

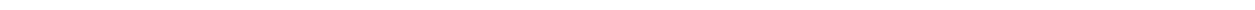
TUFTS-CS Technical Report 2004-10

November 2004

by

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Maximum Margin Algorithms with Boolean Kernels

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Abstract

Recent work has introduced Boolean kernels with which one can learn linear threshold functions over a feature space containing all conjunctions of length up to k (for any $1 \leq k \leq n$) over the original n Boolean features in the input space. This motivates the question of whether maximum margin algorithms such as Support Vector Machines can learn Disjunctive Normal Form expressions in the Probably Approximately Correct (PAC) learning model using this kernel. We study this question, as well as a variant in which structural risk minimization (SRM) is performed where the class hierarchy is taken over the length of conjunctions.

We show that such maximum margin algorithms do not PAC learn $t(n)$ -term DNF for any $t(n) = \omega(1)$, even when used with such a SRM scheme. We also consider PAC learning under the uniform distribution and show that if the kernel uses conjunctions of length $\tilde{\omega}(\sqrt{n})$ then the maximum margin hypothesis will fail on the uniform distribution as well. Our results concretely illustrate that margin based algorithms may overfit when learning simple target functions with natural kernels.

Keywords: Computational Learning Theory, Kernel Methods, PAC Learning, Boolean Functions, Hardness Results.

1 Introduction

1.1 Background

Maximum margin algorithms, notably Support Vector Machines (SVM) [4], have received considerable attention in recent years (see e.g. [27] for an introduction). In their basic form, SVM learn linear threshold hypotheses and combine two powerful ideas. The first idea is to learn using the linear separator which achieves the *maximum margin* on the training data rather than an arbitrary consistent linear threshold hypothesis. The second idea is to use

*This work has been partly supported by NSF Grant IIS-0099446.

†Much of this work was done while supported by an National Science Foundation Mathematical Sciences Postdoctoral Research Fellowship at Harvard University.

an implicit feature expansion by a *kernel function*. The kernel $K : X \times X \rightarrow \mathbb{R}$, where X is the original space of examples, computes the inner product in the expanded feature space. Given a kernel K which corresponds to some expanded feature space, the SVM hypothesis h is (an implicit representation of) the maximum margin linear threshold hypothesis over this expanded feature space rather than the original feature space. SVM theory (see e.g. [27]) implies that if the kernel K is efficiently computable then it is possible to efficiently construct this maximum margin hypothesis h and that h itself is efficiently computable. Several on-line algorithms have also been proposed which iteratively construct large margin hypotheses in the feature space, see e.g. [7, 8].

Both theoretical and experimental studies suggest that such algorithms may be able to take advantage of properties of the distribution and data to converge faster than what would be required by uniform convergence bounds. In particular, convergence bounds based on the maximum margin of the classifier on the observed data have been obtained [26, 27]. The bounds are independent of the dimension of the expanded space but they depend on the L_2 norm of examples in this space. The learning problems analyzed in this paper include cases where both the dimension and the L_2 norm are large so that the known bounds do not imply rapid convergence. Indeed, we show that overfitting can occur in such cases.

1.2 Can SVMs learn DNF?

Another major focus of research in learning theory is the question of whether various classes of Boolean functions can be learned by computationally efficient algorithms. The canonical open question in this area is whether there exist efficient algorithms in Valiant's Probably Approximately Correct (PAC) learning model [29] for learning Boolean formulas in Disjunctive Normal Form, or DNF. This question has been open since the introduction of the PAC model [29], and has been intensively studied by many researchers (see e.g. [2, 3, 5, 9, 10, 12, 14, 16, 18, 23, 28, 30, 31]).

In this paper we analyze the performance of maximum margin algorithms when used with Boolean kernels to learn DNF formulas. Several authors [13, 22, 32, 15] have recently proposed a family of kernel functions $K_k : \{0, 1\}^n \times \{0, 1\}^n \rightarrow \mathbb{N}$, where $1 \leq k \leq n$, such that $K_k(x, y)$ computes the number of (monotone or unrestricted) conjunctions of length (exactly or up to) k which are true in both x and y . This is equivalent to expanding the original feature space of n Boolean features to include all such conjunctions.¹ Since linear threshold elements can represent disjunctions, one can naturally view any DNF formula as a linear threshold function over this expanded feature space. It is thus natural to ask whether the K_k kernel maximum margin learning algorithms are good algorithms for learning DNF.

Additional motivation for studying DNF learnability with the K_k kernels comes from recent progress on the DNF learning problem. The fastest known algorithm for PAC learning DNF is due to Klivans and Servedio [14]; it works by explicitly expanding each example into a feature space of monotone conjunctions and explicitly learning a consistent linear

¹This Boolean kernel is similar to the well known polynomial kernel in that all monomials of length up to k are represented. The main difference is that the polynomial kernel assigns weights to monomials which depend on certain binomial coefficients; thus the weights of different monomials can differ by an exponential factor. In the Boolean kernel all monomials have the same weight.

threshold function over this expanded feature space. Since the K_k kernel enables us to do such expansions implicitly in a computationally efficient way, it is natural to investigate whether the K_k -kernel maximum margin algorithm yields a computationally efficient algorithm for PAC learning DNF.

As mentioned above standard convergence bounds on large margin classifiers do not imply that the K_k kernel maximum margin algorithm is an efficient algorithm for PAC learning DNF. Indeed, the bound given by, e.g., Theorem 4.18 of [27] only implies nontrivial generalization error for the K_k kernel algorithm if a sample of size $n^{\Omega(k)}$ is used, and with such a large sample the computational advantage of using the K_k kernel is lost. However, such upper bounds do not imply that the K_k kernel maximum margin algorithm must have poor generalization error if run with a smaller sample. The situation is analogous to that of [24] where the generalization error of the Perceptron and Winnow algorithms were studied. For both Perceptron and Winnow the standard bounds gave only an exponential upper bound on the number of examples required to learn various classes, but a detailed algorithm-specific analysis gave positive PAC learning results for Perceptron and negative PAC results for Winnow for the problems considered. Analogously, in this paper we perform detailed algorithm-specific analysis for the K_k kernel maximum margin algorithms.

1.3 Previous work

Kharon *et al.* constructed a simple Boolean function and an example sequence for the online mistake-bound learning model, and showed that this sequence causes the K_n kernel Perceptron algorithm (i.e. the Perceptron algorithm run over a feature space of all 2^n monotone conjunctions) to make $2^{\Omega(n)}$ many mistakes [13]. The current paper differs in several ways from this earlier work: we study the maximum margin algorithm rather than Perceptron, we consider PAC learning from a random sample rather than online learning, and we analyze the K_k kernels for all $1 \leq k \leq n$. We note here that maximum margin linear threshold learning algorithms are generally viewed as being more powerful than the simple Perceptron algorithm, and that PAC learning is generally viewed as being easier than online mistake bound learning (it is well known that any concept class which is efficiently learnable in the mistake bound model is efficiently PAC learnable, but the converse is not true [1]). Thus, the results of this work represent a substantial strengthening and generalization of [13].

1.4 Our results

Throughout this paper we study the kernels corresponding to all monotone monomials of length up to k , which we denote by K_k . In addition to unaugmented maximum margin algorithms we also consider a natural scheme of structural risk minimization (SRM) that can be used with maximum margin algorithms over this family of Boolean kernels. In SRM, given a hierarchy of classes $C_1 \subseteq C_2 \subseteq \dots$, one learns with each class separately and uses a cost function combining the complexity of the class with its observed accuracy to choose the final hypothesis. The cost function typically balances various criteria such as the observed error and the (bound on) generalization error. A natural scheme here is to use SRM over

the classes formed by K_k with $k = 1, \dots, n$.²

We prove several negative results which establish strong limitations on the ability of maximum margin algorithms to PAC learn DNF formulas (or other simple Boolean classes) using the monomial kernels. Variants of these results are shown to hold for the standard polynomial kernel as well. Our first result says essentially that for any $t(n) = \omega(1)$, for all $k = 1, \dots, n$ the K_k kernel maximum margin algorithm cannot PAC learn $t(n)$ -term DNF. More precisely, we prove

Result 1: Let $t(n) = \omega(1)$ and let $\epsilon = \frac{1}{4 \cdot 2^{t(n)}}$. There is a $O(t(n)^{1/3})$ -term monotone DNF over $t(n)$ relevant variables, and a distribution \mathcal{D} over $\{0, 1\}^n$ such that for all $k \in \{1, \dots, n\}$ the K_k maximum margin hypothesis has error larger than ϵ (with overwhelmingly high probability over the choice of a polynomial size random sample from \mathcal{D}).

Note that this result implies that the K_k maximum margin algorithms fail even when combined with SRM *regardless of the cost function*. This is simply because the maximum margin hypothesis has error $> \epsilon$ for all k , and hence the final SRM hypothesis must also have error $> \epsilon$.

