## Machine Learning Foundations

(機器學習基石)



Lecture 5: Training versus Testing

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# Roadmap

1 When Can Machines Learn?

## Lecture 4: Feasibility of Learning

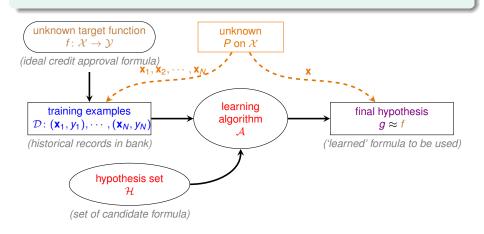
learning is PAC-possible if enough statistical data and finite  $|\mathcal{H}|$ 

Why Can Machines Learn?

## Lecture 5: Training versus Testing

- Recap and Preview
- Effective Number of Lines
- Effective Number of Hypotheses
- Break Point
- 3 How Can Machines Learn?
- 4 How Can Machines Learn Better?

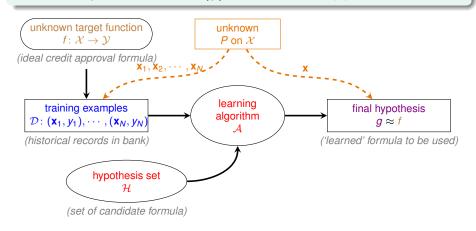
 $\text{if } |\mathcal{H}| = \textit{M} \text{ finite, } \textit{N} \text{ large enough,} \\ \text{for whatever } \textit{g} \text{ picked by } \mathcal{A}, \textit{E}_{\text{out}}(\textit{g}) \approx \textit{E}_{\text{in}}(\textit{g})$ 



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if  $\mathcal{A}$  finds one g with  $E_{\text{in}}(g) \approx 0$ ,

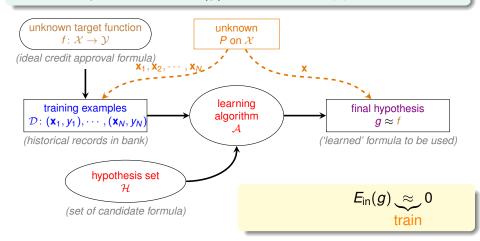
PAC guarantee for  $E_{\text{out}}(g) \approx 0 \Longrightarrow$  learning possible :-)



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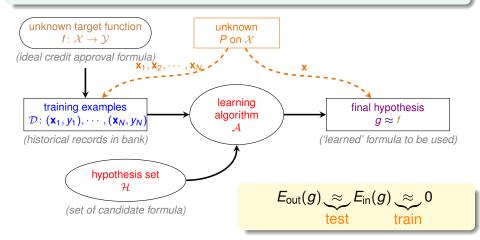
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if  $|\mathcal{H}| = M$  finite, N large enough, for whatever g picked by  $\mathcal{A}$ ,  $E_{\text{out}}(g) \approx E_{\text{in}}(g)$ 

if  ${\mathcal A}$  finds one g with  ${\mathcal E}_{\rm in}(g) \approx {\mathsf 0},$ 

PAC guarantee for  $E_{\text{out}}(g) \approx 0 \Longrightarrow$  learning possible :-)



$$\underbrace{g \approx f}_{\text{lecture 1}} \iff E_{\text{out}}(g) \approx 0$$

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$$E_{\text{in}}(g) \approx 0$$

lecture 2

for batch & supervised binary classification, 
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lecture 3 lecture 1

achieved through 
$$\underbrace{E_{\text{out}}(g) \approx E_{\text{in}}(g)}_{\text{lecture 4}}$$
 and  $\underbrace{E_{\text{in}}(g) \approx 0}_{\text{lecture 2}}$ 

lecture 4

## Two Central Questions

for batch & supervised binary classification, 
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$$\text{lecture 3} \qquad \text{lecture 1}$$
achieved through  $E_{\text{out}}(g) \approx E_{\text{in}}(g)$  and  $E_{\text{in}}(g) \approx 0$ 

#### learning split to two central questions:

1 can we make sure that  $E_{out}(g)$  is close enough to  $E_{in}(g)$ ?

lecture 2

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#### Training versus Testing

### Two Central Questions

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achieved through 
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#### learning split to two central questions:

- 1 can we make sure that  $E_{out}(g)$  is close enough to  $E_{in}(g)$ ?
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what role does M play for the two questions?

