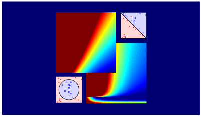
Machine Learning Foundations
(機器學習基石)



Lecture 7: The VC Dimension

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 6: Theory of Generalization

$E_{\text{out}} \approx E_{\text{in}}$ possible

if $m_{\mathcal{H}}(N)$ **breaks somewhere** and N **large enough**

Lecture 7: The VC Dimension

- Definition of VC Dimension
- VC Dimension of Perceptrons
- Physical Intuition of VC Dimension
- Interpreting VC Dimension

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

Recap: More on Growth Function

$$m_{\mathcal{H}}(N) \text{ of break point } k \le B(N,k) = \underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}_{\text{highest term } N^{k-1}}$$

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

N^{k-1}	k=1	2	3	4	5
1	1	1	1	1	1
2	1	2	4	8	16
3	1	3	9	27	81
4	1	4	16	64	256
5	1	5	25	125	625
6	1	6	36	216	1296

provably & loosely, for $N \ge 2, k \ge 3$,

$$m_{\mathcal{H}}(N) \le B(N,k) = \sum_{i=0}^{k-1} \binom{N}{i} \le N^{k-1}$$

Recap: More on Vapnik-Chervonenkis (VC) Bound

For any $g = \mathcal{A}(\mathcal{D}) \in \mathcal{H}$ and 'statistical' large $\mathcal{D}$, for ~~$N \geq 2$,~~ $k \geq 3$

$$
\begin{aligned}
& \mathbb{P}_{\mathcal{D}}\Big[\big|E_{\text{in}}(g) - E_{\text{out}}(g)\big| > \epsilon\Big] \\
\leq \quad & \mathbb{P}_{\mathcal{D}}\Big[\exists h \in \mathcal{H} \text{ s.t. } \big|E_{\text{in}}(h) - E_{\text{out}}(h)\big| > \epsilon\Big] \\
\leq \quad & 4 m_{\mathcal{H}}(2N) \exp\left(-\tfrac{1}{8}\epsilon^2 N\right) \\
\overset{\text{if } k \text{ exists}}{\leq} \quad & 4(2N)^{k-1} \exp\left(-\tfrac{1}{8}\epsilon^2 N\right)
\end{aligned}
$$

if (1) $m_{\mathcal{H}}(N)$ breaks at k (**good** $\mathcal{H}$)

(2) N large enough (**good** $\mathcal{D}$)

$\Longrightarrow$ probably generalized '$E_{\text{out}} \approx E_{\text{in}}$', and

if (3) $\mathcal{A}$ picks a g with small E_{in} (**good** $\mathcal{A}$)

$\Longrightarrow$ probably learned! (**:-) good luck**)

VC Dimension

the formal name of **maximum non-**break point

Definition

VC dimension of $\mathcal{H}$, denoted $d_{\text{VC}}(\mathcal{H})$ is

$$\textbf{largest } N \text{ for which } m_{\mathcal{H}}(N) = 2^N$$

- the **most** inputs $\mathcal{H}$ that can shatter
- $d_{\text{VC}} =$ 'minimum k' - 1

$N \le d_{\text{VC}} \implies \mathcal{H}$ can shatter some N inputs

$k > d_{\text{VC}} \implies k$ is a break point for $\mathcal{H}$

if $N \ge 2, d_{\text{VC}} \ge 2$, $m_{\mathcal{H}}(N) \le N^{d_{\text{VC}}}$

The Four VC Dimensions

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

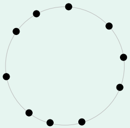
  $d_{\mathrm{VC}} = 1$

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

  $d_{\mathrm{VC}} = 2$

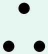
- convex sets: $m_{\mathcal{H}}(N) = 2^N$