While our accuracy bound in the above result is small (it is $o(1)$ since $t(n) = \omega(1)$), a simple variant of the construction used for Result 1 also proves:

Result 2: Let $f(x) = x_1$ be the target function. There is a distribution \mathcal{D} over $\{0, 1\}^n$ such that for any $k = \omega(1)$ the K_k maximum margin hypothesis has error at least $\frac{1}{2} - 2^{-n^{\Omega(1)}}$ (with overwhelmingly high probability over the choice of a polynomial size random sample from \mathcal{D}).

Thus any attempt to learn using monomials of non-constant size can provably lead to overfitting. Note that for any $k = \Theta(1)$, standard bounds on maximum margin algorithms show that the K_k kernel algorithm can learn $f(x) = x_1$ from a polynomial size sample.

Given these strong negative results for PAC learning under arbitrary distributions, we next consider the problem of PAC learning monotone DNF under the uniform distribution. This is one of the few frameworks in which some positive results have been obtained for learning DNF from random examples only (see e.g. [6, 25]). In this scenario a simple variant of the construction for Result 1 shows that learning must fail if k is too small:

Result 3: Let $t(n) = \omega(1)$ and $\epsilon = \frac{1}{4 \cdot 2^{t(n)}}$. There is a $O(t(n))$ -term monotone DNF over $t(n)$ relevant variables such that for all $k < t(n)$ the K_k maximum margin hypothesis has error at least ϵ (with probability 1 over the choice of a random sample from the uniform distribution).

This result is representation based; we show that no possible hypothesis output by the K_k algorithm can have error less than ϵ . On the other hand, we also show that the K_k algorithm fails under the uniform distribution for large k :

Result 4: Let $f(x) = x_1$ be the target function. For any $k = \tilde{\omega}(\sqrt{n})$, the K_k maximum margin hypothesis will have error $\frac{1}{2} - 2^{-\Omega(n)}$ with probability at least 0.028 over the choice of a polynomial size random sample from the uniform distribution.

²This is standard practice in experimental work with the polynomial kernel, where typically small values of k are tried (e.g. 1 to 5) and the best is chosen.

Note that there is a substantial gap between the “low” values of k (for which learning is guaranteed to fail) and the “high” values of k (for which we show that learning fails with constant probability). It is of significant interest to characterize the performance of the K_k maximum margin algorithm under the uniform distribution for these intermediate values of k ; a discussion of this point is given in Section 5.

2 Preliminaries

We consider learning Boolean functions over the Boolean cube $\{0, 1\}^n$ so that $f : \{0, 1\}^n \rightarrow \{0, 1\}$. It is convenient to consider instead the range $\{-1, 1\}$ with 0 mapped to -1 and 1 mapped to 1. This is easily achieved by the transformation $f'(x) = 1 - 2f(x)$ and since we deal with linear function representations this can be done without affecting the results. For the rest of the paper we assume this representation.

For $x, y \in \mathbb{R}^n$ we write $x \cdot y$ to denote the standard inner product $\sum_{i=1}^n x_i y_i$. Note that for $x, y \in \{0, 1\}^n$, $x \cdot y$ calculates the number of bits which are 1 in both x and y . Our arguments will refer to L_1 and L_2 norms of vectors for which we use the notation $|x| = \sum |x_i|$ and $\|x\| = \sqrt{\sum x_i^2}$.

Definition 1 Let $h : \mathbb{R}^N \rightarrow \{-1, 1\}$ be a linear threshold function $h(x) = \text{sign}(W \cdot x - \theta)$ for some $W \in \mathbb{R}^N, \theta \in \mathbb{R}$. The margin of h on $\langle z, b \rangle \in \mathbb{R}^N \times \{-1, 1\}$ is

$$m_h(z, b) = \frac{b(W \cdot z - \theta)}{\|W\|}.$$

Note that $|m_h(z, b)|$ is the Euclidean distance from z to the hyperplane $W \cdot x = \theta$.

Definition 2 Let $S = \{\langle x^i, b_i \rangle\}_{i=1, \dots, m}$ be a set of labeled examples where each $x^i \in \mathbb{R}^N$ and each $b_i \in \{-1, 1\}$. Let $h(x) = \text{sign}(W \cdot x - \theta)$ be a linear threshold function. The margin of h on S is

$$m_h(S) = \min_{\langle x, b \rangle \in S} m_h(x, b).$$

The maximum margin classifier for S is the linear threshold function $h(x) = \text{sign}(W \cdot x - \theta)$ such that

$$m_h(S) = \max_{W' \in \mathbb{R}^N, \theta' \in \mathbb{R}} \min_{\langle x, b \rangle \in S} \frac{b(W' \cdot x - \theta')}{\|W'\|}. \quad (1)$$

The quantity (1) is called the margin of S and is denoted m_S .

Note that $m_S > 0$ iff S is consistent with some linear threshold function. If $m_S > 0$ then the maximum margin classifier for S is unique [27].

Let ϕ be a transformation which maps $\{0, 1\}^n$ to \mathbb{R}^N and let $K : \{0, 1\}^n \times \{0, 1\}^n \rightarrow \mathbb{R}$ be the corresponding kernel function $K(x, y) = \phi(x) \cdot \phi(y)$. Given a set of labeled examples $S = \{\langle x^i, b_i \rangle\}_{i=1, \dots, m}$ where each x^i belongs to $\{0, 1\}^n$ we write $\phi(S)$ to denote the set of transformed examples $\{\langle \phi(x^i), b_i \rangle\}_{i=1, \dots, m}$.

We refer to the following learning algorithm as the K -maximum margin learner:

- The algorithm first draws a sample $S = \{\langle x^i, f(x^i) \rangle\}_{i=1, \dots, m}$ of $m = \text{poly}(n)$ (i.e. $m = n^{\Theta(1)}$) many labeled examples from some fixed probability distribution \mathcal{D} over $\{0, 1\}^n$; here $f : \{0, 1\}^n \rightarrow \{-1, 1\}$ is the unknown function to be learned. Note that we assume both a lower and upper bound on the number of examples. The upper bound as usual limits the resources the algorithm uses. The lower bound is simply used to rule out degenerate cases from the analysis.
- The algorithm's hypothesis is $h : \{0, 1\}^n \rightarrow \{-1, 1\}$, $h(x) = \text{sign}(W \cdot \phi(x) - \theta)$ where $\text{sign}(W \cdot x - \theta)$ is the maximum margin classifier for $\phi(S)$. Without loss of generality we assume that W is normalized, that is $\|W\| = 1$. We also assume that S contains both positive and negative examples since otherwise the maximum margin classifier is not defined.

SVM theory tells us that if $K(x, y)$ can be computed in $\text{poly}(n)$ time then the K -maximum margin learning algorithm runs in $\text{poly}(n, m) = \text{poly}(n)$ time and the output hypothesis $h(x)$ can be evaluated in $\text{poly}(n, m) = \text{poly}(n)$ time [27].

Our goal is to analyze the PAC learning ability of various kernel maximum margin learning algorithms. Recall (see e.g. [11]) that a PAC learning algorithm for a class \mathcal{C} of functions over $\{0, 1\}^n$ is an algorithm which runs in time polynomial in n and $\frac{1}{\delta}, \frac{1}{\epsilon}$ where δ is a confidence parameter and ϵ is an accuracy parameter. We assume here, as is the case throughout the paper, that each function in \mathcal{C} has a description of size $\text{poly}(n)$. Given access to random labeled examples $\langle x, f(x) \rangle$ for any $f \in \mathcal{C}$ and any distribution \mathcal{D} over $\{0, 1\}^n$, with probability at least $1 - \delta$ a PAC learning algorithm must output an efficiently computable hypothesis h such that $\Pr_{x \in \mathcal{D}}[h(x) \neq f(x)] \leq \epsilon$. If an algorithm only satisfies this criterion for a particular distribution such as the uniform distribution on $\{0, 1\}^n$, we say that it is a uniform distribution PAC learning algorithm.

Let $\rho_k(n) = \sum_{i=1}^{i=k} \binom{n}{i}$. Note that the number of nonempty monotone conjunctions (i.e. monomials) of size at most k on n variables is $\rho_k(n)$. For $x \in \{0, 1\}^n$ we write $\phi_k(x)$ to denote the $\rho_k(n)$ -dimensional vector $(x_T)_{T \subseteq \{1, \dots, n\}, 1 \leq |T| \leq k}$ where $x_T = \prod_{i \in T} x_i$, i.e. the components of $\phi_k(x)$ are all monotone conjunctions of the desired size. We note that for an example $x \in \{0, 1\}^n$, the L_1 norm of the expanded example $\phi_k(x)$ is $|\phi_k(x)| = \rho_k(|x|)$.

Definition 3 We write $K_k(x, y)$ to denote $\phi_k(x) \cdot \phi_k(y)$. We refer to K_k as the k -monomials kernel.

