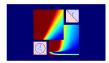
Machine Learning Foundations

(機器學習基石)



Lecture 6: Theory of Generalization

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Roadmap

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

Lecture 5: Training versus Testing

effective price of choice in training: (wishfully) growth function $m_H(N)$ 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: $m_{\mathcal{H}}(N) = N+1$ • × $m_{\mathcal{H}}(2) = 3 < 2^2$: break point at 2

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

 0×0 $m_{\mathcal{H}}(3) = 7 < 2^3$: break point at 3

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

$$\circ \overset{\circ}{\times} \overset{\times}{\circ} m_{\mathcal{H}}(N) = 2^N$$
 always: no break point

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

$$\times$$
 $\stackrel{\circ}{\sim}$ \times $m_{\mathcal{H}}(4) = 14 < 2^4$: break point at 4

break point $k \Longrightarrow$ break point k + 1, ... what else?

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every m_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

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every m_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
0	0	0
0	0	×

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every m_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
0	0	0
0	0	×
0	×	0

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

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

breakpoint=k等价于mH(k)<2^k且mH(K-1)=X^{K-1} 下面要讨论的是k+1的情况

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
0	0	0
0	0	×
0	×	0
-	×	

对于k+1的情况,任意k个x对不能有 2^k种,称为shatter

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every $m_H(N) < 4$ 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
0	0	0
0	0	×
0	×	0
×	0	0

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every $m_H(N) < 4$ 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	X 3
0	0	0
0	0	×
0	×	0
×	0	0
\rightarrow	-	

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every $m_H(N) < 4$ 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	X 3
0	0	0
0	0	×
0	×	0
×	0	0
\rightarrow	\rightarrow	

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every $m_H(N) < 4$ 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

X ₁	\mathbf{x}_2	X 3
0	0	0
0	0	×
0	×	0
×	0	0
\rightarrow	×	

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

- N = 1: every $m_{\mathcal{H}}(N) = 2$ by definition
- N = 2: every $m_H(N) < 4$ 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
0	0	0
0	0	×
0	×	0
×	0	0
:-(:-(:-(

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

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

—break point k restricts maximum possible $m_H(N)$ a lot for N > k

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

 $\leq poly(N)$

Fun Time

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



2 2



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	X 3
0	×	0
-	×	\rightarrow

Bounding Function

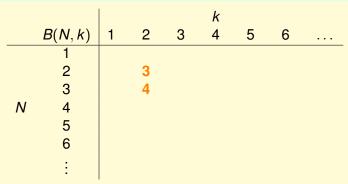
bounding function B(N, k):

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

- combinatorial quantity:
 maximum number of length-N vectors with (o, x)
 while 'no shatter' any length-k subvectors
- irrelevant of the details of H
 e.g. B(N,3) bounds both
 - positive intervals (k = 3)
 - 1D perceptrons (k = 3)

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

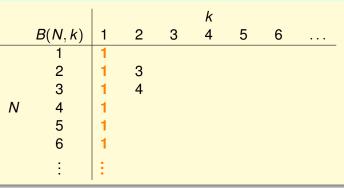
Table of Bounding Function (1/4)



Known

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

Table of Bounding Function (2/4)



Known

• B(N, 1) = 1 (see previous quiz)

Table of Bounding Function (3/4)

					k			
	B(N, k)	1	2	3	4	5	6	
	1	1	2	2	2	2	2	
	2	1	3	4	4	4	4	
	3	1	4		8	8	8	
Ν	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)

					k			
	B(N, 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	
Ν	4	1			15	16	16	
	5	1				31	32	
	6	1					63	
	:	:						$\langle \cdot, \cdot \rangle$

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)

					k			
	B(N, 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	
Ν	4	1		?	15	16	16	
	5	1				31	32	
	6	1					63	
	:	:						٠.,

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 224 sets of dichotomies, the winner is ...

	X ₁	\mathbf{x}_2	\mathbf{x}_3	\mathbf{x}_4	
01	0	0	0	0	
02	×	0	0	0	
03	0	×	0	0	
04	0	0	×	0	
05	0	0	0	×	
06	×	×	0	×	
07	×	0	×	0	
80	×	0	0	×	
09	0	×	×	0	
10	0	×	0	×	
11	0	0	×	×	

					k		
	B(N, 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
Ν	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 2²⁴ sets of dichotomies, the winner is ...

	X ₁	\mathbf{x}_2	\mathbf{x}_3	\mathbf{x}_4
01	0	0	0	0
02	×	0	0	0
03	0	×	0	0
04	0	0	×	0
05	0	0	0	×
06	×	×	0	×
07	×	0	×	0
80	×	0	0	×
09	0	×	×	0
10	0	×	0	×
11	0	0	×	×

_	_
=	$\overline{}$

		x ₁	X 2	x ₃	X ₄
Ī	01	0	0	0	0
	05	0	0	0	×
	02	×	0	0	0
	80	×	0	0	×
	03	0	×	0	0
	10	0	×	0	×
	04	0	0	×	0
	11	0	0	×	×
	06	×	×	0	×
	07	×	0	×	0
	09	0	×	×	0

orange: pair; purple: single

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

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

	X ₁	\mathbf{x}_2	\mathbf{x}_3
α	0	0	0
	×	0	0
	0	×	0
	0	0	×
β	×	×	0
	×	0	×
	0	×	×

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

	X ₁	x ₂	x ₃	x ₄
	0	0	0	0
	0	0	0	×
	×	0	0	0
2α	×	0	0	×
	0	×	0	0
	0	×	0	×
	0	0	×	0
	0	0	×	×
	×	×	0	×
β	×	0	×	0
	0	×	×	0

