

FSAN/ELEG815: Statistical Learning

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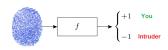
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4: Training vs Testing

#### Review

#### **▶** Error measures:

User specified  $e(h(\mathbf{x}), f(\mathbf{x}))$ 



#### In-sample:

$$E_{in}(h) = \frac{1}{N} \sum_{n=1}^{N} e(h(\mathbf{x}_n), f(\mathbf{x}_n))$$

#### **Out-of-sample:**

$$E_{out}(h) = \mathbb{E}_x[e(h(\mathbf{x}), f(\mathbf{x}))]$$



#### Outline

- ► From training to testing
- ► Illustrative examples
- ► Key notion: break point
- ► Puzzle



### Example - The Final Exam

Before the final exam, a professor may hand out practice problems and solutions to the class (training set).

Why not to give out the exam problems?

The goal is for the students to learn the course material (small  $E_{out}$ ), not to memorize the practice problems (small  $E_{in}$ ).

Having memorized all the practice problems (small  $E_{in}$ ) does not guarantee to learn the course material (small  $E_{out}$ ).



#### The Final Exam

#### Testing:

- ▶ The hypothesis is fixed (you already prepared for the test).
- ▶ The hypothesis is tested over unseen data (the test does not include the same practice problems) i.e.  $E_{in}$  is computed using the hypothesis set.

$$\mathbb{P}[|E_{in} - E_{out}| > \epsilon] \le 2e^{-2\epsilon^2 N}$$

▶ For a large N (number of questions),  $E_{in}$  tracks  $E_{out}$  (your performance gauges how well you learned).

#### The Final Exam

**Training:** Performance on practice problems.

► The hypothesis is adjusted (since you know the answers, you repeat a problem until getting it right).

$$\mathbb{P}[|E_{in} - E_{out}| > \epsilon] \le 2Me^{-2\epsilon^2 N}$$

- $ightharpoonup E_{in}$  is computed using the practice set.
- Small  $E_{in} \rightarrow$  not necessarily small  $E_{out}$ . You may have not learned and have memorized the problems solutions.
- ► M is the number of hypotheses to explore.

  Depending on the times you repeat a problem, your performance may no longer accurately gauge how well you learned.

Goal: We want to replace M by another quantity that is not infinity.

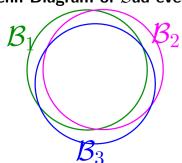


#### Where did the M Come from?

The  $\mathcal{B}$ ad events  $\mathcal{B}_m$  are

$$|E_{in}(h_m) - E_{out}(h_m)| > \epsilon$$

#### Venn Diagram of $\mathcal{B}$ ad events



The union bound consider  $\mathcal{B}_m$  as disjoint events:

$$\mathbb{P}[\mathcal{B}_1 \text{ or } \mathcal{B}_2 \text{ or } \cdots \text{ or } \mathcal{B}_M] \leq \mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \cdots \mathbb{P}[\mathcal{B}_M]$$

It is a poor bound when there is overlap.

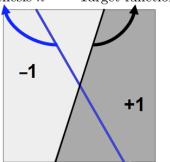


Yes, bad events are very overlapping

Remember the perceptron:

$$h(\mathbf{x}) = \begin{cases} 1 & \text{if 'approved'} \\ -1 & \text{if 'deny credit'} \end{cases}$$
 
$$h(\mathbf{x}) = \operatorname{sign}(\mathbf{w}^T \mathbf{x})$$

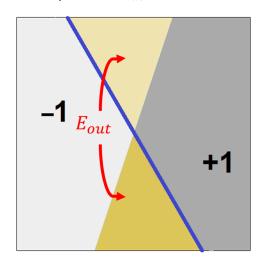
Hypothesis h Target function f

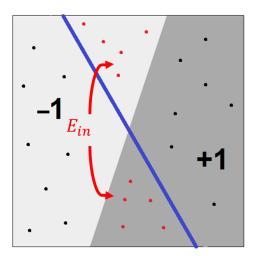


For any perceptron (w): The line  $w_0+w_1x_1+w_2x_2=0$  splits the plane into +1 and -1