The following theorem shows that the k -monomial kernels are easy to compute:

Theorem 4 ([13]) For all $1 \leq k \leq n$ we have $K_k(x, y) = \sum_{i=1}^k \binom{x \cdot y}{i}$.

We will frequently use the following observation which is a direct consequence of the Cauchy-Schwarz inequality:

Observation 5 If $U \in \mathbb{R}^{N_1}$ with $\|U\| = L$ and $I \subseteq \{1, \dots, N_1\}$, $|I| = N_2$, then $\sum_{i \in I} |U_i| \leq L \cdot \sqrt{N_2}$.

As a consequence of Observation 5 we have that if $\rho_k(n) = N_1$ is the number of features in the expanded feature space and $|\phi_k(x)| = \rho_k(|x|) = N_2$, then $U \cdot \phi_k(x) \leq L \cdot \sqrt{N_2}$.

Finally we also use the following well-known tail bound on sums of independent random variables (see e.g. Section 9.3 of [11]):

Fact 6 (Chernoff Bounds) *Let X_1, \dots, X_m be a sequence of m independent 0/1-valued random variables, each of which has $E[X_i] = p$. Let X denote $\sum_{i=1}^m X_i$, so $E[X] = pm$. Then for $0 \leq \gamma \leq 1$, we have*

$$\Pr[X > (1 + \gamma)pm] \leq e^{-mp\gamma^2/3} \quad \text{and} \quad \Pr[X < (1 - \gamma)pm] \leq e^{-mp\gamma^2/2}.$$

3 Distribution-Free Non-Learnability

We give a DNF and a distribution which are such that the maximum margin algorithm using the k -monomials kernel fails to learn, for all $1 \leq k \leq n$. The DNF we consider is a read once monotone DNF over $t(n)$ variables where $t(n) = \omega(1)$ and $t(n) = O(\log n)$. In fact our results hold for any $t(n) = \omega(1)$ but for concreteness we use $t(n) = \log n$ as a running example. We have

$$f(x) = (x_1 \cdots x_{4\ell^2}) \vee (x_{4\ell^2+1} \cdots x_{8\ell^2}) \vee \cdots \vee (x_{4\ell^3-4\ell^2+1} \cdots x_{4\ell^3}) \quad (2)$$

where $4\ell^3 = t(n) = \log n$ so that the number of terms ℓ equals $\Theta(t(n)^{1/3}) = \Theta((\log n)^{1/3})$. For the rest of this section $f(x)$ will refer to the function defined in Equation (2) and ℓ to its size parameter.

A *polynomial threshold function* is defined by a multivariate polynomial $p(x_1, \dots, x_n)$ with real coefficients. The output of the polynomial threshold function is 1 if $p(x_1, \dots, x_n) \geq 0$ and is -1 otherwise. The degree of the function is the degree of the polynomial p . A simple but useful observation is that any hypothesis output by the K_k kernel maximum margin algorithm must be a polynomial threshold function of degree at most k . Minsky and Papert [21] (see also [14]) gave the following lower bound on polynomial threshold function degree for DNF:

Theorem 7 *Any polynomial threshold function for $f(x)$ in Equation (2) must have degree at least ℓ .*

The distribution \mathcal{D} on $\{0, 1\}^n$ we consider is the following:

- With probability $\frac{1}{2}$ the distribution outputs 0^n .
- With probability $\frac{1}{2}$ the distribution outputs a string $x \in \{0, 1\}^n$ drawn from the following product distribution \mathcal{D}' : the first $t(n)$ bits are drawn uniformly, and the last $n - t(n)$ bits are drawn from the product distribution which assigns 1 to each bit with probability $\frac{1}{n^{1/3}}$.

For small values of k the result is representation based and does not depend on the sample drawn:

Lemma 8 *If the maximum margin algorithm uses the kernel K_k for $k < \ell$ when learning $f(x)$ under \mathcal{D} then its hypothesis has error greater than $\epsilon = \frac{1}{4 \cdot 2^{t(n)}} = \frac{1}{4n}$.*

Proof: If hypothesis h has error at most $\epsilon = \frac{1}{4 \cdot 2^{t(n)}}$ under \mathcal{D} then clearly it must have error at most $\frac{1}{2 \cdot 2^{t(n)}}$ under \mathcal{D}' . Since we are using the kernel K_k , the hypothesis h is some polynomial threshold function of degree at most k which has error $\tau \leq \frac{1}{2 \cdot 2^{t(n)}}$ under \mathcal{D}' . So there must be some setting of the last $n - t(n)$ variables which causes h to have error at most τ under the uniform distribution on the first $t(n)$ bits. Under this setting of variables the hypothesis is a degree- k polynomial threshold function on the first $t(n)$ variables. By Minsky and Papert's theorem, this polynomial threshold function cannot compute the target function exactly, so it must be wrong on at least one setting of the first $t(n)$ variables. But under the uniform distribution, every setting of those variables has probability at least $\frac{1}{2^{t(n)}}$. This contradicts $\tau \leq \frac{1}{2 \cdot 2^{t(n)}}$. ■

For larger values of k (in fact for all $k = \omega(1)$) we show that with high probability the maximum margin hypothesis will overfit the sample. The following definition captures typical properties of a sample from distribution \mathcal{D} :

Definition 9 *A sample S is a \mathcal{D} -typical sample if*

- *The sample includes the example 0^n .*
- *Any nonzero example x in the sample has $0.99n^{2/3} \leq |x| \leq 1.01n^{2/3}$.*
- *Every pair of positive and negative examples x^i, x^j in S satisfies $x^i \cdot x^j \leq 1.01n^{1/3}$.*

We can apply Chernoff bounds to analyze the second and third conditions in the definition (with $p = \frac{1}{n^{1/3}}$ and $p = \frac{1}{n^{2/3}}$ respectively) over the last $n - t(n) > n/2$ bits, and absorb the first $t(n)$ bits in the multiplicative (1 ± 0.01) divergence from the expected value in each case (recall that $t(n)$ is only $O(\log n)$). We thus have that the second and third conditions each fail with probability at most $2^{-n^{\Omega(1)}}$. The first condition holds with probability $1 - 2^{-m}$; since the maximum margin algorithm uses $m = \text{poly}(n) = n^{\Omega(1)}$ many examples (see Section 2), the first condition fails with probability at most $2^{-n^{\Omega(1)}}$ as well. A union bound thus gives:

Lemma 10 *For $m = \text{poly}(n)$, with probability $1 - 2^{-n^{\Omega(1)}}$ a random i.i.d. sample of m draws from \mathcal{D} is a \mathcal{D} -typical sample.*

Definition 11 *Let S be a sample. The set $Z(S)$ consists of all positive examples $z \in \{0, 1\}^n$ (i.e. $f(z) = 1$) which have the property that every example x in S satisfies $x \cdot z \leq 1.01n^{1/3}$.*

As above, we can apply Chernoff bounds with $p = \frac{1}{n^{2/3}}$ and use the union bound over all examples $x \in S$ to show that the probability that a random example z drawn from \mathcal{D} will have $x \cdot z > 1.01n^{1/3}$ for any $x \in S$ is at most $2^{-n^{\Omega(1)}}$. Now since $\Pr[f(z) = 1] \geq 1/n$, conditioning on z being a positive example we still have:

Lemma 12 *Let S be a \mathcal{D} -typical sample of size $m = \text{poly}(n)$ examples. Then $\Pr_{\mathcal{D}}[z \in Z(S) | f(z) = 1] = 1 - 2^{-n^{\Omega(1)}}$.*

We now show that for a \mathcal{D} -typical sample one can achieve a very large margin:

Lemma 13 *Let S be a \mathcal{D} -typical sample. Then the maximum margin m_S satisfies*

$$m_S \geq M_{h'} \equiv \frac{1}{2} \cdot \frac{\rho_k(.99n^{2/3}) - m\rho_k(1.01n^{1/3})}{\sqrt{m\rho_k(1.01n^{2/3})}}$$

Proof: We exhibit an explicit linear threshold function h' which has margin at least $M_{h'}$ on the data set. Let $h'(x) = \text{sign}(W' \cdot \phi(x) - \theta')$ be defined as follows:

- $W'_T = 1$ if T is active in some positive example;
- $W'_T = 0$ if T is not active in any positive example.
- θ' is the value that gives the maximum margin on $\phi_k(S)$ for this W' , i.e. θ' is the average of the smallest value of $W' \cdot \phi_k(x^{i,+})$ and the largest value of $W' \cdot \phi_k(x^{j,-})$.

