various results are known in the PAC learning setting. Blum and Kalai [BK98] showed a simple reduction from PAC learning MIL to PAC learning with one-sided noise under the assumption that the instances in each bag were drawn independently from a distribution. Sabato and Tishby [ST12] removed the independence assumption and gave sample complexity bounds for learning future bags. All the above results require the existence of an algorithm for PAC learning with one-sided noise, which is itself a challenging problem and not known to exist for even simple concept classes.

In this work, we do not assume instances within each bag are independently distributed, and we do not require the existence of PAC learning algorithms for one-sided noise. Instead, we give efficient algorithms for labeling future bags when the class labeling instances is an unknown halfspace with a margin or an unknown depth-two neural network. We succeed with respect to general monotone, smooth combining functions.

Notation. Let us denote the space of instances as \( \mathcal{X} \) and the space of bags as \( \mathcal{B} \subseteq \mathcal{X}^* \). Let \( N \) be an upper bound on the size of the bags, that is, \( N = \max_{\beta \in \mathcal{B}} |\beta| \). Let the instance labeling function be \( c: \mathcal{X} \to \mathbb{R} \) and the bag labeling function be \( f_{\text{bag}} \). We assume a distribution \( \mathcal{D} \) over the bags and allow the instances within the bag to be dependent on each other. We consider two variants of the relationship between the instance and bag labeling functions and corresponding learning models.
7.1 Deterministic MIL

In the deterministic case we assume that there is a deterministic map from instance labels to bag labels. This is the standard model that has been studied in literature.

**Definition 7** (Deterministic MI Assumption). Given combining function \( u : \{0,1\}^* \to \{0,1\} \), for bag \( \beta = \{x_1, \ldots, x_r\} \), \( f_{bag}(\beta) \) is a fixed function such that \( f_{bag}(\beta) = u(c(\beta)) \) where \( c(\beta) = (c(x_1), \ldots, c(x_r)) \) and \( c \) is the instance labeling function.

**Definition 8** (Deterministic MIL). The concept class \( \mathcal{C} \) is \((\epsilon, \delta)\)-Deterministic MIL for \( u \) with sample complexity \( M \) and running time \( T \) if under the deterministic MIL assumption for \( u \), there exists an algorithm \( A \) such that for all \( c \in \mathcal{C} \) as the instance labeling function and any distribution \( \mathcal{D} \) on \( \mathcal{B} \), \( A \) draws at most \( M \) iid bags and runs in time \( T \), to output a bag-labeling hypothesis \( h \) such that with probability \( 1 - \delta \),

\[
Pr_{\beta \sim \mathcal{D}}[h(\beta) \neq f_{bag}(\beta)] \leq \epsilon.
\]

The following theorem follows directly from Theorem \( \[ \] \) setting the input space as \( \mathcal{B} \).

**Theorem 11.** The concept class \( \mathcal{C} \) is \((\epsilon, \delta)\)-Deterministic MIL for \( u \) with sample complexity \( C(BL)^2 \cdot \log(1/\delta) \) for sufficiently large constant \( C > 0 \) and running time \( \text{poly}(n,B,L,1/\epsilon,\log(1/\delta)) \) if for all \( c \in \mathcal{C} \), \( u \circ c \) is \( B \)-separated by some kernel \( K \).

Thus, we need to show that \( \text{OR} \) of halfspaces with a margin are \( B \)-separated for an appropriate \( B \) by some kernel function \( K \). We have the following lemma:

**Lemma 17.** The class of \( \text{OR} \) of halfspaces with margin \( \rho \) on bags of size \( \leq N \) with elements in \( \mathbb{S}^{n-1} \) is \( B \)-separated by a kernel \( K \) such that \( \forall \beta \in \mathcal{B}, K(\beta, \beta) \leq 1 \) with \( B = N^{O(\sqrt{1/\rho})} \).