  $d_{\mathrm{VC}} = \infty$



- 2D perceptrons: $m_{\mathcal{H}}(N) \leq N^3$ for $N \geq 2$

  $d_{\mathrm{VC}} = 3$

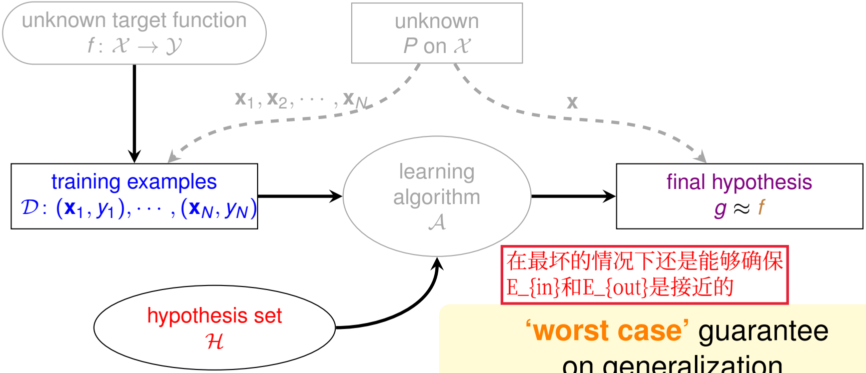


good: **finite** d_{VC}

VC Dimension and Learning

finite $d_{VC} \Longrightarrow g$ 'will' generalize ($E_{out}(g) \approx E_{in}(g)$)

- regardless of learning algorithm $\mathcal{A}$
- regardless of input distribution P
- regardless of target function f



在最坏的情况下还是能够确保E_{in}和E_{out}是接近的

'worst case' guarantee
on generalization

Fun Time

If there is a set of N inputs that cannot be shattered by $\mathcal{H}$. Based only on this information, what can we conclude about $d_{\text{VC}}(\mathcal{H})$?

1. $d_{\text{VC}}(\mathcal{H}) > N$
2. $d_{\text{VC}}(\mathcal{H}) = N$
3. $d_{\text{VC}}(\mathcal{H}) < N$
4. no conclusion can be made

Reference Answer: 4

It is possible that there is another set of N inputs that can be shattered, which means $d_{\text{VC}} \geq N$. It is also possible that no set of N input can be shattered, which means $d_{\text{VC}} < N$. Neither cases can be ruled out by one non-shattering set.

2D PLA Revisited

linearly separable $\mathcal{D}$ $\downarrow$ PLA can converge

with $\mathbf{x}_n \sim P$ and $y_n = f(\mathbf{x}_n)$ $\downarrow$ $\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq \ldots$ by $d_{\text{VC}} = 3$

T large

我们让这个演算法跑了多次的update之后，我们能够找到一条线，把所有的资料都分得好好的，也就是说它的E_{in}是0

N large

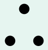
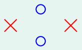
$E_{\text{in}}(g) = 0$

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

$E_{\text{out}}(g) \approx 0$ **:-)**

general PLA for **x** with more than 2 features?

VC Dimension of Perceptrons

- 1D perceptron (pos/neg rays): $d_{\text{VC}} = 2$
- 2D perceptrons: $d_{\text{VC}} = 3$
  - $d_{\text{VC}} \geq 3$: 
  - $d_{\text{VC}} \leq 3$: 
- d-D perceptrons: $d_{\text{VC}} \stackrel{?}{=} d + 1$

two steps:

- $d_{\text{VC}} \geq d + 1$
- $d_{\text{VC}} \leq d + 1$

Extra Fun Time

What statement below shows that $d_{\mathrm{VC}} \geq d + 1$?

1. There are some $d + 1$ inputs we can shatter.
2. We can shatter any set of $d + 1$ inputs.
3. There are some $d + 2$ inputs we cannot shatter.
4. We cannot shatter any set of $d + 2$ inputs.

Reference Answer: 1

d_{VC} is the maximum that $m_{\mathcal{H}}(N) = 2^N$, and $m_{\mathcal{H}}(N)$ is the most number of dichotomies of N inputs. So if we can find 2^{d+1} dichotomies on *some* $d + 1$ inputs, $m_{\mathcal{H}}(d + 1) = 2^{d+1}$ and hence $d_{\mathrm{VC}} \geq d + 1$.