Since each positive example x^+ in S has at least $.99n^{2/3}$ ones, we have $W' \cdot \phi(x^+) \geq \rho_k(.99n^{2/3})$. Since each positive example has at most $1.01n^{2/3}$ ones, each positive example in the sample contributes at most $\rho_k(1.01n^{2/3})$ ones to W' , so $\|W'\| \leq \sqrt{m\rho_k(1.01n^{2/3})}$. Finally, for any negative example x^- in the sample a term T contributes to $W' \cdot \phi(x^-)$ only if T is true in x^- and in some positive example. Now since x^- shares at most $1.01n^{1/3}$ ones with any positive example in the sample, the number of such terms is at most $m\rho_k(1.01n^{1/3})$. We therefore get $W' \cdot \phi(x^-) \leq m\rho_k(1.01n^{1/3})$. Putting these conditions together, we get that the margin of h' on the sample is at least

$$\frac{1}{2} \cdot \frac{\rho_k(.99n^{2/3}) - m\rho_k(1.01n^{1/3})}{\sqrt{m\rho_k(1.01n^{2/3})}}$$

as desired. ■

Lemma 14 *If S is a \mathcal{D} -typical sample, then the threshold θ in the maximum margin classifier for S is at least $M_{h'}$.*

Proof: Let $h(x) = \text{sign}(W \cdot \phi(x) - \theta)$ be the maximum margin hypothesis. Since $\|W\| = 1$ we have

$$\theta = \frac{\theta}{\|W\|} = m_h(\phi_k(0^n), -1) \geq m_{h'}(S) \geq M_{h'}$$

where the second equality holds because $W \cdot \phi(0^n) = 0$ and the last inequality is by Lemma 13. ■

Lemma 15 *If the maximum margin algorithm uses the kernel K_k for $k = \omega(1)$ when learning $f(x)$ under \mathcal{D} then with probability $1 - 2^{-n^{\Omega(1)}}$ its hypothesis has error greater than $\epsilon = \frac{1}{4 \cdot 2^{t(n)}} = \frac{1}{4n}$.*

Proof: Let S be the sample used for learning and let $h(x) = \text{sign}(W \cdot \phi_k(x) - \theta)$ be the maximum margin hypothesis. It is well known (see e.g. Proposition 6.5 of [27]) that the maximum margin weight vector W is a linear combination of the support vectors, i.e. of certain examples $\phi_k(x)$ in the sample $\phi_k(S)$. Hence the only coordinates W_T of W that can be nonzero are those corresponding to features (conjunctions) T such that $x_T = 1$ for some example x in S .

By Lemma 10 we have that with probability $1 - 2^{-n^{\Omega(1)}}$ the sample S is \mathcal{D} -typical. Consider any $z \in Z(S)$. It follows from the above observations on W that $W \cdot \phi_k(z)$ is a sum of at most $m\rho_k(1.01n^{1/3})$ nonzero numbers, and moreover the sum of the squares of these numbers is at most 1. Thus by Observation 5 we have that $W \cdot \phi_k(z) \leq \sqrt{m\rho_k(1.01n^{1/3})}$. The positive example z is erroneously classified as negative by h if $\theta > W \cdot \phi_k(z)$; by Lemma 14 this inequality holds if

$$\frac{1}{2} \cdot \frac{\rho_k(.99n^{2/3}) - m\rho_k(1.01n^{1/3})}{\sqrt{m\rho_k(1.01n^{2/3})}} > \sqrt{m\rho_k(1.01n^{1/3})},$$

i.e. if

$$\rho_k(.99n^{2/3}) > 2m\sqrt{\rho_k(1.01n^{1/3})\rho_k(1.01n^{2/3})} + m\rho_k(1.01n^{1/3}). \quad (3)$$

We prove in Appendix A that this holds for any $k = \omega(1)$.

Finally, observe that positive examples have probability at least $\frac{1}{2^{t(n)}} = \frac{1}{n}$. The above argument shows that any $z \in Z(S)$ is misclassified, and Lemma 12 guarantees that the relative weight of $Z(S)$ in positive examples is $1 - 2^{-n^{\Omega(1)}}$. Thus the overall error rate of h under \mathcal{D} is at least $(1 - 2^{-n^{\Omega(1)}})\frac{1}{2^{t(n)}} > \frac{1}{4 \cdot 2^{t(n)}} = \frac{1}{4n}$ as claimed. ■

Together, Lemma 8 and Lemma 15 imply Result 1:

Theorem 16 *For any value of k , if the maximum margin algorithm uses the kernel K_k when learning $f(x)$ under \mathcal{D} then with probability $1 - 2^{-n^{\Omega(1)}}$ its hypothesis has error greater than $\epsilon = \frac{1}{4 \cdot 2^{t(n)}} = \frac{1}{4n}$.*

With a small modification we can also obtain Result 2. In particular, since we do not need to deal with small k we can use a simple function $f = x_1$ and modify \mathcal{D} as follows. With probability $\frac{1}{4}$ the assignment 0^n is drawn. With probability $\frac{3}{4}$ we draw from \mathcal{D}' where $x_1 = 1$ with probability $\frac{2}{3}$ and as before the other bits are 1 with probability $\frac{1}{n^{1/3}}$. Note that for the modified distribution the probability that $f(x) = 1$ is 0.5. It is easy to see that the previous arguments go through for this case and we get:

Theorem 17 *For $k = \omega(1)$, if the maximum margin algorithm uses the kernel K_k when learning $f(x) = x_1$ under \mathcal{D} then with probability $1 - 2^{-n^{\Omega(1)}}$ its hypothesis has error at least $\epsilon = \frac{1}{2} - 2^{-n^{\Omega(1)}}$.*

Remark 18 The proofs above can be adapted to show the same non-learnability results for the polynomial kernel $K_k(x, y) = (x \cdot y)^k$ which is commonly being used with SVM systems. The low degree argument in Lemma 8 holds directly. We briefly sketch the ideas for the high degree case. First note that Lemmas 10 and 12 hold without modification. The argument

in Lemma 13 does not go through if we use the same value of W' (since W' is defined in the expanded feature space and $\phi(x)$ is not a zero-one vector, it is not as easy to argue about the value of $W' \cdot \phi(x)$). However, we can use a simple modification to get a similar result. First note that for any $x \in \{0, 1\}^n$, all features in $\phi(x)$ take only non-negative values. Now define W' to be $W' = \sum_{x^{i,+} \in S} \phi(x^{i,+})$. As in Lemma 13 we have:

- $W' \cdot \phi(x^+) = \sum_{x^{j,+} \in S} \phi(x^{j,+}) \cdot \phi(x^+) \geq \phi(x^+) \cdot \phi(x^+) \geq (0.99n^{2/3})^k$ where the first inequality uses the fact that all features in the expanded space have a positive value and therefore all inner products in the sum are positive.
- $W' \cdot \phi(x^-) = \sum_{x^{j,+} \in S} \phi(x^{j,+}) \cdot \phi(x^-) \leq m(1.01n^{1/3})^k$.
- $\|W'\| = \sqrt{(\sum_{x^{j,+} \in S} \phi(x^{j,+})) \cdot (\sum_{x^{i,+} \in S} \phi(x^{i,+}))} \leq \sqrt{m^2(1.01n^{2/3})^k}$

So the maximum margin is at least

$$\frac{1}{2} \cdot \frac{(.99n^{2/3})^k - m(1.01n^{1/3})^k}{m\sqrt{(1.01n^{2/3})^k}}. \quad (4)$$

Now the proof of Lemma 14 shows that (4) is a lower bound on the threshold of the maximum margin classifier.

The argument in Lemma 15 needs to be changed since we need a bound on $W \cdot \phi(z)$. This can be derived as follows. Let U be s.t. $U_i \geq 0$ and $U_i = |W_i|$ so weights in U and W have the same magnitude but the weights in U are forced to be non-negative. Then we have that $\|U\| = \|W\| = 1$. For an example $z \in Z(S)$ we now have

$$\begin{aligned} W \cdot \phi(z) &\leq U \cdot \phi(z) \\ &\leq \sum_{x^i \in S} U \cdot \phi(z \cap x^i) \\ &\leq m(1.01n^{1/3})^{k/2}. \end{aligned}$$

The first inequality holds since all entries in $\phi(z)$ are non-negative. The second inequality is true since both vectors do not have negative weights and a monomial contributes to $W \cdot \phi(z)$ only if it is true both in z and in at least one example in the sample (recall that, as in the proof of Lemma 15, the vector W is a linear combination of vectors $\phi(x) \in \phi(S)$). Therefore, each weight in $\phi(z)$ is represented by a weight in one of the intersections, and the value of the weight depends only on the monomial so it is the same in $\phi(z)$ and $\phi(z \cap x^i)$. Summing over all x_i in S gives an upper bound on the total contribution to $W \cdot \phi(z)$. The last inequality follows from the Cauchy-Schwarz inequality.

As a result of this upper bound on $W \cdot \phi(z)$, we have that z is misclassified if

$$\frac{1}{2} \cdot \frac{(.99n^{2/3})^k - m(1.01n^{1/3})^k}{m\sqrt{(1.01n^{2/3})^k}} > m\sqrt{(1.01n^{1/3})^k}.$$

This can be shown to hold for all $k = \omega(1)$.