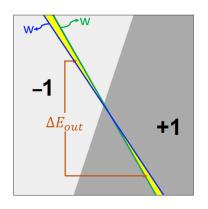
For the given perceptron (w) , consider the out-of-sample error  $E_{out}$  and the in-sample error  $E_{in}$ :

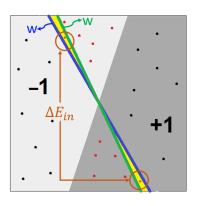






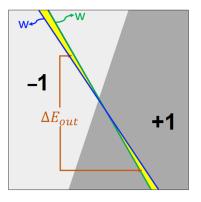
Consider a different perceptron w:

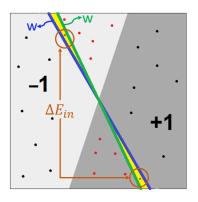




 $\triangle E_{out}$  and  $\triangle E_{in}$  move in the same direction Area of yellow part increases  $\rightarrow$  probability of data points falling in yellow part increases.







$$|E_{in}(h_1) - E_{out}(h_1)| \approx |E_{in}(h_2) - E_{out}(h_2)|$$

(Both exceed  $\epsilon$ )

Many hypotheses are similar. In PLA, if we slowly vary  $\mathbf{w}$ , we get infinitely many hypotheses that differ from each other infinitesimally.



### What can we Replace M with?

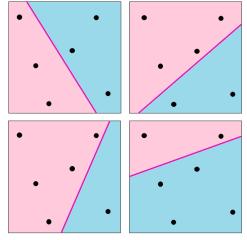
Since the input space  $\mathcal{X}$  is infinity, the possible hypotheses are infinity.

Instead of counting the hypotheses over the whole input space, consider a finite set of input points.

On a finite set of input points, how many different 'hypotheses' can I get?

Classification by the four perceptrons is different in at least one data point, so we have four different 'hypotheses'.

#### Four different perceptrons:





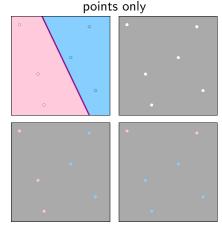
### What can we Replace M with?

Define dichotomy as different 'hypotheses' over the finite set of N input points.

**Definition:** Let  $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathcal{X}$ . The *dichotomies* generated by  $\mathcal{H}$  are

$$\mathcal{H}(\mathbf{x}_1,\cdots,\mathbf{x}_N) = \{(h(\mathbf{x}_1),\cdots,h(\mathbf{x}_N))|h \in \mathcal{H}\}$$

Hypotheses are seen through the eyes of N



Vary perceptron until the line crosses one of the points  $\rightarrow$  different *dichotomy*.



### Dichotomies: Mini-Hypotheses

A hypotheses  $h: \mathcal{X} \to \{-1, +1\}$ 

A dichotomy  $h:\{\mathbf{x}_1,\mathbf{x}_2,,\cdots,\mathbf{x}_N,\} o \{-1,+1\}$ 

Number of hypotheses  $|\mathcal{H}|$  can be infinite.

Number of dichotomies  $|\mathcal{H}(\mathbf{x}_1,\mathbf{x}_2,,\cdots,\mathbf{x}_N)|$  is at most  $2^N$ 

Candidate for replacing M.

**Ex:** The two *dichotomies* in the picture could be:

$$[-1,-1,-1,+1,+1,+1]$$
,  $[-1,-1,+1,+1,+1]$ .



#### The Growth Function

The growth function counts the  $\underline{most}$  dichotomies on any N points

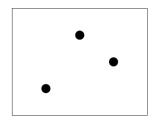
$$m_{\mathcal{H}}(N) = \max_{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N \in \mathcal{X}} |\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)|$$

The value of  $m_{\mathcal{H}}(N)$  is at most  $|\{-1,+1\}^N|$ . Hence, the growth function satisfies:

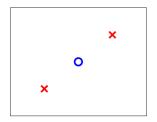
$$m_{\mathcal{H}}(N) \le 2^N$$

Let's apply the definition.

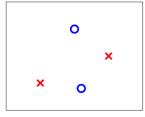
# Applying $m_{\mathcal{H}}(N)$ Definition - 2D Perceptrons



Maximum 8 dichotomies with three points.



