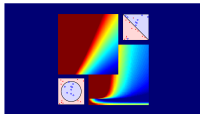


Machine Learning Foundations

(機器學習基石)



Lecture 6: Theory of Generalization

Hsuan-Tien Lin (林軒田)

htlin@csie.ntu.edu.tw

Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)



Roadmap

- 1 When Can Machines Learn?
- 2 **Why** Can Machines Learn?

Lecture 5: Training versus Testing

effective price of choice in training: **(wishfully)**
growth function $m_{\mathcal{H}}(N)$ with **a break point**

Lecture 6: Theory of Generalization

- Restriction of Break Point
- Bounding Function: Basic Cases
- Bounding Function: Inductive Cases
- A Pictorial Proof

- 3 How Can Machines Learn?
- 4 How Can Machines Learn Better?

The Four Break Points

growth function $m_{\mathcal{H}}(N)$: max number of dichotomies

- positive rays: $m_{\mathcal{H}}(N) = N + 1$
 $\circ \times$ $m_{\mathcal{H}}(2) = 3 < 2^2$: break point at 2
- positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$
 $\circ \times \circ$ $m_{\mathcal{H}}(3) = 7 < 2^3$: break point at 3
- convex sets: $m_{\mathcal{H}}(N) = 2^N$
 $\circ \quad \times$
 $\times \quad \circ$ $m_{\mathcal{H}}(N) = 2^N$ always: no break point
- 2D perceptrons: $m_{\mathcal{H}}(N) < 2^N$ in some cases
 $\times \quad \circ \quad \times$ $m_{\mathcal{H}}(4) = 14 < 2^4$: break point at 4

break point $k \implies$ break point $k + 1, \dots$

what else?

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

1 dichotomy , shatter any two points? **no**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

2 dichotomies, shatter any two points? **no**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

3 dichotomies, shatter any two points? **no**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

4 dichotomies, shatter any two points? **yes**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○
○	×	×

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

4 dichotomies, shatter any two points? **no**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○
×	○	○

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

5 dichotomies, shatter any two points? **yes**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○
×	○	○
×	○	×

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible** = 3)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

5 dichotomies, shatter any two points? **yes**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○
×	○	○
×	×	○

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible** = 3)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

5 dichotomies, shatter any two points? **yes**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○
×	○	○
×	×	×

Restriction of Break Point (1/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)

maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$ and $k = 2$?

maximum possible so far: **4 dichotomies**

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
○	○	○
○	○	×
○	×	○
×	○	○
⋮-(⋮-(⋮-(

Restriction of Break Point (2/2)

what 'must be true' when **minimum break point** $k = 2$

- $N = 1$: every $m_{\mathcal{H}}(N) = 2$ by definition
- $N = 2$: every $m_{\mathcal{H}}(N) < 4$ by definition
(so **maximum possible = 3**)
- $N = 3$: **maximum possible = 4** $\ll 2^3$

—break point k **restricts maximum possible** $m_{\mathcal{H}}(N)$ **a lot** for $N > k$

idea:

$$m_{\mathcal{H}}(N)$$

$$\leq \text{maximum possible } m_{\mathcal{H}}(N) \text{ given } k$$

$$\leq \text{poly}(N)$$

Fun Time

When minimum break point $k = 1$, what is the maximum possible $m_{\mathcal{H}}(N)$ when $N = 3$?

① 1

② 2

③ 4

④ 8

Reference Answer: ①

Because $k = 1$, the hypothesis set cannot even shatter one point. Thus, every 'column' of the table cannot contain both \circ and \times . Then, after including the first dichotomy, it is not possible to include any other different dichotomy. Thus, the maximum possible $m_{\mathcal{H}}(N)$ is 1.

