

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** $|\mathcal{H}|$

2 Why Can Machines Learn? 对于无穷大的 \mathcal{H}

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?

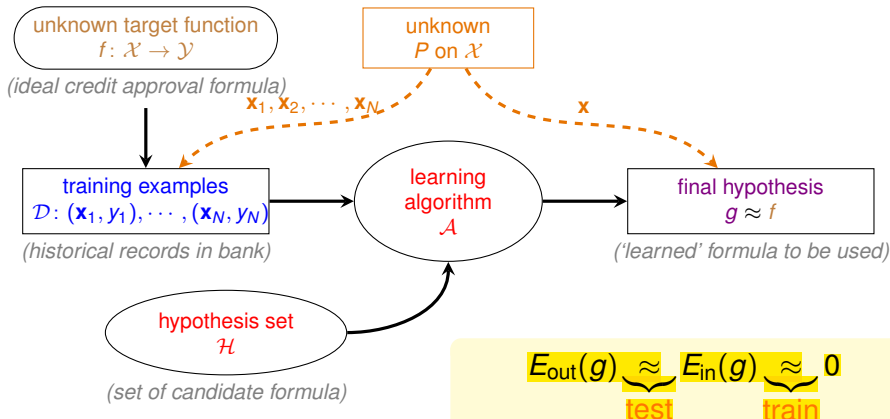
Recap: the 'Statistical' Learning Flow

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

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



Two Central Questions

for batch & supervised binary classification, $\underbrace{g \approx f}_{\text{lecture 1}} \iff E_{\text{out}}(g) \approx 0$
lecture 3

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

前四节课的总结

learning split to two central questions:

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

what role does $\underbrace{M}_{|\mathcal{H}|}$ play for the two questions?

Trade-off on M

- ① can we make sure that $E_{\text{out}}(g)$ is close enough to $E_{\text{in}}(g)$?
- ② can we make $E_{\text{in}}(g)$ small enough?

选择少，不见得可以满足上面的2

small M

- ① Yes!,
 $\mathbb{P}[\text{BAD}] \leq 2 \cdot M \cdot \exp(\dots)$
- ② No!, too few choices

large M

- ① No!,
 $\mathbb{P}[\text{BAD}] \leq 2 \cdot M \cdot \exp(\dots)$
- ② Yes!, many choices

using the right M (or \mathcal{H}) is important
 $M = \infty$ **doomed?**

其实不一定是个No，毕竟只是一个bound，比如即使是PLA里面是无限大，依然有较好的A

Preview

Known

对于所有的H有下式，低于一个则M=1，
即之前的公式

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

Todo

- establish **a finite quantity** that replaces M

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

- justify the feasibility of learning for infinite M
- study $m_{\mathcal{H}}$ to understand its trade-off for ‘right’ \mathcal{H} , just like M

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

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

is to pick a tolerable difference ϵ as well as a tolerable **BAD** probability δ , 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

③ 615

④ 815

Reference Answer: ②

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

Where Did M Come From?

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

- **BAD events** \mathcal{B}_m : $|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon$
- to give \mathcal{A} freedom of choice: bound $\mathbb{P}[\mathcal{B}_1 \text{ or } \mathcal{B}_2 \text{ or } \dots \mathcal{B}_M]$
- worst case: all \mathcal{B}_m non-overlapping

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

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

Where Did Uniform Bound Fail?

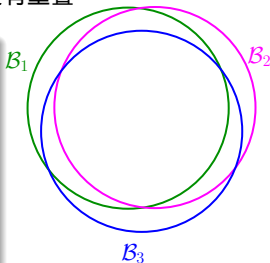
union bound $\mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \dots + \mathbb{P}[\mathcal{B}_M]$

等号成立的条件是，没有重叠

- **BAD events** \mathcal{B}_m : $|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon$

overlapping for similar hypotheses $h_1 \approx h_2$

- why? ① $E_{\text{out}}(h_1) \approx E_{\text{out}}(h_2)$
② for most \mathcal{D} , $E_{\text{in}}(h_1) = E_{\text{in}}(h_2)$
- union bound **over-estimating**

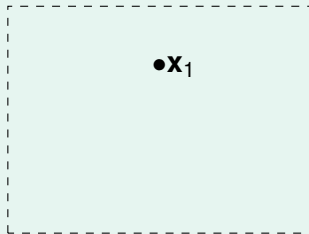


to account for overlap,
can we group similar hypotheses by **kind**?

