

# Examples of the VC Dimension

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## Recall: VC dimension

The previous time we introduced the VC dimension of a hypothesis class  $\mathcal{H}$  as:

The VC dimension of a set of hypotheses  $\mathcal{H}$  is the size of the largest set  $C \subseteq X$  such that  $C$  is shattered by  $\mathcal{H}$ . If  $\mathcal{H}$  can shatter arbitrarily sized sets, its VC dimension is infinite.

Where a finite set is shattered by  $\mathcal{H}$  if

$$|\mathcal{H}_C| = 2^{|C|}$$

We now study the VC dimension of some finite classes, more in particular: classes of boolean functions.

# Finite Hypothesis Classes

If a finite hypothesis class  $\mathcal{H}$  shatters a finite set  $C$  then

$$|\mathcal{H}| \geq |\mathcal{H}_C| = 2^{|C|}$$

This immediately implies that

$$VC(\mathcal{H}) \leq \log(|\mathcal{H}|)$$

Clearly, the VC dimension can be smaller

- ▶ consider threshold functions that can take thresholds in  $\{1, \dots, k\}$
- ▶  $|\mathcal{H}| = k$ , while  $VC(\mathcal{H}) = 1$

In other words,

- ▶ the difference between  $VC(\mathcal{H})$  and  $\log(|\mathcal{H}|)$  can be arbitrarily large
- ▶ but  $\log(|\mathcal{H}|)$  is never the smallest

## Monotone Monomials

Recall the class  $C_n$  of boolean expressions over  $n$  literals. A smaller class  $C_n^+$  (sometimes denoted by  $M_n^+$ ) consists of the monotone (positive) monomials

- ▶ *no negations*, just conjunctions of the variables

Clearly, a variable is either in such an expression or not. Hence,

$$|C_n^+| = 2^n$$

Hence, by the previous page:

$$VC(C_n^+) \leq \log(2^n) = n$$

But, as we noted on the previous page, it could be smaller, a lot smaller.

- ▶ however, it isn't.

To prove that we are going to create a set of  $n$  elements that is shattered by  $C_n^+$ .

$$VC(C_n^+) = n$$

Let  $S$  consist of all 0/1-vectors of length  $n$  that have exactly

- ▶  $n - 1$  1's
- ▶ and 1 0.

Denote by  $x_i$  that element of  $S$  that has 0 for the  $i$ -th coordinate.

- ▶ if  $j = i : \pi_j(x_i) = 0$
- ▶ if  $j \neq i : \pi_j(x_i) = 1$

Let  $R \subseteq S$  be any subset of  $S$ . Define  $h_R \in C_n^+$  as

- ▶ the conjunction of all variables  $u_j$  such that  $x_j \notin R$

Then we have:

$$h_R(x) = \begin{cases} 1 & \text{if } x \in R \\ 0 & \text{if } x \in S \setminus R \end{cases}$$

That is, we have a classifier for any  $R \subseteq S$ :  $S$  is shattered. Hence,

$$VC(C_n^+) = n$$

## How About $C_n$ ?

It is easy to see that

- ▶  $VC(C_1) = 2$

the monomials

- ▶  $x$  and  $\neg x$  will do that for you.

Moreover, since  $C_n^+ \subset C_n : VC(C_n^+) \leq VC(C_n)$

- ▶ any set that can be shattered by  $C_n^+$  can be shattered by  $C_n$

So, it may appear that by allowing negations we increase the VC dimension, because we now have that

$$n \leq VC(C_n) \leq \log(|C_n|) = \log(3^n) = n \log(3)$$

But, we don't

- ▶ except for the case  $n = 1$

No set of size  $n + 1$  can be shattered by  $C_n$  if  $n \geq 2$

$$VC(C_n) = n$$

Let  $S = \{s^1, \dots, s^{n+1}\}$  be a set of  $n + 1$ , 0/1 vectors of length  $n$ , that is shattered by  $C_n$

- ▶ define  $S_i = S \setminus \{s^i\}$

Because  $S$  is shattered by  $C_n$  there exists a  $m_i \in C_n$  such that

- ▶  $S_i = S \cap m_i$ , thus,  $\forall i, j : m_i(s^j) = 0 \leftrightarrow i = j$  ( $0 = \text{false}$ )

But this means that:

- ▶ each  $s^i$  contains a component  $s_{h(i)}^i$
- ▶ each  $m_i$  contains a literal  $l_{k(i)}$
- ▶ such that  $l_{k(i)}$  is false on  $s_{h(i)}^i$ , i.e.,  $l_{k(i)}(s_{h(i)}^i) = 0$

Given that there are only  $n$  variables

- ▶ at least 2 of these literals  $l_{k(1)}, \dots, l_{k(i+1)}$
- ▶ must refer to the same variable, say  $l_{k(1)}$  and  $l_{k(2)}$
- ▶ either  $l_{k(1)} = l_{k(2)}$ , then  $l_{k(1)}(s_{h(1)}^1) = l_{k(1)}(s_{h(2)}^2) = 0$ , i.e.,  $m_1(s^1) = m_1(s^2) = 0$ . Contradiction
- ▶ or  $l_{k(1)} = \neg l_{k(2)}$ , then either  $l_{k(1)}$  or  $l_{k(2)}$  is false on  $s^3$ . Either  $m_1(s^3) = 0$  or  $m_2(s^3) = 0$ . Again a contradiction

# $D_n^{(+)}$ by Duality

Denote by

- ▶  $D_n^+$  the set of all disjunctions over at most  $n$  variables, again no negations
- ▶  $D_n$  the set of disjunctions over at most  $n$  literals

Note that for  $\phi \in C_n$  and  $x \in \{0, 1\}^n$  we have

$$\phi(x) \leftrightarrow \neg\phi(\neg x)$$

That is we have a duality between  $C_n$  and  $D_n$  and similarly between  $C_n^+$  and  $D_n^+$

By this duality we immediately have:

- ▶  $VC(D_n) = n$  and
- ▶  $VC(D_n^+) = n$

In the end, it is just consistently switching

- ▶ 1's to 0's and vice versa



# Monotone Formulas

We have seen that both

- ▶  $C_n^+$ , conjunctions of variables, has VC dimension  $n$
- ▶ and  $D_n^+$ , disjunctions of variables, has VC dimension  $n$

The natural follow up question is

- ▶ what happens if we allow both conjunctions and disjunctions
- ▶ but no negations

This is the class of *monotone boolean formulas*,

- ▶ sometimes denoted by  $M_n$
- ▶ note, without a  $+$ ; perhaps because allowing negations as well yields the class of all boolean functions
  - ▶ which we will discuss later

The problem is thus: determine  $VC(M_n)$

# Sperner's Theorem

To compute the VC dimension of  $M_n$  we need a result from combinatorics known as Sperner's Theorem.

Let  $X$  be a set of  $n$  elements

- ▶ a chain of subsets of  $X$  is a family of subsets  $A_i$  such that  $\emptyset \subseteq A_1 \subset A_2 \subset \dots \subset A_k \subseteq X$
- ▶ an antichain is a family of subsets  $F$  such that for any two elements  $A, B \in F$ :

$$A \not\subseteq B \wedge B \not\subseteq A$$

Sperner: if  $F$  is an antichain of  $X$ , then

$$|F| \leq \binom{n}{\lfloor n/2 \rfloor}$$

Note, an antichain is also known as a Sperner family of subsets.

## Maximal Chains

Without loss of generality we assume that  $X = \{1, \dots, n\}$ . A maximal chain in  $X$  obviously has length  $n + 1$

$$\emptyset = A_0 \subset A_1 \subset \dots \subset A_n = X$$

Such a maximal chain puts a total order on the elements of  $X$

- ▶ the smallest element is the single element of  $A_1$
- ▶ the one-but-smallest is the new element in  $A_2$
- ▶ and so on and so on

Similarly, each total order on  $X$  defines a chain

- ▶  $A_1$  consists of the smallest element
- ▶  $A_2$  consists of the two smallest elements
- ▶ and so on and so on

That is, the total number of maximal chains equals the number of permutations:  $n!$

# Maximal Chains and Antichains

Let  $A \subseteq X$ , with  $|A| = k$ . A maximal chain that contains  $A$

- ▶ i.e.,  $A = A_k$  in that chain

consists of

- ▶ A maximal chain for the set  $A$
- ▶ followed by a chain for  $X \setminus A$ 
  - ▶ each set in the latter chain is extended by the union with  $A$ , of course

This means that there are  $k!(n - k)!$  maximal chains containing  $A$ .