\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
\circ	\times	\circ
\circ	\times	\times

Bounding Function

bounding function $B(N, k)$:

maximum possible $m_{\mathcal{H}}(N)$ when break point = k

- combinatorial quantity:
maximum number of length- N vectors with (\circ, \times)
while ‘**no shatter**’ any **length- k** subvectors
- irrelevant of the details of \mathcal{H}
e.g. $B(N, 3)$ bounds both
 - positive intervals ($k = 3$)
 - 1D perceptrons ($k = 3$)

new goal: $B(N, k) \leq \text{poly}(N)$?

Table of Bounding Function (1/4)

$B(N, k)$		k						
		1	2	3	4	5	6	...
N	1							
	2		3					
	3		4					
	4							
	5							
	6							
	⋮							

Known

- $B(2, 2) = 3$ (maximum < 4)
- $B(3, 2) = 4$ ('pictorial' proof previously)

Table of Bounding Function (2/4)

$B(N, k)$		k						
		1	2	3	4	5	6	...
N	1	1						
	2	1	3					
	3	1	4					
	4	1						
	5	1						
	6	1						
	⋮	⋮						

Known

- $B(N, 1) = 1$ (see previous quiz)

Table of Bounding Function (3/4)

$B(N, k)$		k						...
		1	2	3	4	5	6	
N	1	1	2	2	2	2	2	...
	2	1	3	4	4	4	4	...
	3	1	4		8	8	8	...
	4	1				16	16	...
	5	1					32	...
	6	1						...
	⋮	⋮						...

Known

- $B(N, k) = 2^N$ for $N < k$
—including all dichotomies not violating ‘breaking condition’

Table of Bounding Function (4/4)

$B(N, k)$		k						
		1	2	3	4	5	6	...
N	1	1	2	2	2	2	2	...
	2	1	3	4	4	4	4	...
	3	1	4	7	8	8	8	...
	4	1			15	16	16	...
	5	1				31	32	...
	6	1					63	...
	⋮	⋮						⋱

Known

- $B(N, k) = 2^N - 1$ for $N = k$
 — **removing a single dichotomy** satisfies 'breaking condition'

more than halfway done! :-)

Fun Time

For the 2D perceptrons, which of the following claim is true?

- 1 minimum break point $k = 2$
- 2 $m_{\mathcal{H}}(4) = 15$
- 3 $m_{\mathcal{H}}(N) < B(N, k)$ when $N = k =$ minimum break point
- 4 $m_{\mathcal{H}}(N) > B(N, k)$ when $N = k =$ minimum break point

Reference Answer: ③

As discussed previously, minimum break point for 2D perceptrons is 4, with $m_{\mathcal{H}}(4) = 14$. Also, note that $B(4, 4) = 15$. So bounding function $B(N, k)$ can be 'loose' in bounding $m_{\mathcal{H}}(N)$.

Estimating $B(4, 3)$

$B(N, k)$		k						
		1	2	3	4	5	6	...
N	1	1	2	2	2	2	2	...
	2	1	3	4	4	4	4	...
	3	1	4	7	8	8	8	...
	4	1		?	15	16	16	...
	5	1				31	32	...
	6	1					63	...
	⋮	⋮						⋱

Motivation

- $B(4, 3)$ shall be related to $B(3, ?)$
—‘adding’ one point from $B(3, ?)$

next: reduce $B(4, 3)$ to $B(3, ?)$

'Achieving' Dichotomies of $B(4, 3)$

after checking all 2^{2^4} sets of dichotomies, **the winner is ...**

	x_1	x_2	x_3	x_4
01	○	○	○	○
02	×	○	○	○
03	○	×	○	○
04	○	○	×	○
05	○	○	○	×
06	×	×	○	×
07	×	○	×	○
08	×	○	○	×
09	○	×	×	○
10	○	×	○	×
11	○	○	×	×

$B(N, k)$	k					
	1	2	3	4	5	6
1	1	2	2	2	2	2
2	1	3	4	4	4	4
3	1	4	7	8	8	8
N 4	1		11	15	16	16
5	1				31	32
6	1					63

how to reduce $B(4, 3)$ to $B(3, ?)$ cases?