Dichotomy on 3 colinear points cannot be generated  $\left(N=4\right)$ 



Dichotomy here cannot be generated

$$m_{\mathcal{H}}(3) = 8$$
  $m_{\mathcal{H}}(4) = 14$ 

**Note**: At most 14 out of the possible 16 dichotomies on any 4 points can be generated.



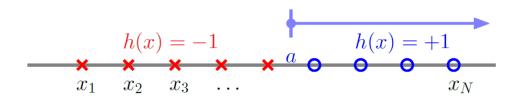
#### Outline

- ► From training to testing
- ▶ Illustrative examples

  These examples confirm the intuition that  $m_{\mathcal{H}}(N)$  grows faster when  $\mathcal{H}$  becomes more complex.
- ► Key notion: break point
- ► Puzzle



### Example 1: Positive Rays



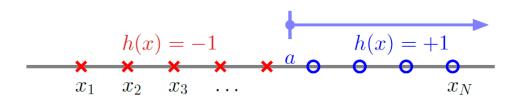
$$\mathcal{H}$$
 is set of  $h: \mathbb{R} \to \{-1, +1\}$ 

$$h(x) = \mathsf{sign}(x - a)$$

Hypotheses are defined on a one-dimensional input space, and they return -1 to the left of a and +1 to the right of a.



### Example 1: Positive Rays



N points, split line into N+1 regions. As we vary a we get different dichotomies.

The growth function:  $m_{\mathcal{H}}(N) = N + 1$ 

At most N+1 dichotomies given any N points.



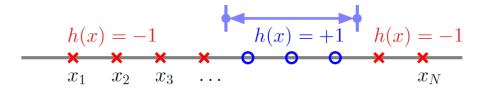
# Example 2: Positive Intervals

$$\mathcal{H}$$
 is set of  $h: \mathbb{R} \to \{-1, +1\}$ 

Hypotheses defined on a one-dimensional input space, and they return +1 over some interval and -1 otherwise.



### Example 2: Positive Intervals

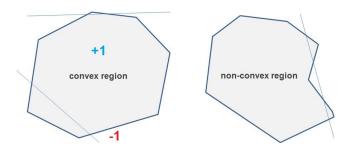


N points, split line into N+1 regions.

$$m_{\mathcal{H}}(N) = {N+1 \choose 2} + 1 = \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

Dichotomies are decided by end values of interval, we have  $\binom{N+1}{2}$  possibilities. Add the case in which both end values fall in the same region.

A set is **convex** if a line segment connecting any two points in the set lies entirely within the set



 ${\cal H}$  consists of all hypotheses in two dimensions that are positive inside some convex set and negative elsewhere

$$\mathcal{H}$$
 is set of  $h: \mathbb{R}^2 \to \{-1, +1\}$   $h(\mathbf{x}) = +1$  is convex

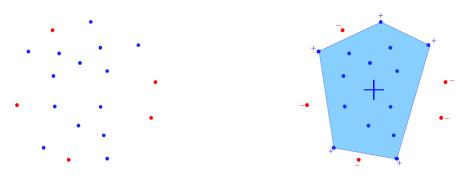
$$h(\mathbf{x}) = +1$$
 is convex



How many patterns can I get out of these data points using convex regions?



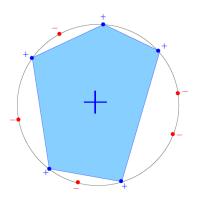
How many patterns can I get out of these data points using convex regions?



If we consider some outer points to be +1, then all interior points are +1 (not many dichotomies).



Find another distribution of points to get all possible dichotomies using convex regions?



Place N points over the perimeter of the circle. We get all possible combinations (maximum number of dichotomies).

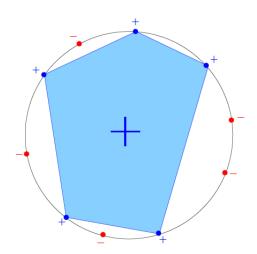


$$m_{\mathcal{H}}(N) = 2^N$$

Any dichotomy on these N points can be realized using a convex hypothesis.

The N points are 'shattered' by convex sets.