Note that if  $F$  is an antichain, then any chain can contain at most one element of  $F$

- ▶ If  $A$  and  $B$  are in a chain, then either  $A \subset B$  or  $B \subset A$
- ▶ If  $A$  and  $B$  are in  $F$ , then both  $A \not\subset B$  and  $B \not\subset A$

## Proving Sperner

Recall that  $F$  is an antichain. The number of maximal chains that contain an element of  $F$  (and thus exactly 1) is

$$\blacktriangleright \sum_{A \in F} |A|!(n - |A|)! = \sum_{A \in F} n! \frac{|A|!(n - |A|)!}{n!} = n! \sum_{A \in F} \frac{1}{\binom{n}{|A|}}$$

Because there are in total  $n!$  maximal chains, we have

$$\blacktriangleright \sum_{A \in F} \frac{1}{\binom{n}{|A|}} \leq 1$$

For binomial coefficients, the middle ones are the largest, hence

$$\blacktriangleright \sum_{A \in F} \frac{1}{\binom{n}{\lfloor n/2 \rfloor}} \leq \sum_{A \in F} \frac{1}{\binom{n}{|A|}} \leq 1$$

Since

$$\blacktriangleright \sum_{A \in F} \frac{1}{\binom{n}{\lfloor n/2 \rfloor}} = \frac{|F|}{\binom{n}{\lfloor n/2 \rfloor}}$$

We have that

$$|F| \leq \binom{n}{\lfloor n/2 \rfloor}$$

## Back to Monotone Formula's

Let  $S$  be the set of all assignments to  $\{x_1, \dots, x_n\}$  such that exactly

- ▶  $\lfloor n/2 \rfloor$  variables are mapped to 1 (true)

Clearly,  $|S| = \binom{n}{\lfloor n/2 \rfloor}$

- ▶ this is the definition of  $\binom{a}{b}$

Now choose some 0/1 labelling on  $S$

- ▶ i.e., choose an arbitrary function  $g : S \rightarrow \{0, 1\}$
- ▶ we need to show that  $M_n$  contains that function

Define  $T$  (from true) by

$$T = \{A \in S \mid g(A) = 1\}$$

We need to construct a monotone formula  $f$  such that

$$f(A) = 1 \leftrightarrow A \in T \leftrightarrow g(A) = 1$$

## Two Special Cases and $f$

$g$  maps all variables to 0 (false)

- ▶ iff  $S = \emptyset$

Clearly, the function  $\text{false} \in M_n$ . Hence we can assume  $S \neq \emptyset$

If  $n = 1$ , we have only 1 variable which is either mapped to 1 or to 0

- ▶ a function that is obviously in  $M_1$

Hence we may assume that  $n > 1$

Let  $f$  be the monotone function

$$f(z_1, \dots, z_n) = \bigvee_{A \in T} \bigwedge_{i: A(x_i)=1} x_i$$

Given the assumptions made above, the disjunction isn't empty and neither is the conjunction

$$VC(M_n) \geq \binom{n}{\lfloor n/2 \rfloor}$$

Let  $B \in T$ , then the monomial

$$\bigwedge_{i: B(x_i)=1} x_i$$

is mapped to 1 by  $B$  and, thus, by  $f$

For  $B \in S \setminus T$ , note that each monomial

$$\bigwedge_{i: A(x_i)=1} x_i$$

in  $f$  assigns 1 to exactly  $\lfloor n/2 \rfloor$  variables and 0 to the rest. Since

$B \in S \setminus T$

- ▶ it assigns 0 to at least one of these  $\lfloor n/2 \rfloor$  variables

Which means that  $f$  assigns 0 to  $B$ ,

In other words,  $M_n$  shatters  $S$  which has  $\binom{n}{\lfloor n/2 \rfloor}$  elements. Hence

$$VC(M_n) \geq \binom{n}{\lfloor n/2 \rfloor}.$$



$$VC(M_n) \leq \binom{n}{\lfloor n/2 \rfloor}$$

Let  $S$  be a set of assignments such that  $|S| > \binom{n}{\lfloor n/2 \rfloor}$ . For each  $A \in S$  define:

$$V_A = \{i \mid A(x_i) = 1\}$$

Because of the size of  $S$ , Sperner's theorem tells us the  $V_A$ 's cannot be an antichain. Hence, there are  $A_1, A_2 \in S$  such that

$$A_1(x_i) = 1 \rightarrow A_2(x_i) = 1$$

Since the functions in  $M_n$  are monotone, this means:

$$\forall f \in M_n : f(A_1) = 1 \rightarrow f(A_2) = 1$$

In other words a labelling that maps  $A_1$  to 1 and  $A_2$  to 0 cannot be constructed in  $M_n$ . In other words:  $VC(M_n) \leq \binom{n}{\lfloor n/2 \rfloor}$  Hence

$$VC(M_n) = \binom{n}{\lfloor n/2 \rfloor}$$

## Adding Negations

In the case of  $C_n$  and  $D_n$  we saw that

- ▶ adding negation did not increase the VC dimension

So, it is reasonable to expect that

- ▶ the VC dimension of all boolean functions is the same as that of  $M_n$

This is, however,

*not true!*

The VC dimension of that set of hypotheses is strictly bigger.