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small M

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#### small M

Yes!,
 P[BAD] ≤ 2 ⋅ M ⋅ exp(...)

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Yes!, many choices

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# large M

- No!,ℙ[BAD] ≤ 2 · M · exp(...)
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using the right M (or  $\mathcal{H}$ ) is important  $M = \infty$  doomed?

#### Known

$$\mathbb{P}\left[\left|E_{\mathsf{in}}(g) - E_{\mathsf{out}}(g)
ight| > \epsilon
ight] \leq 2 \cdot \c M \cdot \exp\left(-2\epsilon^2 N
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#### Todo

establish a finite quantity that replaces M

$$\mathbb{P}\left[\left| \mathsf{E}_{\mathsf{in}}(g) - \mathsf{E}_{\mathsf{out}}(g) \right| > \epsilon\right] \stackrel{?}{\leq} 2 \cdot \mathsf{m}_{\mathcal{H}} \cdot \exp\left(-2\epsilon^2 \mathsf{N}\right)$$

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$$\mathbb{P}\left[\left| \mathsf{E}_{\mathsf{in}}(g) - \mathsf{E}_{\mathsf{out}}(g) 
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• justify the feasibility of learning for infinite M

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- study  $m_{\mathcal{H}}$  to understand its trade-off for 'right'  $\mathcal{H}$ , just like M

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mysterious PLA to be fully resolved after 3 more lectures :-)

#### Fun Time

## Data size: how large do we need?

One way to use the inequality

$$\mathbb{P}\left[\left|E_{\mathsf{in}}(g) - E_{\mathsf{out}}(g)\right| > \epsilon\right] \leq \underbrace{2 \cdot M \cdot \exp\left(-2\epsilon^2 N\right)}_{\delta}$$

is to pick a tolerable difference  $\epsilon$  as well as a tolerable **BAD** probability  $\delta$ , and then gather data with size (N) large enough to achieve those tolerance criteria. Let  $\epsilon = 0.1$ ,  $\delta = 0.05$ , and M = 100. What is the data size needed?

**1** 215

**2** 415

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# Reference Answer: 2

We can simply express N as a function of those 'known' variables. Then, the needed  $N = \frac{1}{2\epsilon^2} \ln \frac{2M}{\delta}$ .

$$\mathbb{P}\left[\left| \textit{E}_{\mathsf{in}}(\textit{g}) - \textit{E}_{\mathsf{out}}(\textit{g}) \right| > \epsilon\right] \leq 2 \cdot \textcolor{red}{\mathsf{M}} \cdot \exp\left(-2\epsilon^2 \textit{N}\right)$$

•  $\mathcal{B}AD$  events  $\mathcal{B}_m$ :  $|E_{in}(h_m) - E_{out}(h_m)| > \epsilon$ 

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- worst case: all B<sub>m</sub> non-overlapping

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

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**union bound**

where did uniform bound fail to consider for  $M = \infty$ ?

# Where Did Uniform Bound Fail?

union bound 
$$\mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \ldots + \mathbb{P}[\mathcal{B}_M]$$

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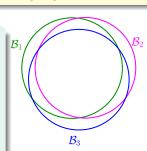
•  $\mathcal{B}$ AD events  $\mathcal{B}_m$ :  $|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon$  overlapping for similar hypotheses  $h_1 \approx h_2$ 

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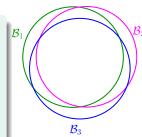
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to account for overlap, can we group similar hypotheses by kind?