$d_{\mathrm{VC}} \geq d + 1$

There are **some $d + 1$ inputs** we can shatter.

- some 'trivial' inputs:

$$
\mathrm{X} = \begin{bmatrix} -\ \mathbf{x}_1^T\ - \\ -\ \mathbf{x}_2^T\ - \\ -\ \mathbf{x}_3^T\ - \\ \vdots \\ -\ \mathbf{x}_{d+1}^T\ - \end{bmatrix} = \begin{array}{c} \begin{array}{ccccc} \text{x\_0} & & & & \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ 1 & 1 & 0 & \ldots & 0 \\ 1 & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & 0 \\ 1 & 0 & \ldots & 0 & 1 \end{bmatrix} \end{array}
$$

- visually in 2D: 

invertible adj. 可逆的

note: X **invertible!**

Can We Shatter X?

$$\mathrm{X} = \begin{bmatrix} -\mathbf{x}_1^T- \\ -\mathbf{x}_2^T- \\ \vdots \\ -\mathbf{x}_{d+1}^T- \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & & \ddots & 0 \\ 1 & 0 & \dots & 0 & 1 \end{bmatrix} \text{ invertible}$$

to shatter . . .

for any $\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_{d+1} \end{bmatrix}$, find $\mathbf{w}$ such that

$$\text{sign}\,(\mathrm{X}\mathbf{w}) = \mathbf{y} \quad \Longleftarrow \quad (\mathrm{X}\mathbf{w}) = \mathbf{y} \overset{\mathrm{X}\text{ invertible!}}{\Longleftrightarrow} \mathbf{w} = \mathrm{X}^{-1}\mathbf{y}$$

'special' X can be shattered $\Longrightarrow d_{\text{VC}} \geq d + 1$

Extra Fun Time

What statement below shows that $d_{\text{VC}} \leq d + 1$?

1. There are some $d + 1$ inputs we can shatter.
2. We can shatter any set of $d + 1$ inputs.
3. There are some $d + 2$ inputs we cannot shatter.
4. We cannot shatter any set of $d + 2$ inputs.

Reference Answer: 4

d_{VC} is the maximum that $m_{\mathcal{H}}(N) = 2^N$, and $m_{\mathcal{H}}(N)$ is the most number of dichotomies of N inputs. So if we cannot find 2^{d+2} dichotomies on *any* $d + 2$ inputs (i.e. break point), $m_{\mathcal{H}}(d + 2) < 2^{d+2}$ and hence $d_{\text{VC}} < d + 2$. That is, $d_{\text{VC}} \leq d + 1$.

$d_{\mathrm{VC}} \le d + 1$ (1/2)

A 2D Special Case

$$\mathrm{X} = \begin{bmatrix} — \mathbf{x}_1^T — \\ — \mathbf{x}_2^T — \\ — \mathbf{x}_3^T — \\ — \mathbf{x}_4^T — \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

数学上没有办法产生的理由，如果把x4表示成其它三个的线性组合的话，我们叫linear dependency线性依赖的关系会限制我们产生dichotomy的数量

○ ?

× ○

如果问号处为x, 这种dichotomy没有办法产生

? cannot be ×

$$\mathbf{w}^T\mathbf{x}_4 = \underbrace{\mathbf{w}^T\mathbf{x}_2}_{\circ} + \underbrace{\mathbf{w}^T\mathbf{x}_3}_{\circ} - \underbrace{\mathbf{w}^T\mathbf{x}_1}_{\times} > 0$$

linear dependence **restricts dichotomy**

$d_{\text{VC}} \le d + 1$ (2/2)

d-D General Case

$$\mathrm{X} = \begin{bmatrix} -\ \mathbf{x}_1^T\ - \\ -\ \mathbf{x}_2^T\ - \\ \vdots \\ -\ \mathbf{x}_{d+1}^T\ - \\ -\ \mathbf{x}_{d+2}^T\ - \end{bmatrix}$$

more rows than columns:

linear dependence (some a_i non-zero)

$$\mathbf{x}_{d+2} = a_1\mathbf{x}_1 + a_2\mathbf{x}_2 + \ldots + a_{d+1}\mathbf{x}_{d+1}$$