How Many Lines Are There? (1/2)

$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

- how many lines? ∞
- how many **kinds of** lines if viewed from one input vector \mathbf{x}_1 ?

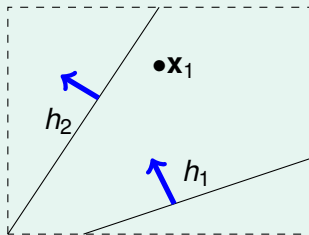


2 kinds: $h_1\text{-like}(\mathbf{x}_1) = \circ$ or $h_2\text{-like}(\mathbf{x}_1) = \times$

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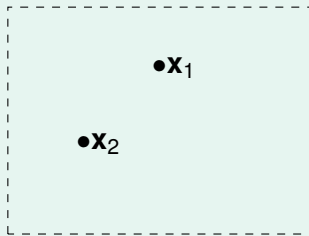


2 kinds: h_1 -like(\mathbf{x}_1) = \circ or h_2 -like(\mathbf{x}_1) = \times

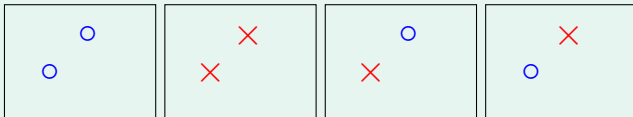
How Many Lines Are There? (2/2)

$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

- how many **kinds of** lines if viewed from two inputs $\mathbf{x}_1, \mathbf{x}_2$?



4:

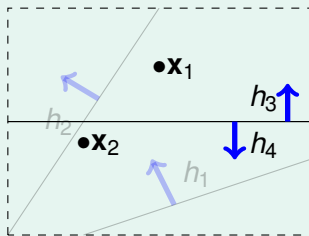


one input: 2; two inputs: 4; **three inputs?**

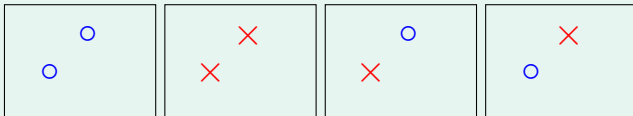
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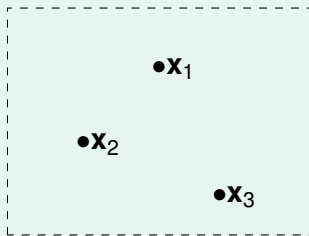


one input: 2; two inputs: 4; **three inputs?**

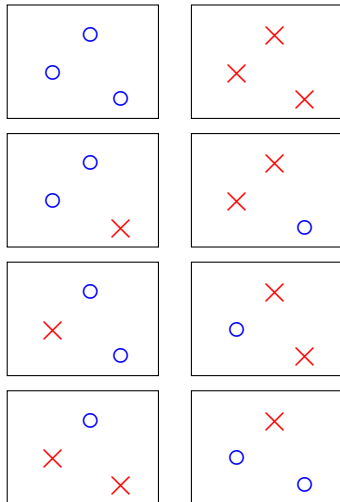
How Many Kinds of Lines for Three Inputs? (1/2)

$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

for three inputs $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$



8:

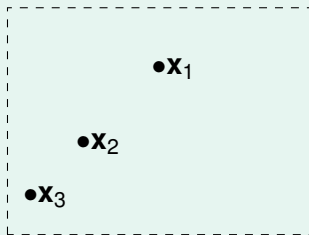


always 8 for three inputs?