# How Many Lines Are There? (1/2)

$$\mathcal{H} = \left\{ \mathsf{all\ lines\ in\ } \mathbb{R}^2 
ight\}$$

• how many lines?  $\infty$ 

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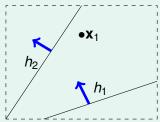
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**2 kinds**: 
$$h_1$$
-like( $\mathbf{x}_1$ ) =  $\circ$  or  $h_2$ -like( $\mathbf{x}_1$ ) =  $\times$ 

## How Many Lines Are There? (2/2)

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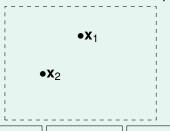
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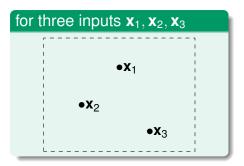




one input: 2; two inputs: 4; three inputs?

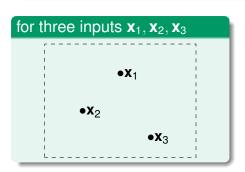
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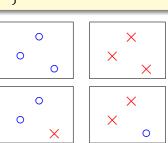


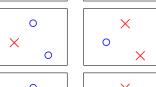
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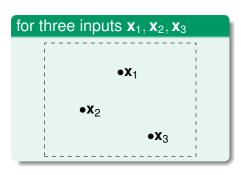




X

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8:

0

× × 0

× .

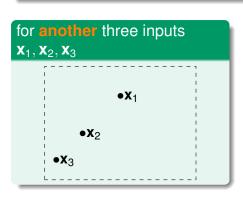
X

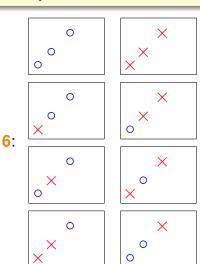
always 8 for three inputs?

X

# How Many Kinds of Lines for Three Inputs? (2/2)

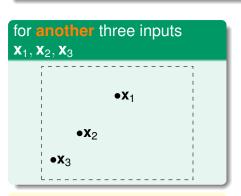
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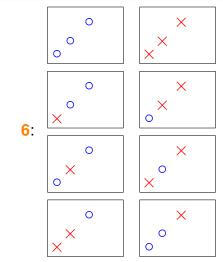


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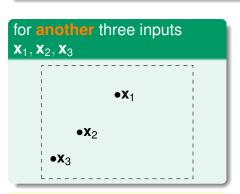


'fewer than 8' when degenerate (e.g. collinear or same inputs)

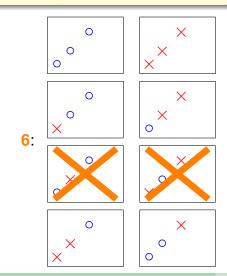


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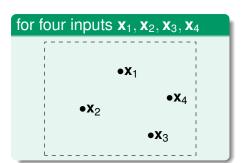


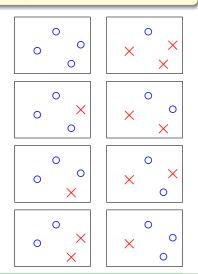
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## How Many Kinds of Lines for Four Inputs?

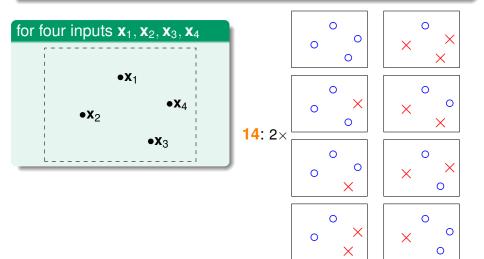
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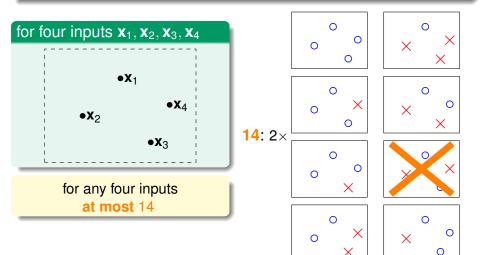
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maximum kinds of lines with respect to N inputs  $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N$   $\iff$  effective number of lines

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lines in 2D			
N effective(N)			
1	2		
2	4		
3	8		
4	14 < 2 <sup>N</sup>		

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• must be  $\leq 2^N$  (why?)