4 Uniform Distribution

While Theorem 16 tells us that the K_k -maximum margin learner is not a PAC learning algorithm for monotone DNF in the distribution-free PAC model, it does not rule out the possibility that the K_k -maximum margin learner might succeed for particular probability distributions such as the uniform distribution on $\{0, 1\}^n$. In this section we investigate the uniform distribution.

It is easy to observe that the proof of Lemma 8 goes through for the uniform distribution as well (we actually gain a factor of 2). This therefore proves Result 3: if the algorithm uses too low a degree k then its hypothesis cannot possibly be a sufficiently accurate approximation of the target. In contrast, the next result will show that if a rather large k is used then the algorithm is likely to overfit.

The case of large k is more complex. In Section 3 we took advantage of the fact that 0^n occurred with high weight under the distribution \mathcal{D} . This provided a lower bound (of 0) on the value of $W \cdot \phi_k(x)$ for some negative example in the sample, and we then could argue that the value of θ in the maximum margin classifier must be at least as large as m_S . For the uniform distribution, though, this lower bound no longer holds, so we must use a more subtle analysis.

For the next result, we consider the target function $f(x) = x_1$. Let $S = S^+ \cup S^-$ be a data set drawn from the uniform distribution \mathcal{U} and labeled according to the function $f(x)$ where $S^+ = \{\langle x^{i,+}, 1 \rangle\}_{i=1, \dots, m_+}$ are the positive examples and $S^- = \{\langle x^{j,-}, -1 \rangle\}_{j=1, \dots, m_-}$ are the negative examples. Let u_i denote $|x^{i,+}|$ the weight of the i -th positive example, and let the positive examples be ordered so that $u_1 \leq u_2 \leq \dots \leq u_{m_+}$. Similarly let v_j denote $|x^{j,-}|$ the weight of the j -th negative example with $v_1 \leq v_2 \leq \dots \leq v_{m_-}$.

4.1 Positive-Skewed Samples

We first establish a technical condition that will allow us to give a bound on θ . It turns out that the relative sizes of u_1 and v_1 , the weights of the lightest positive and negative examples in S , play an important role.

Definition 19 *A sample S of size m is positive-skewed if $u_1 \geq v_1 + B$, i.e. the lightest positive example in S weighs at least B more than the lightest negative example, where $B = \frac{1}{66} \sqrt{\frac{n}{\log m}}$.*

The following theorem shows that a random sample is positive skewed with constant probability:

Theorem 20 *Let S be a sample of size $m = \text{poly}(n)$ drawn from the uniform distribution. Then S is positive-skewed with probability at least 0.029.*

Proof: Our first step is to reduce to a situation in which the positive examples and negative examples are independent from each other.³

³Note that this is not the case in S because the total number of examples is m . So, for example, if we condition on the lightest positive example weighing much more than $n/2$, then this biases m_+ (the number

Let M_-, M_+ be any two positive integers. Consider the following new probabilistic experiment which we call E_{M_-, M_+} : first M_- draws are made from a binomial distribution $B(n-1, \frac{1}{2})$ to obtain (sorted) values $v_1 \leq \dots \leq v_{M_-}$, and then M_+ draws are made from $1 + B(n-1, \frac{1}{2})$ to obtain (sorted) values $u_1 \leq \dots \leq u_{M_+}$. The values v_1, \dots, v_{M_-} are thus distributed identically to the weights of the negative examples in the scenario of Theorem 20 conditioned on $m_- = M_-$, and likewise for the u_1, \dots, u_{M_+} and the positive examples. We define the following event:

- Event A_{M_-, M_+} : $u_1 \geq v_1 + B$.

For succinctness let us write A_m for the event (in our original scenario of a size- m sample S drawn from \mathcal{U}) that S is positive-skewed. We then have

$$\begin{aligned} \Pr[A_m] &\geq \Pr[.49m < m_-, m_+ < .51m] \cdot \Pr[A_m \mid .49m < m_-, m_+ < .51m] \\ &\geq (1 - 2^{-\Omega(m)}) \Pr[A_m \mid .49m < m_-, m_+ < .51m] \\ &\geq (1 - 2^{-\Omega(m)}) \min_{.49m < M_-, M_+ < .51m} \Pr[A_m \mid m_- = M_- \text{ and } m_+ = M_+] \\ &= (1 - 2^{-\Omega(m)}) \min_{.49m < M_-, M_+ < .51m} \Pr[A_{M_-, M_+}]. \end{aligned}$$

where the second inequality holds by Chernoff bound.

It thus suffices to show that for any values M_-, M_+ in $(.49m, .51m)$ we have $\Pr[A_{M_-, M_+}] \geq 0.0291$. Fix any M_-, M_+ in this range; we will henceforth only consider the experiment E_{M_-, M_+} in which any event involving only the u_i 's is independent from any event involving only v_i 's.

Let n' denote $n-1$. The idea of the next part of the proof is to show that with some probability v_1 falls into a relatively small left tail of the distribution while u_1 is bounded away from this tail. This gives us a gap between u_1 and v_1 as desired.

We consider u_1 first. For $1 \leq i \leq n'$ let $\psi(i)$ denote $\sum_{j=0}^{i-1} \binom{n'}{j} 2^{-n'}$. Note that $\psi(i)$ is precisely the weight in the “left tail up to i ” of the distribution $1 + B(n', \frac{1}{2})$. Let X be the event that $\psi(u_1) \geq \frac{1}{2m}$ and $u_1 \leq n'/2$. In order to have $\psi(u_1) < \frac{1}{2m}$, at least one of the $M_+ < .51m$ draws from $1 + B(n', \frac{1}{2})$ must land in the “left tail” of weight less than $\frac{1}{2m}$; by a union bound the probability that this occurs is less than $\frac{0.51}{2}$ and hence $\Pr[\psi(u_1) \geq \frac{1}{2m}] \geq 1 - \frac{0.51}{2} > 0.745$. The probability that $u_1 \geq n'/2$ is $2^{-\Omega(m)}$ and thus $\Pr[X] > 0.745 - 2^{-\Omega(m)} > 0.74$.

Next consider v_1 . For $1 \leq i \leq n'$ let $\varphi(i)$ denote $\sum_{j=0}^i \binom{n'}{j} 2^{-n'}$; similar to $\psi(i)$ we have that $\varphi(i)$ captures the weight in the left tail of $B(n', \frac{1}{2})$. Let Y be the event that $\varphi_n(v_1) \leq \frac{1}{4m}$. This event fails to occur only if each of the M_- draws from $B(n', \frac{1}{2})$ misses the left tail of weight at most $\frac{1}{4m}$. We need to be slightly careful; note that $\varphi(\cdot)$ takes discrete values, so this tail may actually weigh less than $\frac{1}{4m}$ (e.g. conceivably $\varphi(22) = \frac{1}{m^2}$ and $\varphi(23) = \frac{1}{m}$.) To take care of this we will now show that this tail cannot weigh much less than $\frac{1}{4m}$.

For $c \geq 1$ let $\sigma(c)$ denote the largest integer such that $\varphi(\sigma(c)) \leq \frac{1}{cm}$.

Lemma 21 *For any constant $c \geq 1$ we have $\varphi(\sigma(c)) \geq \frac{1}{3cm}$.*

of positive examples) down, hence biases m_- up, and thus biases the weight of the lightest negative example down.

Proof: Suppose not; then we have $\varphi(\sigma(c)) < \frac{1}{3cm}$ and $\varphi(\sigma(c) + 1) > \frac{1}{cm}$. This implies that $\binom{n'}{\sigma(c)+1} > 2 \sum_{j=0}^{\sigma(c)} \binom{n'}{j}$ so in particular $\binom{n'}{\sigma(c)+1} > 2 \binom{n'}{\sigma(c)}$. This implies that $n' - \sigma(c) > 2\sigma(c) + 2$ which implies $\sigma(c) < (n' - 2)/3$. But then Chernoff bound implies that for such values of $\sigma(c)$, $\varphi(\sigma(c) + 1) = 2^{-\Omega(n')}$ which contradicts the inequality $\varphi(\sigma(c) + 1) > \frac{1}{cm}$ since c is constant and m is polynomial in n . \blacksquare (proof of Lemma 21)

The lemma implies that the left tail of weight at most $\frac{1}{4m}$ must have weight at least $\frac{1}{12m}$. Hence the probability that each of the $M_- > .49m$ draws from $B(n', \frac{1}{2})$ misses this left tail is at most $(1 - \frac{1}{12m})^{.49m}$. This is at most 0.96 and hence $\Pr[Y] \geq 0.04$.

We next show that if events X and Y both occur then event A_{M_-, M_+} occurs. This will complete the proof of the theorem since the events X and Y are independent and we have that $\Pr[A_{M_-, M_+}] \geq \Pr[X] \Pr[Y] \geq 0.0296$.