- can you generate $(\text{sign}(a_1), \text{sign}(a_2), \ldots, \text{sign}(a_{d+1}), \times)$? if so, what $\mathbf{w}$?

$$\mathbf{w}^T\mathbf{x}_{d+2} = a_1 \underbrace{\mathbf{w}^T\mathbf{x}_1}_{\circ} + a_2 \underbrace{\mathbf{w}^T\mathbf{x}_2}_{\times} + \ldots + a_{d+1} \underbrace{\mathbf{w}^T\mathbf{x}_{d+1}}_{\times} > 0$$

cannot generate (sign(a1),sign(a2), ...,sign(a_{d+1}, ×)

$$> 0 \text{(contradition!)}$$

'general' X no-shatter $\Longrightarrow d_{\text{VC}} \le d + 1$

Fun Time

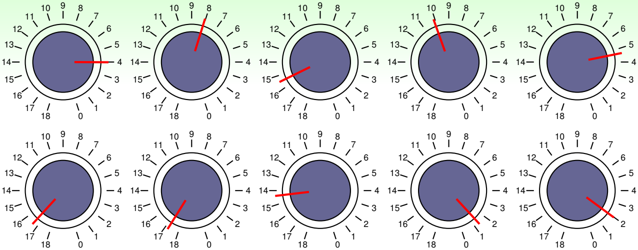
Based on the proof above, what is d_{VC} of 1126-D perceptrons?

1. 1024
2. 1126
3. 1127
4. 6211

Reference Answer: 3

Well, **too much fun for this section! :-)**

Degrees of Freedom



(modified from the work of Hugues Vermeiren on `http://www.texample.net`)

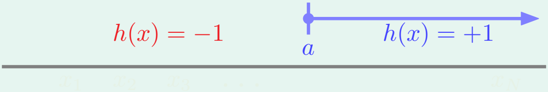
- hypothesis parameters $\mathbf{w} = (w_0, w_1, \cdots, w_d)$:
  creates degrees of freedom
- hypothesis quantity $M = |\mathcal{H}|$:
  'analog' degrees of freedom
- hypothesis 'power' $d_{\mathrm{VC}} = d + 1$:
  effective 'binary' degrees of freedom

$d_{\mathrm{VC}}(\mathcal{H})$: powerfulness of $\mathcal{H}$

Two Old Friends

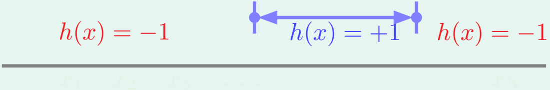
Positive Rays ($d_{VC} = 1$)

有一个可以调的旋钮



free parameters: a

Positive Intervals ($d_{VC} = 2$)



free parameters: ℓ, r

practical rule of thumb:

VC dimension 大概是可以说有多少可以调的旋钮

$d_{VC} \approx$ #free parameters (but not always)

M and d_{VC}

copied from Lecture 5 :-)

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

small M

1. Yes!, $\mathbb{P}[\textbf{BAD}] \le 2 \cdot M \cdot \exp(\ldots)$
2. No!, too few choices

large M

1. No!, $\mathbb{P}[\textbf{BAD}] \le 2 \cdot M \cdot \exp(\ldots)$
2. Yes!, many choices

可能可以选到一个E_in很小的hypothesis, 但坏事情发生的几率就变大了

small d_{VC} 自由度被受到限制

1. Yes!, $\mathbb{P}[\textbf{BAD}] \le 4 \cdot (2N)^{d_{\mathrm{VC}}} \cdot \exp(\ldots)$
2. No!, too limited power

large d_{VC}

1. No!, $\mathbb{P}[\textbf{BAD}] \le 4 \cdot (2N)^{d_{\mathrm{VC}}} \cdot \exp(\ldots)$
2. Yes!, lots of power

using the right d_{VC} (or $\mathcal{H}$) is important

Fun Time

Origin-crossing Hyperplanes are essentially perceptrons with w_0 fixed at 0. Make a guess about the d_{VC} of origin-crossing hyperplanes in $\mathbb{R}^d$.