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- · wish:

$$\begin{split} & \mathbb{P}\left[\left| \textit{E}_{\mathsf{in}}(g) - \textit{E}_{\mathsf{out}}(g) \right| > \epsilon\right] \\ \leq & 2 \cdot \mathsf{effective}(\textit{N}) \cdot \mathsf{exp}\left(-2\epsilon^2\textit{N}\right) \end{split}$$

#### lines in 2D

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- finite 'grouping' of infinitely-many lines  $\in \mathcal{H}$
- wish:

$$\mathbb{P}\left[\left|E_{\mathsf{in}}(g) - E_{\mathsf{out}}(g)\right| > \epsilon\right] \\ \leq 2 \cdot \mathsf{effective}(N) \cdot \exp\left(-2\epsilon^2 N\right)$$

#### lines in 2D

N	effective(N)	
1	2	
2	4	
3	8	
4	$14 < 2^N$	

- if (1) effective (N) can replace M and
  - (2) effective(N)  $\ll 2^N$

learning possible with infinite lines :-)

#### Fun Time

What is the effective number of lines for five inputs  $\in \mathbb{R}^2$ ?

- **1**4

**2** 16

- 3 22

4 32

#### Fun Time

### What is the effective number of lines for five inputs $\in \mathbb{R}^2$ ?

**1**4

**2** 16

3 22

4 32

# Reference Answer: (3)

If you put the inputs roughly around a circle, you can then pick any consecutive inputs to be on one side of the line, and the other inputs to be on the other side. The procedure leads to effectively 22 kinds of lines, which is **much** smaller than  $2^5 = 32$ . You shall find it difficult to generate more kinds by varying the inputs, and we will give a formal proof in future lectures.

•x<sub>1</sub> •x<sub>5</sub> •x<sub>4</sub>

$$\mathcal{H} = \{ \text{hypothesis } h \colon \mathcal{X} \to \{\times, \circ\} \}$$

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call

$$h(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = (h(\mathbf{x}_1), h(\mathbf{x}_2), \dots, h(\mathbf{x}_N)) \in \{\times, \circ\}^N$$

a **dichotomy**: hypothesis 'limited' to the eyes of  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ 

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$$\mathcal{H} = \{\text{hypothesis } h \colon \mathcal{X} \to \{\times, \circ\}\}$$

call

$$h(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)=(h(\mathbf{x}_1),h(\mathbf{x}_2),\ldots,h(\mathbf{x}_N))\in\{\times,\circ\}^N$$

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•  $\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ : all dichotomies 'implemented' by  $\mathcal{H}$  on  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ 

	hypotheses ${\cal H}$	dichotomies $\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$
e.g.	all lines in $\mathbb{R}^2$	{0000,000×,00××,}
size	possibly infinite	upper bounded by 2 <sup>N</sup>

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	hypotheses ${\cal H}$	dichotomies $\mathcal{H}(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)$
e.g.	all lines in $\mathbb{R}^2$	{0000,000×,00××,}
size	possibly infinite	upper bounded by 2 <sup>N</sup>

$$|\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)|$$
: candidate for **replacing**  $M$ 

•  $|\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)|$ : depend on inputs  $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ 