Reorganized Dichotomies of $B(4, 3)$

after checking all 2^{2^4} sets of dichotomies, **the winner is ...**

	x_1	x_2	x_3	x_4
01	o	o	o	o
02	x	o	o	o
03	o	x	o	o
04	o	o	x	o
05	o	o	o	x
06	x	x	o	x
07	x	o	x	o
08	x	o	o	x
09	o	x	x	o
10	o	x	o	x
11	o	o	x	x



	x_1	x_2	x_3	x_4
01	o	o	o	o
05	o	o	o	x
02	x	o	o	o
08	x	o	o	x
03	o	x	o	o
10	o	x	o	x
04	o	o	x	o
11	o	o	x	x
06	x	x	o	x
07	x	o	x	o
09	o	x	x	o

orange: pair; purple: single

Estimating Part of $B(4, 3)$ (1/2)

$$B(4, 3) = 11 = 2\alpha + \beta$$

	\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
α	○	○	○
	×	○	○
	○	×	○
	○	○	×
β	×	×	○
	×	○	×
	○	×	×

- $\alpha + \beta$: dichotomies on $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$
- $B(4, 3)$ 'no shatter' any 3 inputs
 $\implies \alpha + \beta$ 'no shatter' any 3

	\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3	\mathbf{x}_4
2α	○	○	○	○
	○	○	○	×
	×	○	○	○
	×	○	○	×
	○	×	○	○
	○	×	○	×
	○	○	×	○
	○	○	×	×
β	×	×	○	×
	×	○	×	○
	○	×	×	○

$$\alpha + \beta \leq B(3, 3)$$

Estimating Part of $B(4, 3)$ (2/2)

$$B(4, 3) = 11 = 2\alpha + \beta$$

	\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3
α	○	○	○
	×	○	○
	○	×	○
	○	○	×

- α : dichotomies on $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ with \mathbf{x}_4 **paired**
- $B(4, 3)$ 'no shatter' any 3 inputs $\implies \alpha$ 'no shatter' any 2

	\mathbf{x}_1	\mathbf{x}_2	\mathbf{x}_3	\mathbf{x}_4
2α	○	○	○	○
	○	○	○	×
	×	○	○	○
	×	○	○	×
	○	×	○	○
	○	×	○	×
	○	○	×	○
	○	○	×	×
β	×	×	○	×
	×	○	×	○
	○	×	×	○

$$\alpha \leq B(3, 2)$$

Putting It All Together

$$B(4, 3) = 2\alpha + \beta$$

$$\alpha + \beta \leq B(3, 3)$$

$$\alpha \leq B(3, 2)$$

$$\Rightarrow B(4, 3) \leq B(3, 3) + B(3, 2)$$

$B(N, k)$		k					
		1	2	3	4	5	6
N	1	1	2	2	2	2	2
	2	1	3	4	4	4	4
	3	1	4	7	8	8	8
	4	1	≤ 5	11	15	16	16
	5	1	≤ 6	≤ 16	≤ 26	31	32
	6	1	≤ 7	≤ 22	≤ 42	≤ 57	63

now have **upper bound** of bounding function

Putting It All Together

$$B(N, k) = 2\alpha + \beta$$

$$\alpha + \beta \leq B(N - 1, k)$$

$$\alpha \leq B(N - 1, k - 1)$$

$$\Rightarrow B(N, k) \leq B(N - 1, k) + B(N - 1, k - 1)$$

$B(N, k)$		k					
		1	2	3	4	5	6
N	1	1	2	2	2	2	2
	2	1	3	4	4	4	4
	3	1	4	7	8	8	8
	4	1	≤ 5	11	15	16	16
	5	1	≤ 6	≤ 16	≤ 26	31	32
	6	1	≤ 7	≤ 22	≤ 42	≤ 57	63

now have **upper bound** of bounding function

Bounding Function: The Theorem

$$B(N, k) \leq \underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}_{\text{highest term } N^{k-1}}$$