Computing the exact dimension is pretty hard

- ▶ in fact, I am not aware of an exact expression

Bounding the dimension is easier

- ▶ for  $k$ -DNF we can compute a  $\Theta$  bound

For the general case, we need some extra machinery. But first we look at  $k$ -DNF

# k-DNF

Recall that  $k$ -DNF consists of disjunctions

- ▶ each component (disjunct, consisting of conjunctions) is the conjunction of at most  $k$  literals.

Computing the VC dimension exactly isn't easy, giving a bound is:

For  $n, k \in \mathbb{N}$ , let  $D_{n,k}$  be the set of  $k$ -DNF functions (expressions) over  $\{0, 1\}^n$  (i.e., in  $n$  variables). Then  $VC(D_{n,k}) = \Theta(n^k)$

Recall:

- ▶  $g(n) = O(f(n))$  if there exist  $c, n_0$  such that  $\forall n \geq n_0 : g(n) \leq cf(n)$  (i.e., upper bound)
- ▶  $g(n) = \Omega(f(n))$  if there exist  $c, n_0$  such that  $\forall n \geq n_0 : g(n) \geq cf(n)$  (i.e., lower bound)
- ▶  $g(n) = \Theta(f(n))$  if  $g(n) = O(f(n))$  and  $g(n) = \Omega(f(n))$

$$VC(D_{n,k}) = O(n^k)$$

The number of monomials of degree at most  $k$  (not identical false or empty) is:

$$\sum_{i=1}^k \binom{n}{i} 2^i = O(n^k) \text{ for fixed } k$$

( $2^i$ , since the literals you choose are either a variable or its negation).

Each  $k$ -DNF formula is the disjunction of a set of such terms

$$|D_{n,k}| = 2^{O(n^k)}$$

Which means:

$$VC(D_{n,k}) = O(n^k)$$

$$VC(D_{n,k}) = \Omega(n^k)$$

Let  $S \subseteq \{0, 1\}^n$  consist of those vectors

- ▶ that have exactly  $k$  entries equal to 1

Let  $R \subseteq S$

- ▶ for each  $y = (y_1, \dots, y_n) \in R$
- ▶ form the term  $t_y$  as the conjunction of the literals  $u_i$  such that  $y_i = 1$
- ▶  $t_y$  has exactly  $k$  literals and
- ▶  $\forall z \in S : t_y(z) = 1 \leftrightarrow z = y$

Hence,

$$\bigvee_{y \in R} t_y \text{ is a classifier for } R$$

That is,  $S$  is shattered by  $D_{n,k}$ . Since  $|S| = \binom{n}{k} = \Omega(n^k)$  (for fixed  $k$ ). We have:

$$VC(D_{n,k}) = \Omega(n^k)$$

## An Observation

From the results we have reached – perhaps even more from the proofs of these results – one sees that

- ▶ the richer the model class, the higher the VC dimension.

This is, of course, completely logical as we have by definition that

$$\mathcal{H}_1 \subseteq \mathcal{H}_2 \rightarrow VC(\mathcal{H}_1) \leq VC(\mathcal{H}_2)$$

This observation, however, hints at a way to find good models:

- ▶ start with a very simple model class and pick the best hypothesis
- ▶ if that is good, you are done. If not take a slightly richer class

This line of thought gives rise to structural risk minimization

- ▶ rather than empirical risk minimization

which we'll later in this course

# The Growth Function

Exact bounds for larger classes of boolean functions are not known. We do, however, have a more general result which is based on the *growth function*.