- |\(\mathcal{H}(\mathbf{x}\_1, \mathbf{x}\_2, ..., \mathbf{x}\_N)\)|: depend on inputs
   (\mathbf{x}\_1, \mathbf{x}\_2, ..., \mathbf{x}\_N)
- growth function: remove dependence by taking max of all possible (x<sub>1</sub>, x<sub>2</sub>,...,x<sub>N</sub>)

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

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1	lines in 2D		
ı	Ν	$m_{\mathcal{H}}(N)$	
ı	1	2	
ı	2	4	
l	3	$\max(\ldots,6,8) \\ = 8$	
	4	14 < 2 <sup>N</sup>	

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finite, upper-bounded by 2<sup>N</sup>

how to 'calculate' the growth function?

## lines in 2D $m_{\mathcal{H}}(N)$ 2 3 $max(\ldots,6,8)$ = 8 $14 < 2^N$

4

$$h(x) = -1$$

$$x$$

$$x_1$$

$$x_2$$

$$x_3$$

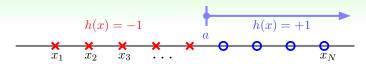
$$x_3$$

$$x_N$$

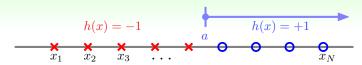
$$h(x) = +1$$

$$x_N$$

- $\mathcal{X} = \mathbb{R}$  (one dimensional)
- $\mathcal{H}$  contains h, where each h(x) = sign(x a) for threshold a



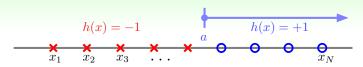
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$$m_{\mathcal{H}}(N) = N + 1$$



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<i>X</i> <sub>1</sub>	<i>X</i> <sub>2</sub>	<i>X</i> <sub>3</sub>	<i>X</i> <sub>4</sub>
0	0	0	0
×	0	0	0
×	×	0	0
×	×	×	0
X	×	×	×

# Growth Function for Positive Rays

$$h(x) = -1$$

$$x_1 \quad x_2 \quad x_3 \quad \dots$$

$$h(x) = +1$$

$$a \quad b(x) = +1$$

$$x_1 \quad x_2 \quad x_3 \quad \dots$$

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- 'positive half' of 1D perceptrons

one dichotomy for  $a \in \text{each spot } (x_n, x_{n+1})$ :

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

$$(N+1) \ll 2^N$$
 when N large!

$$h(x) = -1$$

$$x_1 \quad x_2 \quad x_3 \quad \dots$$

$$h(x) = +1$$

$$h(x) = -1$$

$$x_1 \quad x_2 \quad x_3 \quad \dots$$

- $\mathcal{X} = \mathbb{R}$  (one dimensional)
- $\mathcal{H}$  contains h, where each h(x) = +1 iff  $x \in [\ell, r)$ , -1 otherwise

$$h(x) = -1$$

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- $\mathcal{H}$  contains h, where each h(x) = +1 iff  $x \in [\ell, r)$ , -1 otherwise

### one dichotomy for each 'interval kind'

$$m_{\mathcal{H}}(N) = \underbrace{\begin{pmatrix} N+1 \\ 2 \end{pmatrix}}_{\text{interval ends in } N+1 \text{ spots}} + \underbrace{1}_{\text{all } \times}_{\text{all } \times}$$

$$= \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

$$h(x) = -1$$

$$x_1 \quad x_2 \quad x_3 \quad \dots$$

$$h(x) = +1$$

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<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>
0	X	X	×
0	0	×	×
0	0	0	×
0	0	0	0
×	0	×	×
×	0	0	×
×	0	0	0
×	×	0	×
×	×	0	0
×	×	×	0
×	×	×	×

$$h(x) = -1$$

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$$(\frac{1}{2}N^2 + \frac{1}{2}N + 1) \ll 2^N$$
 when N large!