- simple induction using **boundary and inductive formula**
- for fixed k , $B(N, k)$ upper bounded by $\text{poly}(N)$
 $\implies m_{\mathcal{H}}(N)$ is $\text{poly}(N)$ if **break point exists**

‘ \leq ’ can be ‘=’ actually,
go play and prove it if math lover! :-)

The Three Break Points

$$B(N, k) \leq \underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}_{\text{highest term } N^{k-1}}$$

- positive rays: $m_{\mathcal{H}}(N) = N + 1 \leq N + 1$
 $\circ \times$ $m_{\mathcal{H}}(2) = 3 < 2^2$: break point at 2
- positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1 \leq \frac{1}{2}N^2 + \frac{1}{2}N + 1$
 $\circ \times \circ$ $m_{\mathcal{H}}(3) = 7 < 2^3$: break point at 3
- 2D perceptrons: $m_{\mathcal{H}}(N) = ? \leq \frac{1}{6}N^3 + \frac{5}{6}N + 1$
 $\times \circ \times$ $m_{\mathcal{H}}(4) = 14 < 2^4$: break point at 4

can bound $m_{\mathcal{H}}(N)$ by only **one break point**

Fun Time

For 1D perceptrons (positive and negative rays), we know that $m_{\mathcal{H}}(N) = 2N$. Let k be the minimum break point. Which of the following is not true?

- ① $k = 3$
- ② for some integers $N > 0$, $m_{\mathcal{H}}(N) = \sum_{i=0}^{k-1} \binom{N}{i}$
- ③ for all integers $N > 0$, $m_{\mathcal{H}}(N) = \sum_{i=0}^{k-1} \binom{N}{i}$
- ④ for all integers $N > 2$, $m_{\mathcal{H}}(N) < \sum_{i=0}^{k-1} \binom{N}{i}$

Reference Answer: ③

The proof is generally trivial by listing the definitions. For ②, $N = 1$ or 2 gives the equality. One thing to notice is ④: the upper bound can be 'loose'.

BAD Bound for General \mathcal{H}

want:

$$\mathbb{P}\left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\right] \leq 2 m_{\mathcal{H}}(N) \cdot \exp\left(-2 \epsilon^2 N\right)$$

actually, when N large enough,

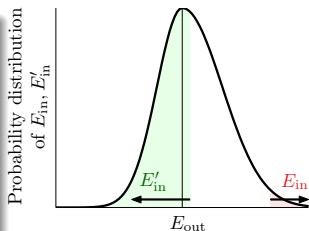
$$\mathbb{P}\left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\right] \leq 2 \cdot 2m_{\mathcal{H}}(2N) \cdot \exp\left(-2 \cdot \frac{1}{16} \epsilon^2 N\right)$$

next: **sketch** of proof

Step 1: Replace E_{out} by E'_{in}

$$\begin{aligned} & \frac{1}{2} \mathbb{P} \left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon \right] \\ \leq & \mathbb{P} \left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E'_{\text{in}}(h)| > \frac{\epsilon}{2} \right] \end{aligned}$$

- $E_{\text{in}}(h)$ finitely many, $E_{\text{out}}(h)$ infinitely many
—replace the evil E_{out} first
- how? sample verification set \mathcal{D}' of size N to calculate E'_{in}
- BAD h of $E_{\text{in}} - E_{\text{out}}$
probably \implies BAD h of $E_{\text{in}} - E'_{\text{in}}$

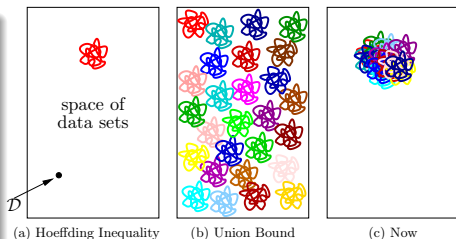


evil E_{out} removed by
verification with 'ghost data'