The VC dimension only looks at the largest set that  $\mathcal{H}$  can shatter. The growth function  $\tau_{\mathcal{H}} : \mathbb{N} \rightarrow \mathbb{N}$  looks much broader to the classifications  $\mathcal{H}$  contains:

$$\tau_{\mathcal{H}}(m) = \max_{C \subset X: |C|=m} |\mathcal{H}_C|$$

That is,

$$\tau_{\mathcal{H}}(m) = \max_{C \subset X: |C|=m} |\{f(c_1), \dots, f(c_m)\}_{f \in \mathcal{H}}|$$

each  $f \in \mathcal{H}$  produces a 0/1 vector of length  $m$  and  $\tau_{\mathcal{H}}$  tells you

- ▶ how many different vectors  $\mathcal{H}$  can produce maximally

## Growth Above VC

Clearly, if  $m \leq d = VC(\mathcal{H})$  then  $\tau_{\mathcal{H}}(m) = 2^m$

- ▶ if there is a  $d$  sized set that  $\mathcal{H}$  can shatter, then for each smaller integer there is also a set that  $\mathcal{H}$  can shatter
- ▶ restrict (actually project) the shattering to the lower dimensional space.

It is more instructive what happens if  $m > d$ . The fact that  $\mathcal{H}$  cannot shatter a set of size  $m$

- ▶ doesn't mean that it is completely useless for sets of that size

It might, e.g., classify almost always almost correctly

- ▶ or it might do a horrible job for any  $m$  sized set.

Sauer's Lemma tells us what to expect above  $d$ .

- ▶ and for Sauer we need Pajor



## Pajor's Lemma

Let  $\mathcal{H}$  be any hypothesis class with  $VC(\mathcal{H}) = d < \infty$ . For any  $C = \{c_1, \dots, c_m\}$

$$|\mathcal{H}_C| \leq |\{B \subseteq C \mid \mathcal{H} \text{ shatters } B\}|$$

To prove this by induction, first note that for  $m = 1$ , either both sides are 1 or both are 2

- ▶ the empty set is shattered by all hypothesis classes.

Now assume that the inequality holds for all  $k < m$

- ▶ Let  $C = \{c_1, c_2, \dots, c_m\}$  and
- ▶ let  $C' = \{c_2, \dots, c_m\}$

Define the two sets

$$Y_0 = \{(y_2, \dots, y_m) \mid (0, y_2, \dots, y_m) \in \mathcal{H}_C \vee (1, y_2, \dots, y_m) \in \mathcal{H}_C\}$$

$$Y_1 = \{(y_2, \dots, y_m) \mid (0, y_2, \dots, y_m) \in \mathcal{H}_C \wedge (1, y_2, \dots, y_m) \in \mathcal{H}_C\}$$

Note that  $|\mathcal{H}_C| = |Y_0| + |Y_1|$ , because  $Y_1$  contains those vectors of  $\mathcal{H}_C$  that generate a vector in  $Y_0$  twice rather than once.

## Proof Part 1

Since  $Y_0 = \mathcal{H}_{C'}$ , we have by the induction assumption that

$$\begin{aligned} |Y_0| &= |\mathcal{H}_{C'}| \leq |\{B \subseteq C' \mid \mathcal{H} \text{ shatters } B\}| \\ &= |\{B \subseteq C \mid c_1 \notin B \wedge \mathcal{H} \text{ shatters } B\}| \end{aligned}$$

Next, define  $\mathcal{H}'$  to contain pairs of hypotheses that agree on  $C'$  but disagree on  $c_1$ :

$$\begin{aligned} \mathcal{H}' &= \{h \in \mathcal{H} \mid \exists h' \in \mathcal{H} : (1 - h'(c_1), h_2(c_2), \dots, h_m(c_m)) \\ &= (h(c_1), h(c_2), \dots, h_m(c_m))\} \end{aligned}$$

Note that

- ▶ if  $\mathcal{H}'$  shatters  $B \subseteq C'$  it also shatters  $B \cup \{c_1\}$  and vice versa
- ▶  $Y_1 = \mathcal{H}'_{C'}$

So, by induction we can compute  $|Y_1|$

## Proof Part 2

Because  $|C'| < m$  our induction assumption yields

$$\begin{aligned} |Y_1| &= |\mathcal{H}'_{C'}| \leq |\{B \subseteq C' \mid \mathcal{H}' \text{ shatters } B\}| \\ &= |\{B \subseteq C' \mid \mathcal{H}' \text{ shatters } B \cup \{c_1\}\}| \\ &= |\{B \subseteq C \mid c_1 \in B \wedge \mathcal{H}' \text{ shatters } B\}| \\ &\leq |\{B \subseteq C \mid c_1 \in B \wedge \mathcal{H} \text{ shatters } B\}| \end{aligned}$$

Bringing all intermediate results together gives us:

$$\begin{aligned} |\mathcal{H}_C| &= |Y_0| + |Y_1| \\ &\leq |\{B \subseteq C \mid c_1 \notin B \wedge \mathcal{H} \text{ shatters } B\}| \\ &\quad + |\{B \subseteq C \mid c_1 \in B \wedge \mathcal{H} \text{ shatters } B\}| \\ &= |\{B \subseteq C \mid \mathcal{H} \text{ shatters } B\}| \end{aligned}$$

Which was to be proven.

