

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

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

$B(N, k)$		k				
		1	2	3	4	5
N	1	1	2	2	2	2
	2	1	3	4	4	4
	3	1	4	7	8	8
	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 $N \geq 2, k \geq 3$,

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

Recap: More on Vapnik-Chervonenkis (VC) Bound

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

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

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

② N large enough (good \mathcal{D})

\Rightarrow probably generalized ‘ $E_{\text{out}} \approx E_{\text{in}}$ ’, and

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

\Rightarrow probably learned! (:-) good luck)

VC Dimension

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

Definition

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

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

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

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

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

if $N \geq 2, d_{VC} \geq 2, m_{\mathcal{H}}(N) \leq N^{d_{VC}}$

The Four VC Dimensions

- positive rays:

$$d_{VC} = 1$$



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

- positive intervals:

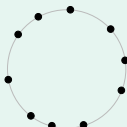
$$d_{VC} = 2$$



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

- convex sets:

$$d_{VC} = \infty$$



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

- 2D perceptrons:

$$d_{VC} = 3$$



$$m_{\mathcal{H}}(N) \leq N^3 \text{ for } N \geq 2$$

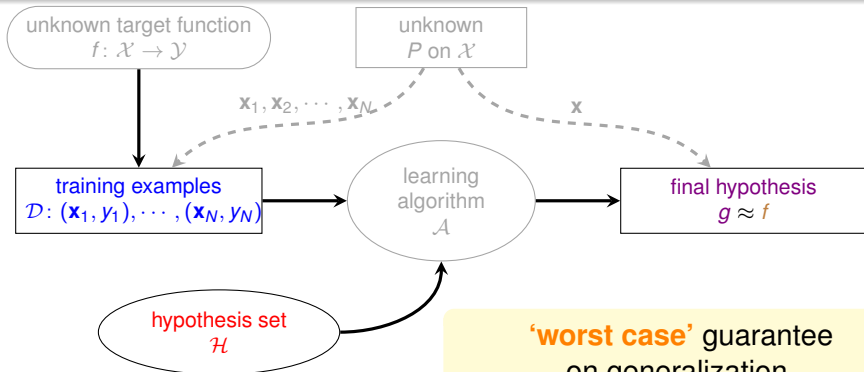
good: **finite** d_{VC}

VC Dimension and Learning

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

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



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} with $\mathbf{x}_n \sim P$ and $y_n = f(\mathbf{x}_n)$

PLA can converge

 $\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq \dots$ by $d_{\text{VC}} = 3$ T large N large



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

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

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

general PLA for \mathbf{x} with more than 2 features?

VC Dimension of Perceptrons

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

two steps:

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

Extra Fun Time

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

- 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 $d_{VC} \geq d + 1$.

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

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

- some 'trivial' inputs:

$$X = \begin{bmatrix} -\mathbf{x}_1^T - \\ -\mathbf{x}_2^T - \\ -\mathbf{x}_3^T - \\ \vdots \\ -\mathbf{x}_{d+1}^T - \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & 0 \\ 1 & 0 & \dots & 0 & 1 \end{bmatrix}$$

- visually in 2D: 

note: **X invertible!**

Can We Shatter X?

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

to shatter ...

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

$$\text{sign}(\mathbf{X}\mathbf{w}) = \mathbf{y} \iff (\mathbf{X}\mathbf{w}) = \mathbf{y} \overset{\text{X invertible!}}{\iff} \mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$$

‘special’ X can be shattered $\implies d_{VC} \geq d + 1$

Extra Fun Time

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

- 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 $d_{VC} < d + 2$. That is, $d_{VC} \leq d + 1$.

$$d_{VC} \leq d + 1 \quad (1/2)$$

A 2D Special Case

$$\begin{matrix} \bullet & \bullet \\ \bullet & \bullet \end{matrix} \quad X = \begin{bmatrix} -\mathbf{x}_1^T - \\ -\mathbf{x}_2^T - \\ -\mathbf{x}_3^T - \\ -\mathbf{x}_4^T - \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

○ ?
× ○

? 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**

$$d_{VC} \leq d + 1 \quad (2/2)$$

d -D General Case

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

more rows than columns:

linear dependence (some a_i non-zero)