**Note:**  $m_{\mathcal{H}}(N)$  is an upper bound. The number of possible dichotomies for given data points may be less than  $2^N$  because of interior points.



The hypothesis shatters all points

#### The 3 Growth Functions

 $ightharpoonup \mathcal{H}$  is positive rays:

$$m_{\mathcal{H}}(N) = N + 1$$

 $\triangleright \mathcal{H}$  is positive intervals:

$$m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

 $\triangleright \mathcal{H}$  is convex sets:

$$m_{\mathcal{H}}(N) = 2^N$$

 $m_{\mathcal{H}}(N)$  grows faster when  $\mathcal{H}$  becomes more complex.



### Back to the Big Picture

Remember this inequality?

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2Me^{-2\epsilon^2 N}$$

What happens if  $m_{\mathcal{H}}(N)$  replaces M?

 $m_{\mathcal{H}}(N)$  polynomial  $\Longrightarrow$  Good

If  $m_{\mathcal{H}}(N)$  can be bounded by any polynomial, the generalization error will go to zero as  $N \to \infty \implies$  Learning is feasible.

Just prove that  $m_{\mathcal{H}}(N)$  can be bounded by a polynomial?



#### Outline

- ► From training to testing
- ► Illustrative examples
- lacktriangle Key notion: break point It would enable us to proof that  $m_{\mathcal{H}}(N)$  can be bounded by a polynomial
- Puzzle



#### Break Point of ${\cal H}$

#### **Definition:**

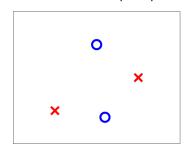
If data set of size k cannot be shattered by  $\mathcal{H}$ , then k is a break point for  $\mathcal{H}$ 

$$m_{\mathcal{H}}(k) < 2^k$$

The break point k is the number of data points at which we fail to get all possible dichotomies.

A bigger data set cannot be shattered either.

#### Remember the 2D perceptrons



At most 14 out of 16 dichotomies on any 4 points can be generated.

$$k = 4$$



# Break Point - the 3 Examples

$$m_{\mathcal{H}}(k) < 2^k$$

▶ Positive rays  $m_{\mathcal{H}}(N) = N + 1$ 

$$k=1$$
  $m_{\mathcal{H}}(1)=2 \not< 2^1$   $k=2$   $m_{\mathcal{H}}(2)=3 < 2^2$   $o$  break point

Intuitively, remember the positive rays:

$$h(x) = -1$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

There is no way for the positive ray to generate:



# Break Point - the 3 Examples

Positive intervals 
$$m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

$$k = 1$$
  $m_{\mathcal{H}}(1) = 2 \nleq 2^{1}$   
 $k = 2$   $m_{\mathcal{H}}(2) = 4 \nleq 2^{2}$   
 $k = 3$   $m_{\mathcal{H}}(3) = 7 < 2^{3}$ 

break point

Intuitively, remember the positive intervals:

$$h(x) = -1$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_2$$

$$x_3$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_5$$

$$x_5$$

$$x_5$$

There is no way to generate:

Convex sets

$$m_{\mathcal{H}}(N) = 2^N$$

break point  $k = \infty$ 



#### Main Result

We observe how the break point increases with the complexity of the model.

No break point 
$$\rightarrow m_{\mathcal{H}}(N) = 2^N$$

Any break point  $\to$  Use k to bound  $m_{\mathcal{H}}(N)$  by a polynomial in N

Remember: If  $m_{\mathcal{H}}(N)$  can be bounded by any polynomial, the generalization error will go to zero as  $N \to \infty \implies$  Learning is feasible.

To consider learning feasible, all that we need to know now is that there exist a break point.



#### What we Want

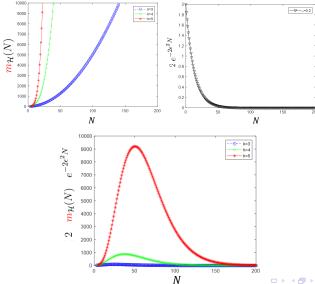
Instead of:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad \mathbf{M} \quad e^{-2\epsilon^2 N}$$

We want:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad \mathbf{m}_{\mathcal{H}}(N) \quad e^{-2\epsilon^2 N}$$

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad \mathbf{m}_{\mathcal{H}}(N) \quad e^{-2\epsilon^2 N}$$

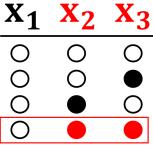




#### Puzzle

Let's consider 3 data points and a break point k=2, i.e. we cannot get 4 dichotomies out of any pair of points. How many dichotomies can we get on these 3 data points?