**Proof.** Let \( w \) correspond to the weight vector of the halfspace that generates the instance labeling function. Since \( \text{OR} \) is the combining function, we consider \( P_{\text{OR}} \) given by Lemma \( \[ \] \) for given \( \rho \) and bag size (sets of size) \( \leq N \) which separates the required class.

\[
P_{\text{OR}}(\beta) = \frac{1}{2} - N + \frac{N}{|\beta|} \sum_{x \in \beta} p(w \cdot x)
\]

where \( p(a) = T_r(1 + a) \) for \( r = O(\sqrt{1/\rho}) \). From the proof of Lemma \( \[ \] \) we know that the sum of squares of the coefficients of \( p(a) \) are bounded by \( 2^{O(r \log 2N^2)} = N^{O(r)} \). Now using Lemma \( \[ \] \) we know that \( \forall x \in \beta, p(w \cdot x) = \langle v, \psi_d(x) \rangle \) for the feature vector \( \psi_d \) of the multinomial kernel \( MK_d \) for \( d = r \log 2N \). We also have \( ||v|| \leq N^{O(r)} \). Thus, \( \frac{N}{|\beta|} \sum_{x \in \beta} p(w \cdot x) = \langle Nv, \frac{1}{|\beta|} \sum_{x \in \beta} \psi(s) \rangle = \langle Nv, \psi_{\text{mean}}(\beta) \rangle \) where \( \psi_{\text{mean}} \) is the feature vector of the mean map kernel of \( MK_d \). The constant term \( 1/2 \) can be incorporated by adding an additional entry to the mean map feature vector \( \psi_{\text{mean}} \) corresponding to constant 1, that is, consider new feature vector \( \psi'(S) = [\psi_{\text{mean}}(S), 1] \). Observe that the corresponding kernel \( K'(S,T) = K_{\text{mean}}(S,T) + 1 \). Note that \( ||\psi'(S)||^2 = ||\psi_{\text{mean}}(S)||^2 + 1 = O(r \log 2N) \). We can normalize this to norm 1 by scaling the weight vector appropriately as before. Thus, \( \text{OR} \circ c \) is \( N^{O(r)} \)-separated by kernel \( K' \). \( \square \)

---

\(^6\)The mean map kernel is essential for our analysis as it handles varying bag sizes requiring only an upper bound on the size of the bags. An alternative would be to concatenate the feature vectors of each instance in a bag to form a new kernel but this would only work if all bags had the same fixed size.
This in turn implies deterministic MIL for the concept class of halfspaces with a constant margin and OR as the combining function. A similar proof can be given for AND. Note that for the proof we do not require independence among the instances but just among the bags as we can embed each possible bag in $\mathcal{B}$ into an RKHS.

**Corollary 5.** The concept class of halfspaces with constant margin is $(\epsilon, \delta)$-Deterministic MIL for OR/AND and bag size $\leq N$ with sample complexity and running time $\text{poly}(n, N, 1/\epsilon, \log(1/\delta))$.

Similarly, following Lemma 11, we can extend the above result to majority.

**Corollary 6.** The concept class of halfspaces with constant margin is $(\epsilon, \delta)$-Deterministic MIL for majority and bag size $\leq N$ with sample complexity and running time $\text{poly}(n, N, 1/\epsilon, \log(1/\delta))$.

### 7.2 Probabilistic MIL

We generalize the deterministic model to allow the labeling function to induce a probability distribution over the labels. This assumption seems more intuitive and less restrictive than the deterministic case as it allows for noise in the labels.

**Definition 9** (Probabilistic MI Assumption). Given combining function $u : \mathbb{R} \rightarrow [0, 1]$, for bag $\beta$, $f_{\text{bag}}(\beta)$ is a random variable such that $\Pr[f_{\text{bag}}(\beta) = 1] = u\left(\frac{1}{|\beta|} \cdot \sum_{x \in \beta} c(x)\right)$ where $c$ is the instance labeling function.

**Definition 10** (Probabilistic MIL). The concept class $\mathcal{C}$ is $(\epsilon, \delta)$-Probabilistic MIL for $u$ with sample complexity $M$ and running time $T$ if under the probabilistic MI assumption for $u$, there exists an algorithm $A$ such that for all $c \in \mathcal{C}$ as the instance labeling function and any distribution $D$ on $\mathcal{B}$, $A$ draws at most $M$ iid bags and runs in time at most $T$ to return a bag-labeling hypothesis $h$ such that with probability $1 - \delta$,

$$\mathbb{E}_{\beta \sim D} \left[ \left( h(\beta) - u\left(\frac{1}{|\beta|} \cdot \sum_{x \in \beta} c(x)\right) \right)^2 \right] \leq \epsilon.$$

The following lemma along with Theorem 5 give us learnability results in the Probabilistic MIL setting.