Suppose, for the sake of contradiction, that events X and Y both occur but $u_1 \leq v_1 + (B - 1)$. Since X occurs we have $\psi(u_1) \geq \frac{1}{2m}$, i.e.

$$\psi(u_1) = \sum_{j=0}^{u_1-1} \binom{n'}{j} 2^{-n'} \geq \frac{1}{2m}.$$

On the other hand since Y occurs we have $\varphi(v_1) \leq \frac{1}{4m}$, so

$$\sum_{j=0}^{v_1} \binom{n'}{j} 2^{-n'} \leq \frac{1}{4m}. \quad (5)$$

These two inequalities together clearly imply $u_1 > v_1$. In fact they imply

$$\sum_{j=v_1+1}^{u_1-1} \binom{n'}{j} 2^{-n'} \geq \frac{1}{4m}. \quad (6)$$

Thus we see that the weights between $v_1 + 1$ and $u_1 - 1$ have a substantial size. We next show that this implies that the weights below v_1 also have a substantial size, contradicting Equation (5). The following lemma is useful:

Lemma 22 *For all j such that $u_1 - 3B \leq j \leq u_1 - 1$ we have $\binom{n'}{j} \geq \frac{1}{2} \binom{n'}{u_1-1}$.*

Proof: Clearly it suffices to prove that $2 \binom{n'}{u_1-3B} \geq \binom{n'}{u_1-1}$. By event X we know that $\psi(u_1) \geq \frac{1}{2m}$. But the left tail Chernoff bound implies that unless

$$u_1 - 1 \geq \frac{n'}{2} - 2\sqrt{n' \log m} \quad (7)$$

we have $\psi(u_1) < \frac{1}{m^4} < \frac{1}{2m}$ so (7) must hold. Let $c = \frac{n'}{2} - (u_1 - 1)$ so $0 < c \leq 2\sqrt{n' \log m}$. Now observe that for any b such that $b < 0.1n'$ we have

$$\frac{\binom{n'}{n'/2-b}}{\binom{n'}{n'/2-b-1}} = \frac{n'/2 + b + 1}{n'/2 - b} = 1 + \frac{2b + 1}{n'/2 - b} < 1 + \frac{2b + 1}{0.4n'} = 1 + \frac{5b + 2.5}{n'}$$

We thus have

$$\begin{aligned}
\frac{\binom{n'}{u_1-1}}{\binom{n'}{u_1-3B}} &= \frac{\binom{n'}{u_1-1}}{\binom{n'}{u_1-2}} \cdot \frac{\binom{n'}{u_1-2}}{\binom{n'}{u_1-3}} \cdots \frac{\binom{n'}{u_1-3B+1}}{\binom{n'}{u_1-3B}} \\
&= \frac{\binom{n'}{\frac{n'}{2}-c}}{\binom{n'}{\frac{n'}{2}-c-1}} \cdot \frac{\binom{n'}{\frac{n'}{2}-c-1}}{\binom{n'}{\frac{n'}{2}-c-2}} \cdots \frac{\binom{n'}{\frac{n'}{2}-(c+3B-2)}}{\binom{n'}{\frac{n'}{2}-(c+3B-3)}} \\
&< \left(1 + \frac{5c+2.5}{n'}\right) \left(1 + \frac{5(c+1)+2.5}{n'}\right) \cdots \left(1 + \frac{5(c+3B-2)+2.5}{n'}\right) \\
&< \left(1 + \frac{5(c+3B)+2.5}{n'}\right)^{3B} \\
&\leq e^{\frac{5(c+3B)+2.5}{n'} 3B}
\end{aligned}$$

where we have used the inequality $1+x \leq e^x$. The last quantity is at most $\sqrt{e} < 2$ provided that

$$3B < \frac{n'}{10(c+3B)+5}. \quad (8)$$

Now since $c \leq 2\sqrt{n' \log m}$ and we can bound $5 < \sqrt{n' \log m}$ and $30B < 0.5\sqrt{n' \log m}$ this holds if

$$3B = \frac{1}{22} \sqrt{\frac{n'}{\log m}} < \frac{n'}{21.5\sqrt{n' \log m}} = \frac{1}{21.5} \sqrt{\frac{n'}{\log m}}$$

which is clearly true. ■(proof of Lemma 22)

Recalling that $u_1 \leq v_1 + (B-1)$, we have that the sum in Equation (6) has at most $B-2$ terms. Now since $u_1 < \frac{n'}{2}$ the largest of these terms is $\binom{n'}{u_1-1} 2^{-n'}$. By Equation (6) we thus have that

$$\binom{n'}{u_1-1} 2^{-n'} \geq \frac{1}{4(B-2)m}. \quad (9)$$

Now Lemma 22 together with Equation (9), implies that we have

$$\sum_{j=u_1-3B}^{v_1-1} \binom{n'}{j} 2^{-n'} > \sum_{j=u_1-3B}^{u_1-B-1} \binom{n'}{j} 2^{-n'} \geq \sum_{j=u_1-3B}^{u_1-B-1} \frac{1}{2} \binom{n'}{u_1-1} 2^{-n'} \geq \frac{2B}{2} \frac{1}{4(B-2)m} > \frac{1}{4m}$$

but this contradicts Equation (5). ■

4.2 Lower Bound for Large k

Using the fact that the sample is likely to be positive-skewed we can prove the lower bound along the same lines as before.

Definition 23 *A sample S is a \mathcal{U} -typical sample if*

- Every example $x \in S$ satisfies $0.49n \leq |x| \leq 0.51n$.
- Every pair of positive and negative examples $x^{i,+}, x^{j,-}$ in S satisfy $x^{i,+} \cdot x^{j,-} \leq 0.26n$.

As above we can apply Chernoff bounds to derive the next two lemmas:

Lemma 24 For $m = \text{poly}(n)$, with probability $1 - 2^{-\Omega(n)}$ a random i.i.d. sample of m draws from \mathcal{U} is a \mathcal{U} -typical sample.

Definition 25 Let S be a sample. The set $Z(S)$ includes all positive examples z such that every example x in S satisfies $x \cdot z \leq 0.26n$.

Lemma 26 Let S be a \mathcal{U} -typical sample of size $m = \text{poly}(n)$ examples. Then $\Pr_{\mathcal{U}}[z \in Z(S) | f(z) = 1] = 1 - 2^{-\Omega(n)}$.

The following lemma is analogous to Lemma 13:

Lemma 27 Let S be a \mathcal{U} -typical sample of size m . Then the maximum margin m_S satisfies

$$m_S \geq \frac{1}{2} \left(\frac{1}{\sqrt{m}} \sqrt{\rho_k(u_1)} - \sqrt{m\rho_k(.26n)} \right).$$

Proof: We exhibit an explicit linear threshold function h' which has this margin. Let $h'(x) = \text{sign}(W' \cdot \phi_k(x) - \theta')$ be defined as follows:

- For each positive example $x^{i,+}$ in S , pick a set of $\rho_k(u_1)$ features (monomials) which take value 1 on $x^{i,+}$. This can be done since each positive example $x^{i,+}$ has at least u_1 bits which are 1. For each feature T in each of these sets, assign $W'_T = 1$.
- For all remaining features T set $W'_T = 0$.
- Set θ' to be the value that gives the maximum margin on $\phi_k(S)$ for this W' , i.e. θ' is the average of the smallest value of $W' \cdot \phi_k(x^{i,+})$ and the largest value of $W' \cdot \phi_k(x^{j,-})$.

Note that since each positive example contributes at most $\rho_k(u_1)$ nonzero coefficients to W' , the number of 1's in W' is at most $m\rho_k(u_1)$, and hence $\|W'\| \leq \sqrt{m\rho_k(u_1)}$. By construction we also have that each positive example $x^{i,+}$ satisfies $W' \cdot \phi_k(x^{i,+}) \geq \rho_k(u_1)$.

Since S is a \mathcal{U} -typical sample, each negative example $x^{j,-}$ in S shares at most $.26n$ ones with any positive example in S . Hence the value of $W' \cdot \phi_k(x^{j,-})$ is a sum of at most $m\rho_k(.26n)$ numbers whose squares sum to at most $m\rho_k(u_1)$. By Observation 5 we have that $W' \cdot \phi_k(x^{j,-}) \leq \sqrt{m\rho_k(.26n)}\sqrt{m\rho_k(u_1)}$.

The lemma follows by combining the above bounds on $\|W'\|$, $W' \cdot \phi_k(x^{i,+})$ and $W' \cdot \phi_k(x^{j,-})$.

■

Now we can give a lower bound on the threshold θ for the maximum margin classifier.