We start generating the possible dichotomies.



We stop when we get all possible combinations out of two points.

We cannot include this last dichotomy!



### Puzzle

We tried another one:

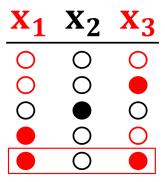
| $\mathbf{x_1}$ | $\mathbf{x_2}$ | $\mathbf{X_3}$ |
|----------------|----------------|----------------|
| 0              | 0              | 0              |
| 0              | $\circ$        |                |
| 0              |                | 0              |
|                | $\circ$        | 0              |

We can add this one!



### Puzzle

Let's continue!



We stop again when we get all possible combinations out of two points. We cannot include this last dichotomy either!



#### Puzzle

If we continue trying, we'll see that none of the other dichotomies work.

| $\mathbf{X_1}$ | $\mathbf{X_2}$ | $\mathbf{X_3}$ |
|----------------|----------------|----------------|
| 0              | 0              | 0              |
| 0              | 0              |                |
| 0              |                | 0              |
|                | $\circ$        | 0              |

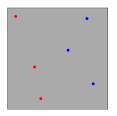
At most 4 dichotomies out of 8.

If we start different, are we going to be able to achieve more? No!

Note: Knowing only N and k, we can determine the maximum number of dichotomies (complexity).

### Review

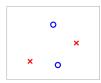
Dichotomies:



**▶** Growth Function:

$$m_{\mathcal{H}}(N) = \max_{\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathcal{X}} |\mathcal{H}(\mathbf{x}_1, \dots, \mathbf{x}_N)|$$

**Break Point** k:



At most 14 out of the possible 16 dichotomies on any 4 points can be generated. k=4

► Maximum # of dichotomies

$$\begin{array}{c|cccc} x_1 & x_2 & x_3 \\ \hline \bigcirc & \bigcirc & \bigcirc \\ \bigcirc & \bigcirc & \bullet \\ \bigcirc & \bullet & \bigcirc \\ \bullet & \bigcirc & \bigcirc \\ \end{array}$$

### Bounding the Growth Function

For a given  $\mathcal{H}$ , if the break point k is fixed,  $m_{\mathcal{H}}(N)$  can be bounded by a polynomial<sup>(\*)</sup>:

#### Theorem:

If  $m_{\mathcal{H}}(k) < 2^k$  for some value k, then

$$m_{\mathcal{H}}(N) \le \sum_{i=0}^{k-1} \binom{N}{i}$$

for all N. The RHS is polynomial of degree k-1.

Note: This ensures good generalization on the Hoeffding's Inequality.

(\*) Proof can be found on the book: Learning from Data, Yaser S. Abu-Mostafa, Malik Magdon-Ismail and Hsuan-Tien Lin, AMLbook 2012.

### Three examples

Let's take the hypothesis sets for which we compute the growth function:

 $\triangleright \mathcal{H}$  is positive rays:

$$h(x) = -1$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_3$$

$$x_4$$

$$x_4$$

$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_1$$

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$$x_5$$

$$x_1$$

$$x_2$$

$$x_3$$

$$x_4$$

$$x_5$$

$$x_5$$

$$x_1$$

We compute before:

$$m_{\mathcal{H}}(N) = N + 1$$

No need to know anything about the hypothesis set just that break point  $k=2\,$ 

$$m_{\mathcal{H}}(N) \le \sum_{i=0}^{1} {N \choose i} = N+1$$



### Three examples

$$m_{\mathcal{H}}(N) \le \sum_{i=0}^{k-1} \binom{N}{i}$$

 $ightharpoonup \mathcal{H}$  is positive intervals: (break point k=3)

$$m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1 \le \sum_{i=0}^{2} {N \choose i} = \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