## Sauer's Lemma

Let  $\mathcal{H}$  be any hypothesis class with  $VC(\mathcal{H}) = d < \infty$ .

- ▶  $\forall m : \tau_{\mathcal{H}}(m) \leq \sum_{i=0}^d \binom{m}{i}$
- ▶ if  $m \geq d : \tau_{\mathcal{H}}(m) < (em/d)^d$

**Proof:** Since  $VC(\mathcal{H}) = d$ ,  $\mathcal{H}$  shatters *no* set with more than  $d$  elements. Thus

$$|\{B \subseteq C \mid \mathcal{H} \text{ shatters } B\}| \leq \sum_{i=0}^d \binom{m}{i}$$

$$\begin{aligned} \sum_{i=0}^d \binom{m}{i} &= \sum_{i=0}^d \binom{m}{i} \left(\frac{m}{d}\right)^i \left(\frac{d}{m}\right)^i \leq \left(\frac{m}{d}\right)^d \sum_{i=0}^d \binom{m}{i} \left(\frac{d}{m}\right)^i \\ &\leq \left(\frac{m}{d}\right)^d \sum_{i=0}^m \binom{m}{i} \left(\frac{d}{m}\right)^i = \left(\frac{m}{d}\right)^d \left(1 + \frac{d}{m}\right)^m < \left(\frac{em}{d}\right)^d \end{aligned}$$

For last inequality use  $x > 0 \rightarrow (1 + x/m)^m < e^x$

## A Simple Consequence

Let  $\mathcal{H}$  be a finite hypothesis set with at least two hypothesis, defined on a finite domain  $X$

- ▶ unfortunately, 1 hypothesis isn't going to work because:

Two hypothesis  $h_1, h_2 \in \mathcal{H}$  are different if

- ▶  $\exists x \in X : h_1(x) \neq h_2(x)$

That is,  $h_1$  and  $h_2$  are different if they are different classifications on the complete domain  $X$

- ▶ there are, by definition,  $\tau_{\mathcal{H}}(|X|)$  such classifications.

That is:

$$\tau_{\mathcal{H}}(|X|) = |\mathcal{H}|$$

By Sauer's lemma we have  $|\mathcal{H}| < \left(\frac{e|X|}{d}\right)^d$ . Which means that

$$VC(\mathcal{H}) \geq \frac{\log |\mathcal{H}|}{n + \log e}$$

## Back to Boolean Functions

If  $VC(\mathcal{H}) \geq 3$  the inequality of the previous slide can be improved to  $VC(\mathcal{H}) \geq \frac{\log |\mathcal{H}|}{n}$ .

Hence, for any large enough class  $B_n$  of boolean functions on  $\{0, 1\}^n$  we have that

$$\frac{\log |B|}{n} \leq VC(B_n) \leq \log |B|$$

Clearly, these bounds are much weaker than the ones we had for  $M_n$

- ▶ but, then again, we talk about (almost) arbitrary sets here

Until now we studied classes of functions from  $\{0, 1\}^n$  to  $\{0, 1\}$ . An obvious generalization is to study sets of functions

- ▶ from  $\mathbb{R}^n$  to  $\{0, 1\}$ .

We look at one such class, polynomials on  $\mathbb{R}$

# Polynomials as Classifiers

Recall how we saw lines and hyperplanes as classifiers

- ▶ simply by distinguishing the half spaces above and below the line/hyper plane

For polynomials we can do the same. First we define the set of polynomials of degree at most  $n$  by

$$P_n = \sum_{i=0}^n a_i x^i$$

for  $a_i \in \mathbb{R}$ . Next, for any  $p \in P_n$  define the function  $p_+ : \mathbb{R} \rightarrow \{0, 1\}$  by

$$p_+(x) = \begin{cases} 1 & \text{if } f(x) > 0 \\ 0 & \text{if } f(x) \leq 0 \end{cases}$$

The set of all these classifiers is known as  $\text{pos}(P_n)$  which we denote by  $P_n^{>0}$ . The question now is: determine  $VC(P_n^{>0})$ ?