Step 2: Decompose \mathcal{H} by Kind

$$\begin{aligned} \text{BAD} &\leq 2\mathbb{P}\left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E'_{\text{in}}(h)| > \frac{\epsilon}{2}\right] \\ &\leq 2m_{\mathcal{H}}(2N)\mathbb{P}\left[\text{fixed } h \text{ s.t. } |E_{\text{in}}(h) - E'_{\text{in}}(h)| > \frac{\epsilon}{2}\right] \end{aligned}$$

- E_{in} with \mathcal{D} , E'_{in} with \mathcal{D}'
—now $m_{\mathcal{H}}$ comes to play
- how? infinite \mathcal{H} becomes
 $|\mathcal{H}(\mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{x}'_1, \dots, \mathbf{x}'_N)|$
kinds
- union bound on $m_{\mathcal{H}}(2N)$ kinds

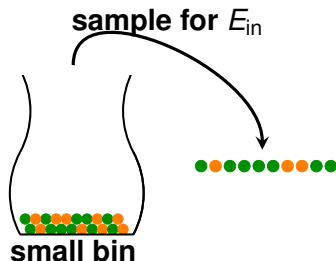


use $m_{\mathcal{H}}(2N)$ to calculate BAD-overlap properly

Step 3: Use Hoeffding without Replacement

$$\begin{aligned} \text{BAD} &\leq 2m_{\mathcal{H}}(2N)\mathbb{P}\left[\text{fixed } h \text{ s.t. } |E_{\text{in}}(h) - E'_{\text{in}}(h)| > \frac{\epsilon}{2}\right] \\ &\leq 2m_{\mathcal{H}}(2N) \cdot 2 \exp\left(-2\left(\frac{\epsilon}{4}\right)^2 N\right) \end{aligned}$$

- consider bin of $2N$ examples, choose N for E_{in} , leave others for E'_{in}
 $|E_{\text{in}} - E'_{\text{in}}| > \frac{\epsilon}{2} \Leftrightarrow \left|E_{\text{in}} - \frac{E_{\text{in}} + E'_{\text{in}}}{2}\right| > \frac{\epsilon}{4}$
- so? just 'smaller bin', 'smaller ϵ ', and Hoeffding without replacement



use Hoeffding after zooming to fixed h

That's All!

Vapnik-Chervonenkis (VC) bound:

$$\begin{aligned} & \mathbb{P}\left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\right] \\ & \leq 4m_{\mathcal{H}}(2N) \exp\left(-\frac{1}{8}\epsilon^2 N\right) \end{aligned}$$

- replace E_{out} by E'_{in}
- decompose \mathcal{H} by kind
- use Hoeffding without replacement

2D perceptrons:

- break point? 4
- $m_{\mathcal{H}}(N)$? $O(N^3)$

learning with 2D perceptrons feasible! :-)

Fun Time

For positive rays, $m_{\mathcal{H}}(N) = N + 1$. Plug it into the VC bound for $\epsilon = 0.1$ and $N = 10000$. What is VC bound of BAD events?

$$\mathbb{P}\left[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\right] \leq 4m_{\mathcal{H}}(2N) \exp\left(-\frac{1}{8}\epsilon^2 N\right)$$

- 1 2.77×10^{-87}
- 2 5.54×10^{-83}
- 3 2.98×10^{-1}
- 4 2.29×10^2

Reference Answer: 3

Simple calculation. Note that the BAD probability bound is not very small even with 10000 examples.

Summary

- 1 When Can Machines Learn?
- 2 **Why** Can Machines Learn?

Lecture 5: Training versus Testing

Lecture 6: Theory of Generalization

- Restriction of Break Point
break point 'breaks' consequent points
- Bounding Function: Basic Cases
 $B(N, k)$ **bounds** $m_{\mathcal{H}}(N)$ **with break point** k
- Bounding Function: Inductive Cases
 $B(N, k)$ **is** $\text{poly}(N)$
- A Pictorial Proof
 $m_{\mathcal{H}}(N)$ **can replace** M **with a few changes**

- **next: how to 'use' the break point?**

- 3 How Can Machines Learn?
- 4 How Can Machines Learn Better?