1. 1
2. d
3. $d+1$
4. ∞

Reference Answer: 2

The proof is almost the same as proving the d_{VC} for usual perceptrons, but it is the **intuition** ($d_{\text{VC}} \approx \#$free parameters) that you shall use to answer this quiz.

VC Bound Rephrase: Penalty for Model Complexity

For any $g = \mathcal{A}(\mathcal{D}) \in \mathcal{H}$ and 'statistical' large $\mathcal{D}$, for $\cancel{N \geq 2,}\ d_{\mathrm{VC}} \geq 2$

$$\mathbb{P}_{\mathcal{D}}\Big[\underbrace{\big|E_{\text{in}}(g) - E_{\text{out}}(g)\big| > \epsilon}_{\textbf{BAD}}\Big] \leq \underbrace{4(2N)^{d_{\mathrm{VC}}} \exp\left(-\frac{1}{8}\epsilon^2 N\right)}_{\delta}$$

Rephrase

..., with probability $\geq 1 - \delta$, **GOOD**: $\big|E_{\text{in}}(g) - E_{\text{out}}(g)\big| \leq \epsilon$

$$\begin{aligned}
\text{set} \quad \delta &= 4(2N)^{d_{\mathrm{VC}}} \exp\left(-\frac{1}{8}\epsilon^2 N\right) \\
\frac{\delta}{4(2N)^{d_{\mathrm{VC}}}} &= \exp\left(-\frac{1}{8}\epsilon^2 N\right) \\
\ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right) &= \frac{1}{8}\epsilon^2 N \\
\sqrt{\frac{8}{N}\ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right)} &= \epsilon
\end{aligned}$$

VC Bound Rephrase: Penalty for Model Complexity

For any $g = \mathcal{A}(\mathcal{D}) \in \mathcal{H}$ and 'statistical' large $\mathcal{D}$, for $\cancel{N \geq 2,}\ d_{\mathrm{VC}} \geq 2$

$$\mathbb{P}_{\mathcal{D}}\Big[\underbrace{\big|E_{\mathrm{in}}(g) - E_{\mathrm{out}}(g)\big| > \epsilon}_{\textbf{BAD}}\Big] \leq \underbrace{4(2N)^{d_{\mathrm{VC}}} \exp\left(-\tfrac{1}{8}\epsilon^2 N\right)}_{\delta}$$

Rephrase

..., with probability $\geq 1 - \delta$, **GOOD**!

$$\text{gen. error } \big|E_{\mathrm{in}}(g) - E_{\mathrm{out}}(g)\big| \leq \sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right)}$$

$$E_{\mathrm{in}}(g) - \sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right)} \leq E_{\mathrm{out}}(g) \leq E_{\mathrm{in}}(g) + \sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right)}$$

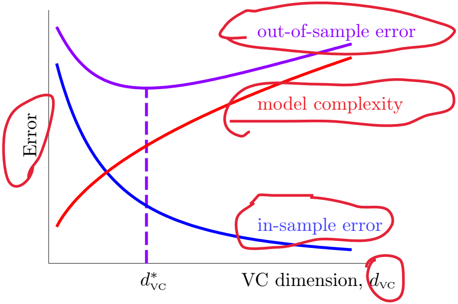
$\underbrace{\sqrt{\ldots}}_{\Omega(N, \mathcal{H}, \delta)}$: penalty for **model complexity**

THE VC Message

with a high probability,

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \underbrace{\sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{\text{VC}}}}{\delta}\right)}}_{\Omega(N,\mathcal{H},\delta)}$$

model complexity



- $d_{\text{VC}} \uparrow$: $E_{\text{in}} \downarrow$ but $\Omega \uparrow$
- $d_{\text{VC}} \downarrow$: $\Omega \downarrow$ but $E_{\text{in}} \uparrow$
- best d^*_{VC} in the middle

powerful $\mathcal{H}$ not always good!