<i>X</i> <sub>1</sub>	<i>X</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>X</i> <sub>4</sub>
0	X	×	×
0	0	×	×
0	0	0	×
0	0	0	0
×	0	X	×
×	0	0	×
×	0	0	0
×	X	0	×
×	X	0	0
×	×	×	0
×	×	×	×





convex region in blue

non-convex region

- $\mathcal{X} = \mathbb{R}^2$  (two dimensional)
- $\mathcal{H}$  contains h, where  $h(\mathbf{x}) = +1$  iff  $\mathbf{x}$  in a convex region, -1 otherwise





convex region in blue

non-convex region

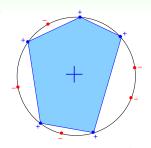
- $\mathcal{X} = \mathbb{R}^2$  (two dimensional)
- $\mathcal{H}$  contains h, where  $h(\mathbf{x}) = +1$  iff x in a convex region, -1 otherwise

what is  $m_{\mathcal{H}}(N)$ ?

one possible set of N inputs:
 x<sub>1</sub>, x<sub>2</sub>,..., x<sub>N</sub> on a big circle

- one possible set of N inputs:
   x<sub>1</sub>, x<sub>2</sub>,..., x<sub>N</sub> on a big circle
- every dichotomy can be implemented by H using a convex region slightly extended from contour of positive inputs

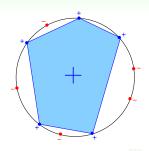
$$m_{\mathcal{H}}(N) = 2^N$$



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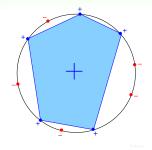
• call those N inputs 'shattered' by  $\mathcal{H}$ 



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• call those N inputs 'shattered' by  $\mathcal{H}$ 



$$m_{\mathcal{H}}(N) = 2^N \Longleftrightarrow$$
 exists  $N$  inputs that can be shattered

#### Fun Time

Consider positive and negative rays as  $\mathcal{H}$ , which is equivalent to the perceptron hypothesis set in 1D. The hypothesis set is often called 'decision stump' to describe the shape of its hypotheses. What is the growth function  $m_{\mathcal{H}}(N)$ ?









#### Fun Time

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# Reference Answer: (3)

Two dichotomies when threshold in each of the N-1 'internal' spots; two dichotomies for the all- $\circ$  and all- $\times$  cases.

### The Four Growth Functions

- positive rays:
- positive intervals:
- convex sets:
- 2D perceptrons:

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

 $m_{\mathcal{H}}(N) < 2^N$  in some cases

### The Four Growth Functions

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

 $m_{\mathcal{H}}(N) < 2^N$  in some cases

## what if $m_{\mathcal{H}}(N)$ replaces M?

$$\mathbb{P}\left[\left|E_{\mathsf{in}}(g) - E_{\mathsf{out}}(g)\right| > \epsilon\right] \stackrel{?}{\leq} 2 \cdot m_{\mathcal{H}}(N) \cdot \exp\left(-2\epsilon^2 N\right)$$

polynomial: good; exponential: bad

### The Four Growth Functions

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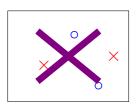
$$\mathbb{P}\left[\left|E_{\mathsf{in}}(g) - E_{\mathsf{out}}(g)\right| > \epsilon\right] \stackrel{?}{\leq} 2 \cdot m_{\mathcal{H}}(N) \cdot \exp\left(-2\epsilon^2 N\right)$$

polynomial: good; exponential: bad

for 2D or general perceptrons,  $m_{\mathcal{H}}(N)$  polynomial?

#### what do we know about 2D perceptrons now?

three inputs: 'exists' shatter; four inputs, 'for all' no shatter

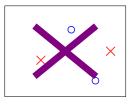


### what do we know about 2D perceptrons now?

three inputs: 'exists' shatter; four inputs, 'for all' no shatter

if no k inputs can be shattered by  $\mathcal{H}$ , call k a **break point** for  $\mathcal{H}$ 

• 
$$m_{\mathcal{H}}(k) < 2^k$$

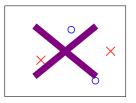


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if no k inputs can be shattered by  $\mathcal{H}$ , call k a **break point** for  $\mathcal{H}$ 

- $m_{\mathcal{H}}(k) < 2^k$
- k+1, k+2, k+3, ... also break points!