**Lemma 18.** Let $c$ be the instance labeling function mapping $\mathcal{X}$ to $\mathbb{R}$ such that $c$ is $(\epsilon, B)$-approximated by kernel $\mathcal{K}$ and feature vector $\psi$. Then the function $f : \mathcal{B} \rightarrow \mathbb{R}$ given by $f(\beta) = \frac{1}{|\beta|} \cdot \sum_{x \in \beta} c(x)$ is $(\epsilon, B)$-approximated by the mean map kernel of $\mathcal{K}$.

**Proof.** We have that $\forall x \in \mathcal{X}, |c(x) - \langle v, \psi(x) \rangle| \leq \epsilon$ for $v$ such that $||v|| \leq B$. Let $\mathcal{K}_{\text{mean}}$ be the mean map kernel of $\mathcal{K}$ and $\psi_{\text{mean}}$ be the corresponding vector. We will show that $v$ $(\epsilon, B)$-approximates $f$ in $\mathcal{K}_{\text{mean}}$. This follows from the following,

$$|f(\beta) - \langle v, \psi_{\text{mean}}(\beta) \rangle| = \left| \frac{1}{|\beta|} \cdot \sum_{x \in \beta} c(x) - \frac{1}{|\beta|} \cdot \sum_{x \in \beta} \langle v, \psi(x) \rangle \right| \leq \frac{1}{|\beta|} \cdot \sum_{x \in \beta} |c(x) - \langle v, \psi(x) \rangle| \leq \epsilon.$$
Theorem 12. The concept class $C$ is $(\epsilon, \delta)$-Probabilistic MIL for monotone $L$-Lipschitz $u$ with sample complexity $(\frac{BL}{\epsilon})^2 \cdot \log(1/\delta)$ and running time $\text{poly}(n, B, L, 1/\epsilon, \log(1/\delta))$ if all $c \in C$ are $(\epsilon/CL, B)$-approximated by some kernel $K$ for large enough constant $C > 0$.

Proof. Consider $c \in C$ that is $(\epsilon/CL, B)$-approximated by some kernel $K$ for large enough constant $C > 0$ (to be chosen later). Using Lemma 18 we know that $f(\beta) = \frac{1}{|\beta|} \cdot \sum_{x \in \beta} c(x)$ is $(\epsilon/CL, B)$-approximated by the mean map kernel $K_{\text{mean}}$ of $K$. Applying Theorem 5, we get that with probability $1 - \delta$,

$$E_{\beta \sim D} \left[ \left( h(\beta) - u \left( \frac{1}{|\beta|} \cdot \sum_{x \in \beta} c(x) \right) \right)^2 \right] \leq \frac{C'}{C} \epsilon,$$

for sufficiently large constant $C' > 0$. Choosing $C \geq C'$ gives the result. \qed

Combining Theorem 12 with learnability Theorems 7 and 9 we can show the following polynomial time Probabilistic MIL results.

Corollary 7. For any monotone $L$-Lipschitz function $u$, the concept class of sigmoids over $S^{n-1}$ are $(\epsilon, \delta)$-Probabilistic MIL with sample complexity and running time $\text{poly}(n, L, 1/\epsilon, \log(1/\delta))$.

Corollary 8. For any monotone $L$-Lipschitz function $u$, the concept class of halfspaces with a constant margin over $S^{n-1}$ are $(\epsilon, \delta)$-Probabilistic MIL with sample complexity and running time $\text{poly}(n, L, 1/\epsilon, \log(1/\delta))$.

8 Conclusions and Future Work

We have given the first assumption-free, polynomial-time algorithm for learning a class of non-linear neural networks with more than one hidden layer. We only require that the conditional mean function is computed by such a network, and therefore our results also capture Boolean learning problems. In contrast, PAC learning corresponding Boolean function classes seems intractable.

Understanding the broadest class of conditional mean functions that admit efficient learning algorithms is a natural open problem. For example, can we learn two hidden layers with multiple hidden units in the second layer?

We remark that while our algorithms are noise-tolerant in the sense that we make assumptions only on the conditional mean function, it is unlikely that our results can be extended to the fully non-realizable (agnostic) setting, as there are hardness results for agnostically learning even a single ReLU in fully-polynomial time [GKKT16].

Finally, it is easy to see that depth-3 neural networks with one hidden layer of ReLUs feeding into a sigmoid can approximate (with negligible error), polynomial-size DNF formulas. Thus, it is unlikely we can obtain polynomial-time algorithms for such architectures [DSS16].

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