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

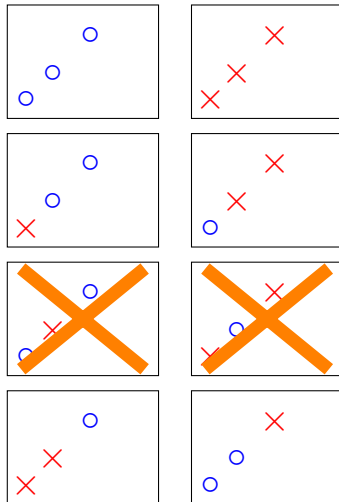
$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

for **another** three inputs
 $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$



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

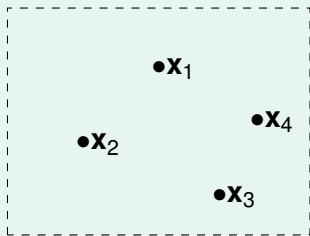
6:



How Many Kinds of Lines for Four Inputs?

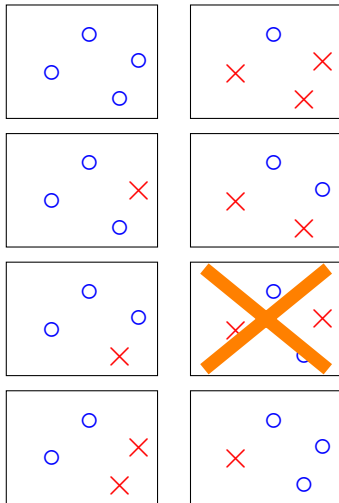
$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

for four inputs $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4$



for any four inputs
at most 14

14: $2 \times$



Effective Number of Lines

maximum kinds of lines with respect to N inputs $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$

\iff **effective number of lines**

- must be $\leq 2^N$ (why?)
- finite 'grouping' of infinitely-many lines $\in \mathcal{H}$
- wish:

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

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 :-)

怎么对应到P(BAD)问题呢？

Fun Time

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

① 14

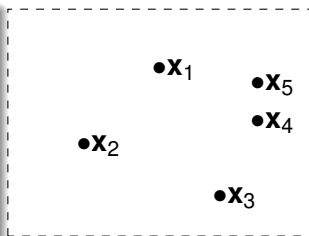
② 16

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.



考虑凸多边形？正多边形，应为考虑最大，不能共线（为什么？）

Dichotomies: Mini-hypotheses

$$\mathcal{H} = \{\text{hypothesis } h: \mathcal{X} \rightarrow \{\times, \circ\}\}$$

- 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 $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$

- $\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$:

all dichotomies ‘implemented’ by \mathcal{H} on $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$

对应到dichotomies来分类

	hypotheses \mathcal{H}	dichotomies $\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$
e.g.	all lines in \mathbb{R}^2	$\{\circ\circ\circ\circ, \circ\circ\circ\times, \circ\circ\times\times, \dots\}$
size	possibly infinite	upper bounded by 2^N

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

Growth Function

- $|\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)|$: depend on inputs $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$
- growth function:
remove dependence by **taking max of all possible $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$**

N的成长函数

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

各种共线会少一些

- finite, upper-bounded by 2^N

lines in 2D

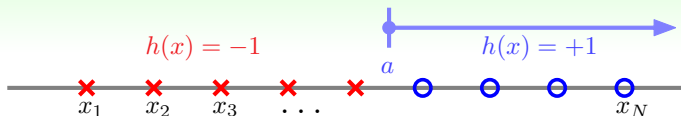
N	$m_{\mathcal{H}}(N)$
1	2
2	4
3	$\max(\dots, 6, 8)$ $= 8$
4	$14 < 2^N$

upper bound

how to 'calculate' the growth function?

\mathbf{x}_i 是选定的所以，为了消除依赖（对以后理论不利，消除之），取max

Growth Function for Positive Rays



找到一种 $h(x)$? 满足 ?