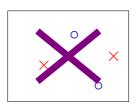


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- will study minimum break point k

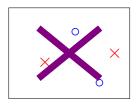


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if no k inputs can be shattered by  $\mathcal{H}$ , call k a **break point** for  $\mathcal{H}$ 

- $m_{\mathcal{H}}(k) < 2^k$
- k + 1, k + 2, k + 3, ... also break points!
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2D perceptrons: break point at 4

• positive rays:  $m_{\mathcal{H}}(\textit{N}) = \textit{N} + 1$  break point at 2

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

break point at 3

• convex sets:  $m_{\mathcal{H}}(N) = 2^N$ 

no break point

• 2D perceptrons:  $m_{\mathcal{H}}(N) < 2^N$  in some cases

break point at 4

• positive rays: 
$$m_{\mathcal{H}}(N) = N + 1 = O(N)$$
 break point at 2

• positive intervals:  $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1 = O(N^2)$ 

break point at 3

• convex sets:  $m_{\mathcal{H}}(\textit{N}) = 2^{\textit{N}}$ 

no break point

• 2D perceptrons:  $m_{\mathcal{H}}(N) < 2^N$  in some cases

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• convex sets:  $m_{\mathcal{H}}(N) = 2^N$ 

no break point

• 2D perceptrons:  $m_{\mathcal{H}}(N) < 2^N$  in some cases

break point at 4

#### conjecture:

- no break point:  $m_{\mathcal{H}}(N) = 2^N$  (sure!)
- break point k:  $m_{\mathcal{H}}(N) = O(N^{k-1})$

• positive rays:  $m_{\mathcal{H}}(N) = N + 1 = O(N)$  break point at 2

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

break point at 3

• convex sets:  $m_{\mathcal{H}}(N) = 2^N$ 

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break point at 4

#### conjecture:

- no break point:  $m_{\mathcal{H}}(N) = 2^N$  (sure!)
- break point k:  $m_{\mathcal{H}}(N) = O(N^{k-1})$

excited? wait for next lecture :-)

#### Fun Time

Consider positive and negative rays as  $\mathcal{H}$ , which is equivalent to the perceptron hypothesis set in 1D. As discussed in an earlier quiz question, the growth function  $m_{\mathcal{H}}(N) = 2N$ . What is the minimum break point for  $\mathcal{H}$ ?









#### **Fun Time**

Consider positive and negative rays as  $\mathcal{H}$ , which is equivalent to the perceptron hypothesis set in 1D. As discussed in an earlier quiz question, the growth function  $m_{\mathcal{H}}(N) = 2N$ . What is the minimum break point for  $\mathcal{H}$ ?







Reference Answer: (3)

At 
$$k = 3$$
,  $m_{\mathcal{H}}(k) = 6$  while  $2^k = 8$ .

# Summary

1 When Can Machines Learn?

# Lecture 4: Feasibility of Learning

Why Can Machines Learn?

## Lecture 5: Training versus Testing

Recap and Preview

two questions:  $E_{\mathsf{out}}(g) \approx E_{\mathsf{in}}(g)$ , and  $E_{\mathsf{in}}(g) \approx 0$ 

- Effective Number of Lines
  - at most 14 through the eye of 4 inputs
- Effective Number of Hypotheses
   at most m<sub>H</sub>(N) through the eye of N inputs
- Break Point when  $m_{\mathcal{H}}(N)$  becomes 'non-exponential'
- next:  $m_{\mathcal{H}}(N) = poly(N)$ ?
- 3 How Can Machines Learn?
- 4 How Can Machines Learn Better?