## The Intuition

The fundamental theorem of algebra tells us that over the complex numbers, a polynomial of degree  $n$  can be written as

$$\beta \prod_{i=1}^n (x - \alpha_i) \quad \alpha_i, \beta \in \mathbb{C}$$

In other words, the graph of a real valued degree  $n$  polynomial

- ▶ crosses the  $x$ -axis at most  $n$  times

Each such crossing

- ▶ switches the classification from 1 to 0 or vice versa

Hence we can shatter at most  $n + 1$  points in  $\mathbb{R}$

Each labelling of  $n + 1$  points on the  $x$ -axis shows a number of adjacent change pairs  $(1, 0)$  or  $(0, 1)$

- ▶ construct your polynomial such that the roots are between the two points of a change pair

This will give you a separating polynomial



# From Intuition to Proof

Making this intuition precise using the language of the graphs of polynomials involves lots of infuriating bookkeeping details

- ▶ wiggly lines are hard to keep under control

To make life easier

- ▶ for those who know some linear algebra

we map (embed) our data into a higher dimensional space

- ▶ and stretch the wiggly line in a linear structure: a hyperplane
- ▶ for the cognoscenti, we are using the "kernel trick", well known from SVMs, with a polynomial kernel

The mapping we use is:

$$\phi : z \rightarrow (1, z, z^2, \dots, z^n)$$

mapping  $c \in \mathbb{R}$  to the vector  $(1, c, c^2, \dots, c^n)^T \in \mathbb{R}^{n+1}$

## Using $\phi$

A polynomial  $p$  is given by

$$p = \sum_{i=0}^n a_i x^i$$

We can rewrite this as a dot product by

$$p = \sum_{i=0}^n a_i x^i = (a_0, a_1, \dots, a_n) \cdot (1, x, x^2, \dots, x^n)$$

The second expression should remind you of a hyperplane, perhaps all the more when evaluated on a particular instance

$$\begin{aligned} p(c) &= (a_0, a_1, \dots, a_n) \cdot (1, c, c^2, \dots, c^n) \\ &= (a_0, a_1, \dots, a_n) \cdot \phi(c) = \phi(p)(\phi(c)) \end{aligned}$$

where  $\phi(p)$  denotes the function on  $\mathbb{R}^{n+1}$

# Polynomials, Hyperplanes, and Thresholds

More in particular, if we turn from  $P_n$  to  $P_n^{>0}$

- ▶ i.e., we turn from functions to classifiers

We see that

- ▶  $p(c) > 0$  on  $\mathbb{R}$  translates to  $\phi(p)(\phi(c)) > 0$  on  $\mathbb{R}^{n+1}$

Now, the expression:  $\phi(p)$  denotes both

- ▶ a threshold function on  $\mathbb{R}^{n+1}$
- ▶ and a hyperplane on  $\mathbb{R}^n$

That is, we have a 1-1 correspondence between

- ▶ polynomial classifiers and
- ▶ threshold/hyperplane classifiers

This correspondence helps us to prove our results "linearly".

$$VC(P_n^{>0}) \leq n + 1$$

Let  $S \subseteq \mathbb{R}^n$  be a set, that is shattered by  $P_n^{>0}$ . That is, for every  $S^+ \subseteq S$  there exists a  $p_+ \in P_n^{>0}$  such that

- ▶  $p_+(s) = 1$  if  $s \in S^+$
- ▶  $p_+(s) = 0$  if  $s \in S \setminus S^+$

In other words, there is a  $p \in P_n$  such that

- ▶  $\sum_{i=0}^n a_i s^i > 0$  if  $s \in S^+$
- ▶  $\sum_{i=0}^n a_i s^i \leq 0$  if  $s \in S \setminus S^+$

Written in the language of dot products this says that there is a vector  $a = (a_1, \dots, a_n)$  and a constant  $a_0$  such that

- ▶  $(a_1, \dots, a_n) \cdot (s, s^2, \dots, s^n) + a_0 > 0$  if  $s \in S^+$
- ▶  $(a_1, \dots, a_n) \cdot (s, s^2, \dots, s^n) + a_0 \leq 0$  if  $s \in S \setminus S^+$

Since  $z \rightarrow (z, z^2, \dots, z^n)$  simply maps  $\mathbb{R} \rightarrow \mathbb{R}^n$ , we have a separating hyperplane on  $\mathbb{R}^n$ . Hence,  $|S| \leq n + 1$

## Independent Vectors are Shattered

To prove that  $VC(P_n^{>0}) \geq n + 1$ , we first prove that a set  $\{x_1, \dots, x_n\} \subset \mathbb{R}^n$  of independent vectors is shattered by threshold functions on  $\mathbb{R}^n$ .