- $\mathcal{X} = \mathbb{R}$ (one dimensional)
- \mathcal{H} contains h , where **each** $h(x) = \text{sign}(x - a)$ **for threshold** a
- 'positive half' of 1D perceptrons

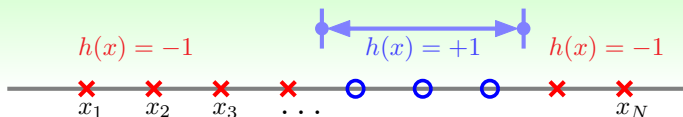
one dichotomy for $a \in$ each spot (x_n, x_{n+1}) :

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

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

x_1	x_2	x_3	x_4
○	○	○	○
×	○	○	○
×	×	○	○
×	×	×	○
×	×	×	×

Growth Function for Positive Intervals



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

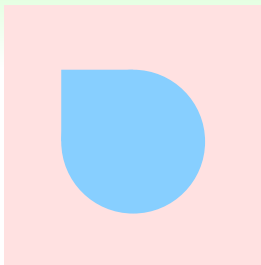
one dichotomy for each 'interval kind'

$$\begin{aligned}
 m_{\mathcal{H}}(N) &= \underbrace{\binom{N+1}{2}}_{\text{interval ends in } N+1 \text{ spots}} + \underbrace{1}_{\text{all } \times} \quad \text{放在一个区域} \\
 &= \frac{1}{2}N^2 + \frac{1}{2}N + 1
 \end{aligned}$$

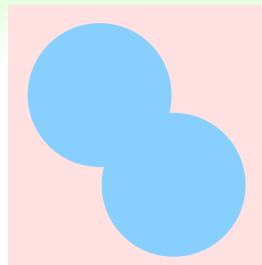
x_1	x_2	x_3	x_4
o	x	x	x
o	o	x	x
o	o	o	x
o	o	o	o
x	o	x	x
x	o	o	x
x	o	o	o
x	x	o	x
x	x	o	o
x	x	x	o
x	x	x	x

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

Growth Function for Convex Sets (1/2)



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

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

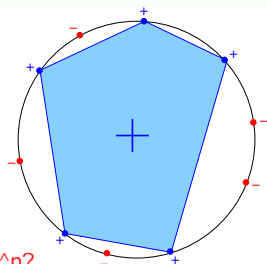
Growth Function for Convex Sets (2/2)

- one possible set of N inputs: $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ on a big circle
- every dichotomy can be implemented** by \mathcal{H} using a convex region slightly extended from **contour of positive inputs**

$$m_{\mathcal{H}}(N) = 2^N \quad \text{为什么是 } 2^N$$

答: $C_n + C_{n-1} + \dots + C_0 = 2^n$

- call those N inputs **'shattered'** by \mathcal{H}



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

1 N

2 $N + 1$

3 $2N$

4 2^N

$2(n-1)+2$ 后面的是全正全负两种情况

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:

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

- positive intervals:

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

- convex sets:

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

- 2D perceptrons:

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

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

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

polynomial: good; exponential: bad

for 2D or general perceptrons,

$m_{\mathcal{H}}(N)$ **polynomial?**

既然之前证明了PLA是有效的，那在这里证明的又是什么呢？

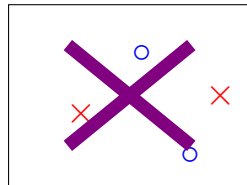
Break Point of \mathcal{H}

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}

- $m_{\mathcal{H}}(k) < 2^k$ 如果 k 是break point的话, 那么:
- $k + 1, k + 2, k + 3, \dots$ also break points!
- will study **minimum break point k**



break point 就是他的 dichotomies 不是 2^k , 开始降下来 (有希望)

2D perceptrons: **break point at 4**

对于线性分

有点像平面上 K 条直线可以讲平面分成多少部分?

The Four Break Points

- 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: $m_{\mathcal{H}}(N) = 2^N$
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 : $m_{\mathcal{H}}(N) = O(N^{k-1})$ 这么强? !
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} ?

1 1

2 2

3 3

4 4

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

2 Why Can Machines Learn?

Lecture 5: Training versus Testing

- Recap and Preview

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

- Effective Number of Lines

at most 14 through the eye of 4 inputs

- Effective Number of Hypotheses

at most $m_{\mathcal{H}}(N)$ through the eye of N inputs

- Break Point

when $m_{\mathcal{H}}(N)$ becomes 'non-exponential'

- next:** $m_{\mathcal{H}}(N) = \text{poly}(N)$?

3 How Can Machines Learn?

4 How Can Machines Learn Better?