 $ightharpoonup \mathcal{H}$  is 2D perceptrons: (break point k=4)

$$m_{\mathcal{H}}(N) = ? \le \sum_{i=0}^{3} {N \choose i} = \frac{1}{6}N^3 + \frac{5}{6}N + 1$$



### What we Want

Instead of:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad \mathbf{M} \quad e^{-2\epsilon^2 N}$$

We want:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad m_{\mathcal{H}}(N) \quad e^{-2\epsilon^2 N}$$

Let's consider a pictorial proof:

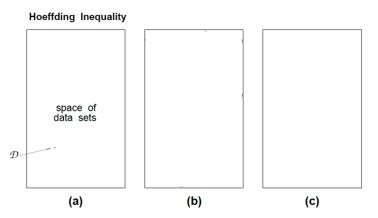


### Pictorial Proof

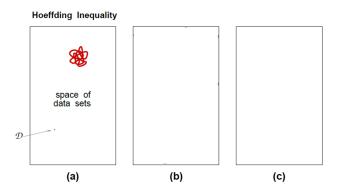
- ▶ How does  $m_{\mathcal{H}}(N)$  relate to overlaps?
- $\blacktriangleright$  What to do about  $E_{out}$ ?
- ▶ Putting it together



The 'canvas' represents space of all possible data sets, with areas corresponding to probabilities. Each data set  $\mathcal D$  is a point on the canvas. The total area of the canvas is 1.



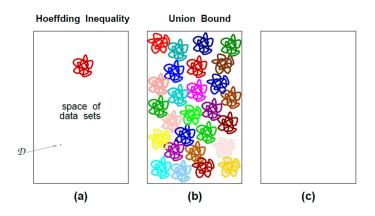




(a) For a given hypothesis  $h \in \mathcal{H}$ , colored points correspond to data sets where  $E_{in}$  does not generalize well to  $E_{out}$  (" $|E_{in}(h) - E_{out}(h)| > \epsilon$ ").

The Hoeffding Inequality guarantees a small colored area.





(b) Considering different hypothesis.

The event " $|E_{in}(h) - E_{out}(h)| > \epsilon$ " may contain different points The union bound assumes no overlap, colored area is large.

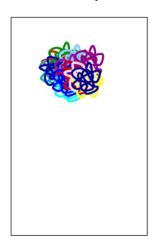


#### How the growth function is going to account for the overlaps?

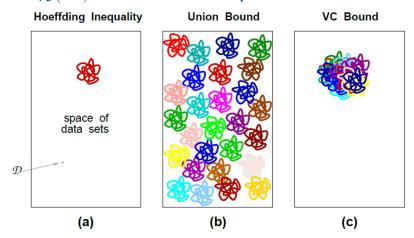
Assume a hypothesis set  $|\mathcal{H}|=100$  that colors same point on the canvas 100 times.

The total colored area is now  $\frac{1}{100}$  of what it would have been without any overlap.

Many hypotheses have same dichotomy on a given  $\mathcal{D}$ .







(c) The VC bound keeps track of overlaps. It estimates the total area of bad generalization to be relatively small.

Learning is Feasible!





Colored (event " $|E_{in}(h) - E_{out}(h)| > \epsilon$ ") depends not only on  $\mathcal{D}$ , but also on the entire  $\mathcal{X}$  because  $E_{out}(h)$  is based on  $\mathcal{X}$ . Instead of:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad \mathbf{M} \quad e^{-2\epsilon^2 N}$$

We wanted:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 2 \quad m_{\mathcal{H}}(N) \quad e^{-2\epsilon^2 N}$$

but rather, we get:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le 4 \quad m_{\mathcal{H}}(2N) \quad e^{-\frac{1}{8}\epsilon^2 N}$$

The Vapnik-Chervonenkis Inequality



### Definition of VC Dimension

The Vapnik-Chervonenkis (VC) dimension  $d_{vc}(H)$  of a hypothesis set  ${\mathcal H}$  is

$$d_{vc}(H) = \text{Largest value of } N \text{ for which } m_{\mathcal{H}}(N) = 2^N$$