样本复杂度, 资料量的复杂度

VC Bound Rephrase: Sample Complexity

For any $g = \mathcal{A}(\mathcal{D}) \in \mathcal{H}$ and 'statistical' large $\mathcal{D}$, for ~~$N \geq 2$,~~ $d_{VC} \geq 2$

$$\mathbb{P}_{\mathcal{D}}\Big[\underbrace{\big|E_{in}(g) - E_{out}(g)\big| > \epsilon}_{\textbf{BAD}}\Big] \leq \underbrace{4(2N)^{d_{VC}} \exp\left(-\frac{1}{8}\epsilon^2 N\right)}_{\delta}$$

E_in和E_out最多差0.1, 坏事情发生的概率为10%, VC dimension为3

given **specs** $\epsilon = 0.1$, $\delta = 0.1$, $d_{VC} = 3$, want $4(2N)^{d_{VC}} \exp\left(-\frac{1}{8}\epsilon^2 N\right) \leq \delta$

N	bound
100	2.82×10^7
1,000	9.17×10^9
10,000	1.19×10^8
100,000	1.65×10^{-38}
29,300	9.99×10^{-2}

$\boxed{\text{VC bound 上限}}$

sample complexity:
need $N \approx 10{,}000 d_{VC}$ in theory

$\boxed{\text{坏事情发生的几率很小}}$

practical rule of thumb:

$N \approx 10 d_{VC}$ **often enough!**

Looseness of VC Bound

来源就是VC Bound到底有多宽松

$$\mathbb{P}_{\mathcal{D}}\Big[\big|E_{\text{in}}(g) - E_{\text{out}}(g)\big| > \epsilon\Big] \quad \leq \quad 4(2N)^{d_{\text{VC}}} \exp\left(-\frac{1}{8}\epsilon^2 N\right)$$

theory: $N \approx 10{,}000 d_{\text{VC}}$; practice: $N \approx 10 d_{\text{VC}}$

Why?

宽松的来源

- Hoeffding for unknown E_{out} — **any distribution, any target**
- $m_{\mathcal{H}}(N)$ instead of $|\mathcal{H}(\mathbf{x}_1, \ldots, \mathbf{x}_N)|$ — **'any' data**
- $N^{d_{\text{VC}}}$ instead of $m_{\mathcal{H}}(N)$ — **'any' $\mathcal{H}$ of same d_{VC}**
- union bound on worst cases — **any choice made by $\mathcal{A}$**

—**but hardly better, and 'similarly loose for all models'**

philosophical message of VC bound
important for improving ML

Fun Time

Consider the VC Bound below. How can we decrease the probability of getting **BAD** data?

$$\mathbb{P}_{\mathcal{D}}\left[\left|E_{\text{in}}(g) - E_{\text{out}}(g)\right| > \epsilon\right] \quad \leq \quad 4(2N)^{d_{\text{VC}}} \exp\left(-\frac{1}{8}\epsilon^2 N\right)$$

1. decrease model complexity d_{VC}
2. increase data size N a lot
3. increase generalization error tolerance ϵ
4. all of the above

Reference Answer: 4

Congratulations on being Master of VC bound! :-)

Summary

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

Lecture 6: Theory of Generalization

Lecture 7: The VC Dimension

- Definition of VC Dimension
  maximum non-break point
- VC Dimension of Perceptrons
  $d_{VC}(\mathcal{H}) = d + 1$
- Physical Intuition of VC Dimension
  $d_{VC} \approx$ **#free parameters**
- Interpreting VC Dimension
  loosely: model complexity & sample complexity

- **next: more than noiseless binary classification?**

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