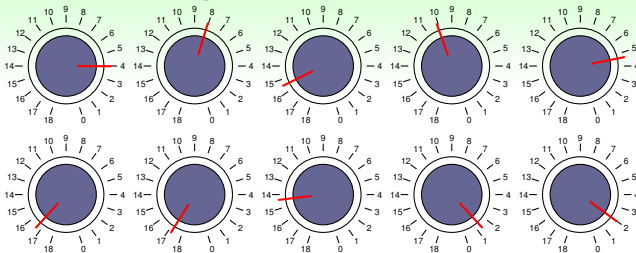
$$\mathbf{x}_{d+2} = a_1 \mathbf{x}_1 + a_2 \mathbf{x}_2 + \dots + a_{d+1} \mathbf{x}_{d+1}$$

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

$$\begin{aligned} \mathbf{w}^T \mathbf{x}_{d+2} &= a_1 \underbrace{\mathbf{w}^T \mathbf{x}_1}_0 + a_2 \underbrace{\mathbf{w}^T \mathbf{x}_2}_{\times} + \dots + a_{d+1} \underbrace{\mathbf{w}^T \mathbf{x}_{d+1}}_{\times} \\ &> 0 \text{ (contradiction!)} \end{aligned}$$

'general' X no-shatter $\implies d_{VC} \leq d + 1$

Degrees of Freedom



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

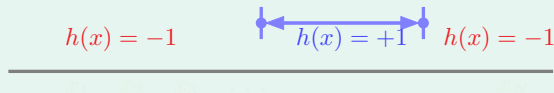
- hypothesis parameters $\mathbf{w} = (w_0, w_1, \dots, w_d)$:
creates degrees of freedom
- hypothesis quantity $M = |\mathcal{H}|$:
'analog' degrees of freedom
- hypothesis 'power' $d_{\text{VC}} = d + 1$:
effective 'binary' degrees of freedom

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

Two Old Friends

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

free parameters: a

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

free parameters: ℓ, r

practical rule of thumb:

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

M and d_{VC}

copied from Lecture 5 :-)

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

small M

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

large M

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

small d_{VC}

- ① Yes!, $\mathbb{P}[\mathbf{BAD}] \leq$
 $4 \cdot (2N)^{d_{VC}} \cdot \exp(\dots)$
- ② No!, too limited power

large d_{VC}

- ① No!, $\mathbb{P}[\mathbf{BAD}] \leq$
 $4 \cdot (2N)^{d_{VC}} \cdot \exp(\dots)$
- 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** ($d_{VC} \approx \# \text{free parameters}$) 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 $N \geq 2, d_{VC} \geq 2$

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

Rephrase

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

$$\text{set } \delta = 4(2N)^{d_{VC}} \exp\left(-\frac{1}{8}\epsilon^2 N\right)$$

$$\frac{\delta}{4(2N)^{d_{VC}}} = \exp\left(-\frac{1}{8}\epsilon^2 N\right)$$

$$\ln\left(\frac{4(2N)^{d_{VC}}}{\delta}\right) = \frac{1}{8}\epsilon^2 N$$

$$\sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{VC}}}{\delta}\right)} = \epsilon$$

VC Bound Rephrase: Penalty for Model Complexity

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

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

Rephrase

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

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

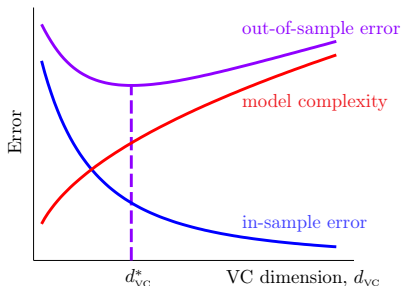
$$E_{in}(g) - \sqrt{\frac{8}{N} \ln \left(\frac{4(2N)^{d_{VC}}}{\delta} \right)} \leq E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{8}{N} \ln \left(\frac{4(2N)^{d_{VC}}}{\delta} \right)}$$

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

THE VC Message

with a high probability,

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



- $d_{\text{VC}} \uparrow$: $E_{\text{in}} \downarrow$ 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!

VC Bound Rephrase: Sample Complexity

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

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

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}

sample complexity:

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

practical rule of thumb:

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

Looseness of VC Bound

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

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

Why?

- Hoeffding for unknown E_{out} **any distribution, any target**
- $m_{\mathcal{H}}(N)$ instead of $|\mathcal{H}(\mathbf{x}_1, \dots, \mathbf{x}_N)|$ **'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?

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

- ❶ decrease model complexity d_{VC}
- ❷ increase data size N a lot
- ❸ increase generalization error tolerance ϵ
- ❹ all of the above

Reference Answer: ❹

**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

$$d_{VC} \approx \# \text{free parameters}$$

- 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?