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

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

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

	X ₁	\mathbf{x}_2	\mathbf{x}_3
	0	0	0
α	×	0	0
	0	×	0
	0	0	×

- α: dichotomies on (x₁, x₂, x₃) with x₄ paired
- B(4,3) 'no shatter' any 3 inputs $\Rightarrow \alpha$ 'no shatter' any 2

	X 1	X 2	x ₃	x ₄
	0	0	0	0 X
	0	0	0	
	×	0	0	0
2α	×	0	0	×
	0	×	0	0
	0	×	0	×
	0	0	×	0
	0	0	×	×
	×	×	0	×
β	×	0	×	0
	0	×	×	0

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

Putting It All Together

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

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

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

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

					k		
	B(N, 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
Ν	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

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

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

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

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

					k		
	B(N, 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
Ν	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

$$B(N,k) \le \sum_{i=0}^{k-1} {N \choose i}$$
highest term N^{k-1}

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

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'≤' can be '=' actually, <sup>等号可以成立</sup>
go play and prove it if math lover! :-)
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The Three Break Points

$$B(N, k) \le \sum_{i=0}^{k-1} {N \choose i}$$
highest term N^{k-1}

• positive rays:
$$m_{\mathcal{H}}(N) = N + 1 \le N + 1$$

• × $m_{\mathcal{H}}(2) = 3 < 2^2$: break point at 2

- positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1 \le \frac{1}{2}N^2 + \frac{1}{2}N + 1$ • × • $m_{\mathcal{H}}(3) = 7 < 2^3$: break point at 3
- $\circ \times \circ$ $m_{\mathcal{H}}(3) = 7 < 2^{\circ}$: break point at 3

• 2D perceptrons:
$$m_{\mathcal{H}}(N) = ? \le \frac{1}{6}N^3 + \frac{5}{6}N + 1$$

$$\times$$
 $\stackrel{\circ}{\sim}$ \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?

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

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:

$$\mathbb{P}\left[\frac{\exists h}{\exists h} \in \mathcal{H} \text{ s.t. } |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\right] \leq 2 \quad m_{\mathcal{H}}(N) \cdot \exp\left(-2 - \epsilon^2 N\right)$$
 是不是放得有点大这个不等式,之前是对于所有的H

actually, when N large enough, ??

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

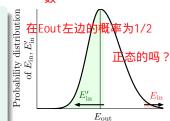
next: sketch of proof

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

这中是一个独立事件变成乘法P(在左边&XXX>epxl)
$$= \mathbb{P} \left[\exists h \in \mathcal{H} \text{ s.t. } \left| E_{\text{in}}(h) - E_{\text{out}}(h) \right| > \epsilon \right]$$

$$\leq \mathbb{P}\Big[\exists h \in \mathcal{H} \text{ s.t. } \big| E_{\mathsf{in}}(h) - E'_{\mathsf{in}}(h) \big| > \frac{\epsilon}{2}\Big]$$

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



由Hxxx不等式Ein'和Eout大概率接近

evil *E*_{out} removed by verification with 'ghost data'

Step 2: Decompose \mathcal{H} by Kind

化为有限种,Eout无限 BAD
$$\leq 2\mathbb{P}\Big[\frac{\exists h}{\exists h} \in \mathcal{H} \text{ s.t. } \big| E_{\text{in}}(h) - E_{\text{in}}'(h) \big| > \frac{\epsilon}{2} \Big]$$
 $\leq 2m_{\mathcal{H}}(2N)\mathbb{P}\Big[\text{fixed } h \text{ s.t. } \big| E_{\text{in}}(h) - E_{\text{in}}'(h) \big| > \frac{\epsilon}{2} \Big]$

- 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, \ldots, \mathbf{x}_N, \mathbf{x}'_1, \ldots, \mathbf{x}'_N)|
 kinds
- union bound on $m_{\mathcal{H}}(2N)$ kinds





(b) Union Bound



(c) Now

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

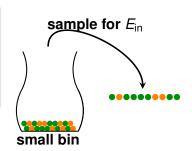
Step 3: Use Hoeffding without Replacement

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

 $\leq 2m_{\mathcal{H}}(2N) \cdot 2\exp\left(-2\left(\frac{\epsilon}{4}\right)^2N\right)$

consider bin of 2N examples, choose N for E_{in}, leave others for E'_{in} |E_{in} - E'_{in} | > ε/4 | E_{in} - E'_{in} | > ε/4 | ε_{in} - E_{in} + E'_{in} |
 so? just 'smaller bin', 'smaller ε', and

Hoeffding without replacement



use Hoeffding after zooming to fixed h

That's All!

Vapnik-Chervonenkis (VC) bound 存在就是说,发生坏事情的,想想反面,反而是不存在坏事情

$$\mathbb{P}\Big[\exists \textit{h} \in \mathcal{H} \text{ s.t. } \big|\textit{E}_{\text{in}}(\textit{h}) - \textit{E}_{\text{out}}(\textit{h})\big| > \epsilon\Big]$$

$$\leq 4m_{\mathcal{H}}(2N)\exp\left(-\frac{1}{8}\epsilon^2N\right)$$

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

2D perceptrons:

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

由此证明N足够多的时候, PLA可以达到学习的效果

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?

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

- 1.77×10^{-87}
- 25.54×10^{-83}
- 32.98×10^{-1}
- 42.29×10^{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?
- 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 poly(N)

- ◆ A Pictorial Proof
 m_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?