Lemma 28 Let S be a labeled sample of size m which is \mathcal{U} -typical and positive skewed, and let $h(x) = \text{sign}(W \cdot \phi_k(x) - \theta)$ be the maximum margin hypothesis for S . Then

$$\theta \geq \frac{1}{2} \left(\frac{1}{\sqrt{m}} \sqrt{\rho_k(u_1)} - \sqrt{m\rho_k(.26n)} \right) - \sqrt{\rho_k(u_1 - B)}.$$

Proof: Since S is positive-skewed we know that $W \cdot \phi_k(x^{1,-})$ is a sum of at most $\rho_k(u_1 - B)$ weights W_T , and since W is normalized the sum of the squares of these weights is at most 1. By Observation 5 we thus have $W \cdot \phi_k(x^{1,-}) \geq -\sqrt{\rho_k(u_1 - B)}$. Now since $\theta \geq W \cdot \phi_k(x^{1,-}) + m_S$, Lemma 27 implies the result. ■

Putting all of the pieces together, we have:

Theorem 29 *If the maximum margin algorithm uses the kernel K_k for $k = \omega(\sqrt{n} \log^{\frac{3}{2}} n)$ when learning $f(x) = x_1$ under the uniform distribution then with probability at least 0.028 its hypothesis has error $\epsilon = \frac{1}{2} - 2^{-\Omega(n)}$.*

Proof: By Lemma 24 and Theorem 20, the sample S used for learning is both \mathcal{U} -typical and positive skewed with probability at least $0.029 - 1/2^{-\Omega(n)} > 0.028$. Consider any $z \in Z(S)$. Using the reasoning from Lemma 15, $W \cdot \phi(z)$ is a sum of at most $m\rho_k(.26n)$ numbers whose squares sum to at most 1, so $W \cdot \phi(z) \leq \sqrt{m\rho_k(.26n)}$. The example z is erroneously classified as negative by h if

$$\frac{1}{2} \left(\frac{1}{\sqrt{m}} \sqrt{\rho_k(u_1)} - \sqrt{m\rho_k(.26n)} \right) - \sqrt{\rho_k(u_1 - B)} > \sqrt{m\rho_k(.26n)}.$$

so it suffices to show that

$$\sqrt{\rho_k(u_1)} > 3m \left(\sqrt{\rho_k(.26n)} + \sqrt{\rho_k(u_1 - B)} \right). \quad (10)$$

Recall that $\rho_k(x) = \sum_{j=0}^k \binom{x}{j}$. Note that for $k = n$ (all-monomials kernel) the above inequality becomes $2^{u_1/2} > 3m (2^{.13n} + 2^{(u_1-B)/2})$ which is clearly true. In Appendix B we show that Equation (10) holds for all $k = \omega(\sqrt{n} \log^{\frac{3}{2}} n)$ as required.

The above argument shows that any $z \in Z(S)$ is misclassified, and Lemma 26 guarantees that the relative weight of $Z(S)$ in positive examples is $1 - 2^{-\Omega(n)}$. Since $\Pr_{x \in \mathcal{U}}[f(x) = 1]$ is $1/2$, we have that with probability at least 0.028 the hypothesis h has error rate at least $\epsilon = \frac{1}{2} - 2^{-\Omega(n)}$, and we are done. ■

Remark 30 Here again we can adapt the proofs to show non-learnability results for the polynomial kernel $K_k(x, y) = (x \cdot y)^k$. We modify the definition of W' in Lemma 27 as follows. For every positive example $x^{i,+}$ in the sample let $\hat{x}^{i,+}$ be the example obtained by picking an arbitrary subset of size u_1 of the original true bits and setting all other bits to 0. Now let $W' = \sum_{x^{i,+} \in S} \phi(\hat{x}^{i,+})$. Arguing as in Remark 18 we get that the maximum margin is at least

$$\frac{1}{2} \cdot \frac{u_1^k - m(0.26n)^k}{m\sqrt{u_1^k}}.$$

Now in Lemma 28 we get that $W' \cdot \phi(x^{1,-}) \geq -(u_1 - B)^{k/2}$ which again implies a lower bound on the threshold.

Finally, following Theorem 29 and the argument in Remark 18 one can show that for an example $z \in Z(S)$ we have $W \cdot \phi(z) \leq m\sqrt{(0.26n)^k}$ so that z is misclassified if

$$u_1^k - m(0.26n)^k - 2m\sqrt{u_1^k} \sqrt{(u_1 - B)^k} \geq 2m^2 \sqrt{u_1^k (0.26n)^k}$$

which is true if

$$u_1^{k/2} > 5m^2(u_1 - B)^{k/2}.$$

Using the reasoning in Case 1 of Appendix B, one can show that this holds for $k = \omega(\sqrt{n} \log^{\frac{3}{2}} n)$.

5 Conclusions and Future Work

Boolean kernels offer an interesting new algorithmic approach to one of the major open problems in computational learning theory, namely learnability of DNF expressions. We have studied the performance of the maximum margin algorithm with the Boolean kernels, giving negative results for several settings of the problem. Our results indicate that the maximum margin algorithm can overfit even when learning simple target functions and using natural and expressive kernels for such functions, and even when combined with structural risk minimization. Our results consider cases where the L_2 norm of examples in the expanded feature space is large. This seems necessary for learning DNF; note that while one can use an exponential function to define a kernel with weighted monomials where the weight decays exponentially depending on the degree k , this implies that the margin for functions of high degree is exponentially small.

While our results are negative there are several interesting avenues suggested by this work which may succeed; we discuss these briefly below. One direction is to modify the basic learning algorithm. Many interesting variants of the basic maximum margin algorithm have been used in recent years, such as soft margin criteria and kernel regularization. It may be possible to prove positive results for some DNF learning problems using these approaches. A starting point would be to test their performance on the counterexamples (functions and distributions) which we have constructed.

A more immediate goal is to close the gap between small and large k in our results for the uniform distribution. It is well known [30] that when learning polynomial size DNF under the uniform distribution, conjunctions of length $\omega(\log n)$ can be ignored with little effect. Hence the most interesting setting of k for the uniform distribution learning problem is $k = \Theta(\log n)$. Learning under the uniform distribution with a $k = \Theta(\log n)$ kernel is qualitatively quite different from learning with the large values of k which we were able to analyze. For example, for $k = \Theta(\log n)$ if a sufficiently large polynomial size sample is taken, then with very high probability all features (monomials of size at most k) are active in the sample.

As a first concrete problem in this scenario, one might consider the question of whether a $k = \Theta(\log n)$ kernel maximum margin algorithm can efficiently PAC learn the target function $f(x) = x_1$. For this problem it is easy to show that the naive hypothesis h' constructed in our proofs achieves both a large margin and high accuracy. Moreover, it is possible to show that with high probability the maximum margin hypothesis has a margin which is within a multiplicative factor of $(1 + o(1))$ of the margin achieved by h' . Though these preliminary results do not answer the above question they suggest that the answer may be positive. A positive answer, in our view, would be strong motivation to analyze the general case.

Finally, the kernel we have used is natural in terms of capturing all monomials of a

certain length but there are other ways to capture natural kernels for Boolean problems. An interesting possibility is using a kernel of parity functions and such a construction can indeed be given. The resulting representation is closely related to learning via the Fourier transform, e.g. as done in [19, 17, 20] but the algorithmic ideas are very different to the ones used by maximum margin algorithms.

Appendix

A Proof of Equation (3)

To show that

$$\rho_k(.99n^{2/3}) > 2m\sqrt{\rho_k(1.01n^{1/3})\rho_k(1.01n^{2/3})} + m\rho_k(1.01n^{1/3})$$

it suffices to show that

$$\rho_k(.99n^{2/3}) > 3m\sqrt{\rho_k(1.01n^{1/3})\rho_k(1.01n^{2/3})}. \quad (11)$$

The proof uses several cases depending on the value of k relative to n .

Case 1: $k \leq 0.505n^{1/3}$. Since $\rho_k(\ell) = \sum_{i=1}^k \binom{\ell}{i}$, for $k \leq \ell/2$ we have that $\rho_k(\ell) \leq k\binom{\ell}{k}$. For all k we have $\rho_k(\ell) \geq \binom{\ell}{k}$ so it suffices to show that

$$\binom{.99n^{2/3}}{k} > 3mk\sqrt{\binom{1.01n^{1/3}}{k}\binom{1.01n^{2/3}}{k}}$$

which is equivalent (clearing denominators from the binomial coefficients) to

$$\prod_{i=0}^{k-1} (.99n^{2/3} - i) > 3mk\sqrt{\prod_{i=0}^{k-1} (1.01n^{1/3} - i)(1.01n^{2/3} - i)}.$$

We now use the fact that for $i \geq 0$ we have $(A - i)(B - i) \leq (\sqrt{AB} - i)^2$ provided that $2\sqrt{AB} < A + B$; it is easy to see that this latter condition holds for $A = 1.01n^{1/3}$, $B = 1.01n^{2/3}$. It thus suffices to show that

$$\prod_{i=0}^{k-1} (.99n^{2/3} - i) > 3mk \prod_{i=0}^{k-1} (1.01n^{1/2} - i)$$

which in turn is implied by

$$\left(\frac{.99n^{2/3}}{1.01n^{1/2}}\right)^k > 3mn$$

(we used the fact that $k \leq n$ to obtain the right-hand side above). This holds as long as $k > \frac{\log(3mn)}{\log 0.98 + \frac{1}{6} \log n} = \Theta(1)$ for any $m = \text{poly}(n)$. Therefore the condition holds for any $k = \omega(1)$.