" the maximum number of points  ${\cal H}$  can shatter"

$$d_{vc}(H) \leq k$$
 is a break point for  $\mathcal{H}$ 

Hence 
$$d_{VC}(\mathcal{H}) = k - 1$$

### The Growth Function

In terms of a break point k:

$$m_{\mathcal{H}}(N) \le \sum_{i=0}^{k-1} \binom{N}{i}$$

In terms of the  $d_{VC}$ :

$$m_{\mathcal{H}}(N) \le \sum_{i=0}^{\mathbf{d_{VC}}} \binom{N}{i}$$

Maximum power is  $N^{d_{VC}}$ 

### **Examples**

 $\triangleright \mathcal{H}$  is positive rays:

 $d_{VC} = 1$ 

if N=2, we cannot have

•

 $\triangleright$   $\mathcal{H}$  is 2D perceptrons:

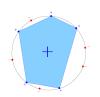
if N=4, we cannot have



 $d_{VC} = 3$ 

 $\triangleright \mathcal{H}$  is convex sets:

$$d_{VC} = \infty$$



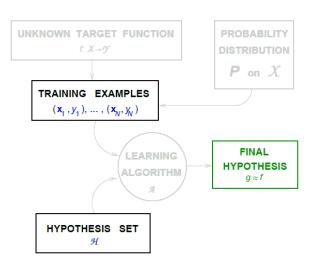


## VC Dimension and Learning

**Result**: If  $d_{VC}(\mathcal{H})$  is finite,  $g \in \mathcal{H}$  will generalize.

This statement is true independently of:

- ► Learning algorithm
- ► Input distribution
- ► Target function



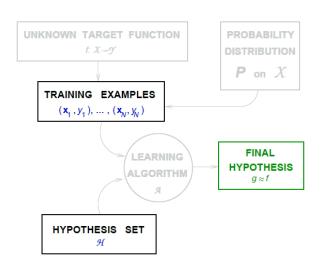


## VC Dimension and Learning

**Result**: If  $d_{VC}(\mathcal{H})$  is finite,  $g \in \mathcal{H}$  will generalize.

#### This statement depends on:

- Hypothesis set
   VC dimension depends only on the hypothesis set.
- Training samples Exist a small chance of having a data set that won't allow generalization.



# VC Dimension of Perceptrons

Consider the 2D perceptron:

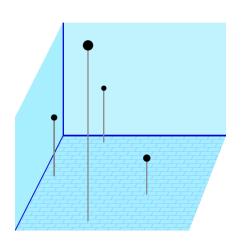
$$d = 2$$
,  $\frac{d_{VC}}{d_{VC}} = 3$ 

In general, for a d-dimensional perceptron:

$$d_{\text{VC}} = d+1$$

To prove this, we are going to show that:

$$\begin{array}{ccc} d_{\text{VC}} & \leq & d+1 \\ d_{\text{VC}} & \geq & d+1 \end{array}$$



# VC Dimension of Perceptrons

Consider a set of N = d + 1 points in  $\mathbb{R}^d$  shattered by the perceptron:

Let's choose input points such as:

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1d} \\ 1 & x_{21} & x_{22} & \dots & x_{2d} \\ 1 & x_{31} & x_{32} & \dots & x_{3d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & x_{N2} & \dots & x_{Nd} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \dots & 0 & 1 \end{bmatrix}$$

- $\mathbf{X} \in \mathbb{R}^{(d+1)\times(d+1)}$
- **X** is invertible  $(\det(\mathbf{X}) = 1)$ .

### Can we Shatter this Data Set?

In vector form, dichotomies are:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{d+1} \end{bmatrix} = \begin{bmatrix} \pm 1 \\ \pm 1 \\ \vdots \\ \pm 1 \end{bmatrix}, \quad \text{and considering the perceptron: } \mathbf{y} = \operatorname{sign}(\mathbf{X}\mathbf{w}).$$

Since X is invertible, for any y, we can find a vector w satisfying:

$$\begin{aligned} \mathsf{sign}(\mathbf{X}\mathbf{w}) &=& \mathbf{y} \\ \mathbf{X}\mathbf{w} &=& \mathbf{y} \\ \mathbf{w} &=& \mathbf{X}^{-1}\mathbf{y} \end{aligned}$$

Note: There exist a perceptron **w** that can generate all possible dichotomies **y**. Hence  $d_{vc} \ge d+1$ 

We cannot shatter any set of d+2 points.

