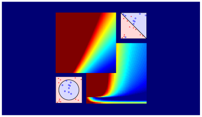
Machine Learning Foundations
(機器學習基石)



Lecture 6: Theory of Generalization

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

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

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

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

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

  ○ ○ × × ○ $m_{\mathcal{H}}(N) = 2^N$ always: no break point

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

  × ○ ○ × $m_{\mathcal{H}}(4) = 14 < 2^4$: break point at 4

break point $k \Longrightarrow$ break point $k + 1, \ldots$

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
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  (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:

$$\begin{aligned} & m_{\mathcal{H}}(N) \\ \leq\ & \text{maximum possible } m_{\mathcal{H}}(N) \text{ given } k \\ \leq\ & poly(N) \end{aligned}$$

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

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							
	$\vdots$							

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	$\ldots$
	1	1						
	2	1	3					
	3	1	4					
N	4	1						
	5	1						
	6	1						
	$\vdots$	$\vdots$						

Known

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

Table of Bounding Function (3/4)

	$B(N,k)$	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	...
N	4	1				16	16	...
	5	1					32	...
	6	1						...
	$\vdots$	$\vdots$						

(columns indexed by k)

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	...
	1	1	2	2	2	2	2	...
	2	1	3	4	4	4	4	...
	3	1	4	7	8	8	8	...
N	4	1			15	16	16	...
	5	1				31	32	...
	6	1					63	...
	$\vdots$	$\vdots$						$\ddots$

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	...
	1	1	2	2	2	2	2	...
	2	1	3	4	4	4	4	...
	3	1	4	7	8	8	8	...
N	4	1		?	15	16	16	...
	5	1				31	32	...
	6	1					63	...
	$\vdots$	$\vdots$						$\ddots$

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 . . .

	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$
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 . . .

	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$
01	○	○	○	○
02	×	○	○	○
03	○	×	○	○
04	○	○	×	○
05	○	○	○	×
06	×	×	○	×
07	×	○	×	○
08	×	○	○	×
09	○	×	×	○
10	○	×	○	×
11	○	○	×	×

$\Rightarrow$

	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$
01	○	○	○	○
05	○	○	○	×
02	×	○	○	○
08	×	○	○	×
03	○	×	○	○
10	○	×	○	×
04	○	○	×	○
11	○	○	×	×
06	×	×	○	×
07	×	○	×	○
09	○	×	×	○

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 $\Longrightarrow \alpha + \beta$ '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 $\Longrightarrow \alpha$ 'no shatter' any 2

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

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

Putting It All Together

$$\begin{aligned} B(4,3) &= 2\alpha + \beta \\ \alpha + \beta &\leq B(3,3) \\ \alpha &\leq B(3,2) \\ \Rightarrow B(4,3) &\leq B(3,3) + B(3,2) \end{aligned}$$

	$B(N,k)$	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

$$\begin{aligned} B(N,k) &= 2\alpha + \beta \\ \alpha + \beta &\leq B(N-1,k) \\ \alpha &\leq B(N-1,k-1) \\ \Rightarrow B(N,k) &\leq B(N-1,k) + B(N-1,k-1) \end{aligned}$$

	$B(N,k)$	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 $poly(N)$
  $\Longrightarrow m_{\mathcal{H}}(N)$ is $poly(N)$ 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: $m_{\mathcal{H}}(N) = N + 1 \leq N + 1$

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

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

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

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

  × ○ ○ × $m_{\mathcal{H}}(4) = 14 < 2^4$: 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:

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

actually, when N large enough,

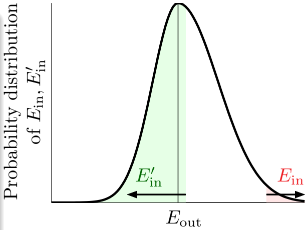
$$\mathbb{P}\Big[\exists h \in \mathcal{H} \text{ s.t. } \big|E_{\text{in}}(h) - E_{\text{out}}(h)\big| > \epsilon\Big] \leq 2 \cdot 2 m_{\mathcal{H}}(2N) \cdot \exp\left(-2 \cdot \frac{1}{16} \epsilon^2 N\right)$$

next: sketch of proof

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

$$\frac{1}{2}\mathbb{P}\Big[\exists h \in \mathcal{H} \text{ s.t. } \big|E_{\text{in}}(h) - E_{\text{out}}(h)\big| > \epsilon\Big]$$
$$\leq \quad \mathbb{P}\Big[\exists h \in \mathcal{H} \text{ s.t. } \big|E_{\text{in}}(h) - E'_{\text{in}}(h)\big| > \frac{\epsilon}{2}\Big]$$

- $E_{\text{in}}(h)$ 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 $E_{\text{in}} - E_{\text{out}}$ $\overset{\text{probably}}{\Longrightarrow}$ BAD h of $E_{\text{in}} - E'_{\text{in}}$

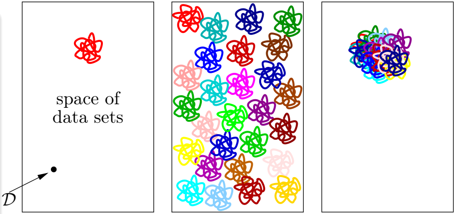


evil E_{out} removed by
verification with 'ghost data'

Step 2: Decompose $\mathcal{H}$ by Kind

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

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



(a) Hoeffding Inequality (b) Union Bound (c) Now

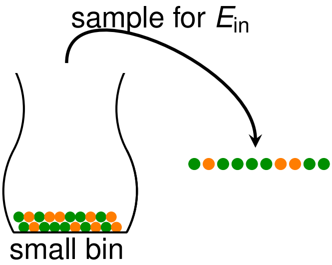
use $m_{\mathcal{H}}(2N)$ to calculate BAD-overlap properly

Step 3: Use Hoeffding without Replacement

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

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

- 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:

$$\mathbb{P}\left[\exists h \in \mathcal{H} \text{ s.t. } \left|E_{\text{in}}(h) - E_{\text{out}}(h)\right| > \epsilon\right]$$

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

- 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?

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

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 $poly(N)$
- 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?