Case 2: $0.505n^{1/3} \leq k \leq 0.25 \cdot 0.99n^{2/3}$. In this case we use the bounds $\left(\frac{\ell}{k}\right)^k \leq \rho_k(\ell) = \sum_{i=1}^k \binom{\ell}{i} \leq \left(\frac{e\ell}{k}\right)^k$ for the first and third occurrences of ρ_k in equation (11) and we use $\rho_k(\ell) \leq 2^\ell$ for the second occurrence. It thus suffices to show that

$$\left(\frac{.99n^{2/3}}{k}\right)^k > 3m \sqrt{\left(\frac{e \cdot 1.01n^{2/3}}{k}\right)^k \cdot 2^{1.01n^{1/3}}}$$

Since $1.01n^{1/3} \leq 2k$ it suffices to show that

$$\left(\frac{.99n^{2/3}}{k}\right)^k > 3m \left(\frac{e \cdot 1.01n^{2/3}}{k}\right)^{k/2} \cdot 2^k$$

which holds (taking k -th roots and rearranging) if and only if

$$\frac{1}{2} \cdot \frac{.99n^{2/3}}{k} \cdot \frac{\sqrt{k}}{n^{1/3} \sqrt{1.01 \cdot e}} = \frac{1}{2} \left(\frac{.99}{\sqrt{1.01 \cdot e}}\right) \frac{n^{1/3}}{\sqrt{k}} > (3m)^{1/k}.$$

Using our upper bound on k on the left side, the previous inequality holds if

$$\frac{.99}{\sqrt{1.01 \cdot e}} \cdot \frac{2}{\sqrt{.99}} > (3m)^{1/k}$$

and since the left side is greater than 1.2 the inequality holds if $k > \frac{\log 3m}{\log 1.2} = \Theta(\log n)$ for $m = \text{poly}(n)$. This obviously holds since $k = \Omega(n^{1/3})$.

Case 3: $0.25 \cdot 0.99n^{2/3} \leq k \leq 0.5 \cdot 0.99n^{2/3}$. We use the following bound (proved later) which holds for $0 < \alpha < 1$:

$$\sum_{i=1}^{\alpha q} \binom{q}{i} \geq \frac{1}{\sqrt{2\pi q}} 2^{H(\alpha)q} \quad (12)$$

where $H(p) = -p \log p - (1-p) \log(1-p)$ is the binary entropy function. Applying this bound to the left side of (11) with $q = .99n^{2/3}$ and $\alpha = k/q$, we have $.25 \leq \alpha \leq .5$ so $H(\alpha) > .81$. Since $\rho_k(\ell)$ is always at most 2^ℓ it suffices to show that

$$\frac{1}{\sqrt{2\pi \cdot .99n^{1/3}}} 2^{0.81 \cdot 0.99n^{2/3}} > 3m \sqrt{2^{1.01n^{2/3} + 1.01n^{1/3}}}.$$

This is easily seen to hold for any $m = \text{poly}(n)$.

To prove the bound (12) we use Stirling's approximation $\sqrt{2\pi n} \left(\frac{n}{e}\right)^n \leq n! \leq \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \sqrt{1 + \frac{1}{2n}}$; in fact we use a weaker form with $\sqrt{2}$ instead of $\sqrt{1 + \frac{1}{2n}}$ in the upper bound. We thus have

$$\begin{aligned} \sum_{i=1}^{\alpha q} \binom{q}{i} &\geq \binom{q}{\alpha q} = \frac{q!}{(\alpha q)!((1-\alpha)q)!} \geq \frac{\sqrt{2\pi q}}{2\sqrt{2\pi \alpha q} \sqrt{2\pi(1-\alpha)q}} \left(\frac{q}{e}\right)^q \left(\frac{e}{\alpha q}\right)^{\alpha q} \left(\frac{e}{(1-\alpha)q}\right)^{(1-\alpha)q} \\ &= \frac{1}{2\sqrt{2\pi \alpha(1-\alpha)q}} \alpha^{-\alpha q} (1-\alpha)^{-(1-\alpha)q} = \frac{1}{2\sqrt{2\pi \alpha(1-\alpha)q}} 2^{qH(\alpha)}. \end{aligned}$$

Equation (12) follows since $\alpha(1 - \alpha) \leq 1/4$.

Note that by using $\sum_{i=0}^{\alpha q} \binom{q}{i} \leq \alpha q \binom{q}{\alpha q}$ one can also obtain $\sum_{i=0}^{\alpha q} \binom{q}{i} \leq \frac{\sqrt{\alpha q}}{\sqrt{\pi(1-\alpha)}} 2^{H(\alpha)q}$.

Case 4: $k \geq 0.5 \cdot 0.99n^{2/3}$. In this case we have $\rho_k(.99n^{2/3}) = \sum_{i=1}^k \binom{.99n^{2/3}}{i} \geq \frac{1}{2} 2^{.99n^{2/3}}$. Thus it suffices to show that

$$\frac{1}{2} \cdot 2^{0.99n^{2/3}} > 3m \sqrt{2^{1.01n^{2/3} + 1.01n^{1/3}}}$$

which is easily seen to hold for any $m = \text{poly}(n)$. Thus Equation (11) holds for all $k = \omega(1)$. ■

B Proof of Equation (10)

We must show that $\sqrt{\rho_k(u_1)} > 3m \left(\sqrt{\rho_k(.26n)} + \sqrt{\rho_k(u_1 - B)} \right)$. Since we are assuming that the sample S is \mathcal{U} -typical, we have $u_1 \geq .49n$ so $u_1 - B > 0.26n$. It thus suffices to show that $\rho_k(u_1) > 36m^2 \rho_k(u_1 - B)$.

Case 1: $k \leq \frac{1}{2}(u_1 - B)$. Since $\rho_k(\ell) = \sum_{i=1}^k \binom{\ell}{i}$, for $k \leq \ell/2$ we have $\rho_k(\ell) \leq k \binom{\ell}{k}$. Also for all k , $\rho_k(\ell) \geq \binom{\ell}{k}$ so it suffices to show that

$$\binom{u_1}{k} > 36m^2 k \binom{u_1 - B}{k}.$$

This inequality is true if

$$\left(\frac{u_1}{u_1 - B} \right)^k > 36m^2 k.$$

Recall that $B = \frac{1}{66} \sqrt{\frac{n}{\log m}}$. Now using the fact that

$$\frac{u_1}{u_1 - B} = 1 + \frac{B}{u_1 - B} > 1 + \frac{B}{n} = 1 + \frac{1}{66\sqrt{n \log m}}$$

it suffices to show that

$$\left(1 + \frac{1}{66\sqrt{n \log m}} \right)^k > 36m^2 k.$$

Using the fact that $1 + x \geq e^{x/2}$ for $0 < x < 1$, we can see that this inequality holds if $k > 132\sqrt{n \log(m)} \ln(36m^2 n)$. Since $m = \text{poly}(n)$, this is the case for $k = \omega(\sqrt{n \log^{\frac{3}{2}} n})$.

Case 2: $\frac{1}{2}(u_1 - B) < k$. Since $\rho_k(u_1 - B) \leq 2^{u_1 - B}$, it suffices to show that

$$\sum_{i=1}^{\frac{u_1 - B}{2}} \binom{u_1}{i} > 36m^2 \cdot 2^{u_1 - B}.$$

Since $\sqrt{u_1} > \sqrt{.049n} > \frac{92}{132}\sqrt{n} > 92\frac{B}{2}$ it suffices to show that

$$\sum_{i=1}^{\frac{u_1 - \sqrt{u_1}}{92}} \binom{u_1}{i} > 36m^2 \cdot 2^{u_1 - B}.$$

Using Stirling approximation it is easy to check that $\binom{q}{q/2} < \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{q}} 2^q$ and this implies that

$$\sum_{i=1}^{\frac{u_1 - \sqrt{u_1}}{92}} \binom{u_1}{i} > \frac{1}{2} 2^{u_1} - \frac{\sqrt{u_1}}{92} \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{u_1}} 2^{u_1} > 0.49 \cdot 2^{u_1}$$

so the condition above holds if

$$0.49 \cdot 2^B > 36m^2.$$

This is clearly true since $m = \text{poly}(n)$ and $B = \frac{1}{66} \sqrt{\frac{n}{\log m}}$. ■

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