Let  $A$  be the  $n \times n$  matrix with the  $x_i$  vectors as columns. This is an invertible matrix

- ▶ otherwise the  $x_i$  would not be independent

Let  $v$  be any of the  $2^n - 1$   $\pm 1$  vectors that denote the labellings of the  $x_i$

- ▶ then, the matrix equation  $Aw = v$  has a unique solution
- ▶  $w = A^{-1}v$

The vector  $w$  gives you the threshold function that shatters the  $x_i$  for labelling  $v$ .

Hence, if we can prove that there exists a set  $\{x_0, \dots, x_n\} \subset \mathbb{R}^n$  that  $\phi$  maps to a set of independent vectors in  $\mathbb{R}^{n+1}$  we are done.

## $P_n$ is a Vector Space

For that we need:

Let  $f, g \in P_n$  and  $\lambda \in \mathbb{R}$ . Then clearly

- ▶  $f + g = \sum_{i=0}^n (a_i + b_i)x^i \in P_n$  and
- ▶  $\lambda f = \sum_{i=0}^n (\lambda a_i)x^i \in P_n$

In other words,  $P_n$  is a vector space over  $\mathbb{R}$

Moreover,  $P_n$  is a  $n + 1$ -dimensional vector space with base

$$\{1, x, \dots, x^n\}$$

For, clearly, these functions are linearly independent

$$[\forall x \in \mathbb{R} : \lambda_0 + \lambda_1 x + \lambda_2 x^2 + \dots + \lambda_n x^n = 0] \Leftrightarrow [\forall i : \lambda_i = 0]$$

and every element of  $P_n$  can (by definition) be written as a linear combination of these functions

## $n + 1$ Independent Vectors

To see that  $\phi$  creates  $n + 1$  independent vectors we argue from contradiction.

Assume that for every  $X = \{x_0, \dots, x_n\} \subset \mathbb{R}$  we have that the set of vectors  $\phi(X) = \{\phi(x_0), \dots, \phi(x_n)\}$  is dependent

- ▶ then the vector subspace spanned by  $\{\phi(x) \mid x \in \mathbb{R}\}$  of  $\mathbb{R}^{n+1}$  has at most dimension  $n$
- ▶ that is, it is contained in some hyperplane
- ▶ this means that there are  $\lambda_i$ , not all equal to 0, such that

$$\forall x \in \mathbb{R} : \sum_{i=0}^n \lambda_i (\phi(x)) = \sum_{i=0}^n \lambda_i x^i = 0$$

But that contradicts that  $\{1, x, \dots, x^n\}$  is a base.

$$VC(P_n^{>0}) \geq n + 1$$

We have:

- ▶ there exists a  $X = \{x_0, \dots, x_n\} \subset \mathbb{R}$
- ▶ such that  $\phi(X) = \{\phi(x_0), \dots, \phi(x_n)\}$  is independent
- ▶ hence,  $\phi(X)$  is shattered by threshold functions
- ▶ hence,  $X$  is shattered by the corresponding polynomials

In other words,  $VC(P_n^{>0}) \geq n + 1$ . We already had that  $VC(P_n^{>0}) \leq n + 1$ , hence we have

$$VC(P_n^{>0}) = n + 1$$

For the more general case, having more variables  $x_1, \dots, x_m$  see exercise 6.12 in the book



## A Simple Consequence

The fact that  $VC(P_n^{>0}) = n + 1$  implies that the set of all polynomials

$$P = \bigcup_{n=1}^{\infty} P_n$$

has  $VC(P) = \infty$

- ▶ if  $VC(P)$  would be finite, say  $k$  we have a contradiction with  $VC(P_k) = k + 1$

Hence, we cannot simply learn the best fitting polynomial using the ERM rule

- ▶ recall that sets with infinite VC dimension are not PAC learnable

For that one needs a more subtle approach

- ▶ Structural Risk Minimization

Which we mentioned before and is discussed later in this course.