For any d+2 points,

$$\mathbf{x}_1, \cdots, \mathbf{x}_{d+1}, \mathbf{x}_{d+2}$$

More points than dimensions  $(\mathbf{x} \in \mathbb{R}^d) \implies$  the vectors must be linearly dependent and

$$\mathbf{x}_j = \sum_{i \neq j} \mathbf{a}_i \mathbf{x}_i$$

where not all the  $a_i$ 's are zeros.

$$\mathbf{x}_j = \sum_{i \neq j} \mathbf{a_i} \mathbf{x}_i$$

Focus on  $\mathbf{x}_i$ 's with non-zero  $a_i$  and construct a dichotomy that cannot be implemented by a perceptron:

 $\mathbf{x}_i$ 's with non-zero  $\mathbf{a}_i$  get  $y_i = \operatorname{sign}(\mathbf{a}_i)$ .

 $\mathbf{x}_j$  gets  $y_j = -1$  and let others either +1 or -1.

No perceptron can implement such dichotomy!

### Why?

The perceptron:

$$\mathbf{x}_j = \sum_{i \neq j} a_i \mathbf{x}_i \implies \mathbf{w}^T \mathbf{x}_j = \sum_{i \neq j} a_i \mathbf{w}^T \mathbf{x}_i$$

If  $y_i = \operatorname{sign}(\mathbf{w}^T \mathbf{x}_i) = \operatorname{sign}(a_i)$ , then  $a_i \mathbf{w}^T \mathbf{x}_i > 0$ 

This forces

$$\mathbf{w}^T \mathbf{x}_j = \sum_{i \neq j} a_i \mathbf{w}^T \mathbf{x}_i > 0$$

Therefore,  $y_j = \operatorname{sign}(\mathbf{w}^T \mathbf{x}_j) = +1$  (impossible to get -1).

**Conclusion**: we cannot shatter any set of d+2 points  $\Longrightarrow d_{VC} \le d+1$ 

# Putting it Together

We proved  $d_{VC} \le d+1$  and  $d_{VC} \ge d+1$ . Thus,

$$d_{VC} = d + 1$$

What is d+1 in the perceptron?

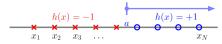
It is the number of parameters  $w_0, w_1, ..., w_d$ ,

Note: The more parameters a model has, the more diverse its hypothesis set is, which is reflected in a larger value of the growth function.

### The Usual Suspects

Let's see if the correspondence between degrees of freedom and VC dimension holds.

Positive rays ( $d_{VC} = 1$ ):

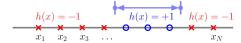


we cannot have

•

Each hypothesis is specified by the parameter a (one degree of freedom).

▶ Positive Intervals  $(d_{VC} = 2)$ 



we cannot have



Each hypothesis is specified by the two end values of the interval (two degrees of freedom).

#### Not Just Parameters

Parameters may not contribute degrees of freedom:

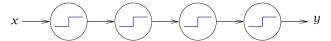
**Example**: consider a one-dimensional perceptron  $h(x) = \text{sign}(w_0 + w_1 x)$  where  $w_0$  is a threshold.

$$y = h(x) = \begin{cases} 1 & \text{if } w_1 x > -w_0 \\ -1 & \text{if } w_1 x < -w_0 \end{cases}$$



2 parameters and 2 degrees of freedom.

Creating a cascade of perceptrons:



Eight parameters in this model and still two degrees of freedom.

 $d_{VC}$  measures the **effective** number of parameters.

### Number of Data Points Needed

Two small quantities in the VC inequality:

$$\mathbb{P}[|E_{in}(g) - E_{out}(g)| > \epsilon] \le \underbrace{4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N}}_{\bullet}$$

If we want certain  $\epsilon$  and  $\delta$ , how does N depend on  $d_{VC}$ 

Let us look at  $N^{\mathbf{d}}e^{-N}$ 

Fix  $N^{\mathbf{d}}e^{-N}=$  small value

How does N change with d? It is basically proportional.

#### Rule of thumb:

$$N \ge 10 d_{\rm VC}$$

