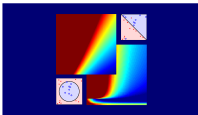


Machine Learning Foundations

(機器學習基石)



Lecture 7: The VC Dimension

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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

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

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	2	1	3	4	4	4
	3	1	4	7	8	8
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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 \mathcal{H} and 'statistical' large \mathcal{D} ,

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

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 (2) N large enough (good \mathcal{D})
 \implies generalized ' $E_{\text{out}} \approx E_{\text{in}}$ '

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

VC Dimension

the formal name of

break point

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

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Definition

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

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

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

The Four VC Dimensions

- positive rays:

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



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- positive intervals:

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• •

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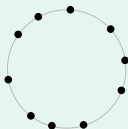
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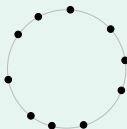
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$$m_{\mathcal{H}}(N) = 2^N$$

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

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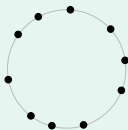
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good: **finite** d_{VC}

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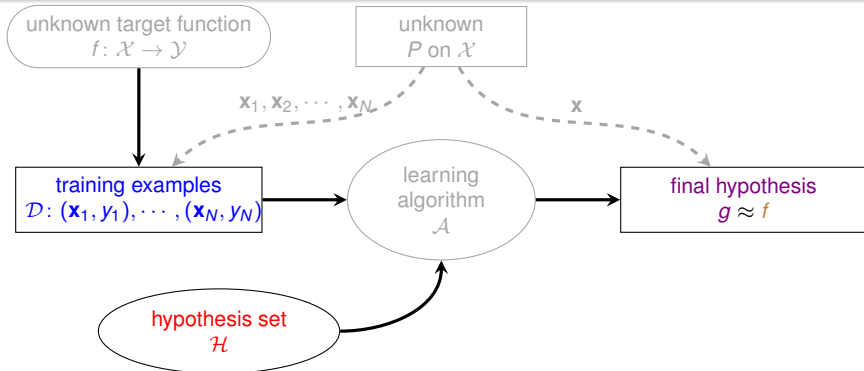
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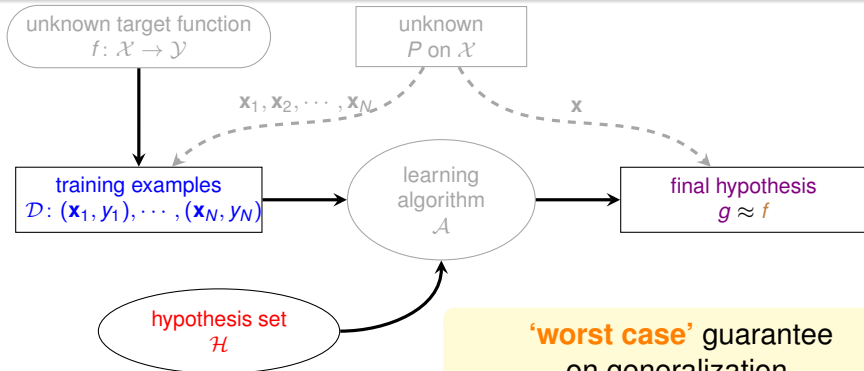
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'worst case' guarantee on generalization

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 $d_{\text{VC}}(\mathcal{H}) = N$
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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.

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linearly separable \mathcal{D}

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

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

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linearly separable \mathcal{D} 

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

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

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 N large

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

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



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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.

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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

$$\text{sign}(X\mathbf{w}) = \mathbf{y}$$

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

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

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

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

'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.

Extra Fun Time

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

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- 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

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

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

A 2D Special Case

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○ ?

× ○

? cannot be ×

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$$\mathbf{x}_4 = \mathbf{x}_2 + \mathbf{x}_3 - \mathbf{x}_1$$

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

A 2D Special Case

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

○ ?

× ○

? cannot be ×

$$\mathbf{w}^T \mathbf{x}_4 = \mathbf{w}^T \mathbf{x}_2 + \mathbf{w}^T \mathbf{x}_3 - \mathbf{w}^T \mathbf{x}_1$$

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

A 2D Special Case

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

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

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○ ?

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

linear dependence **restricts dichotomy**

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

d -D General Case

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

more rows than columns:

linear dependence (some a_i non-zero)

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

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

d -D General Case

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

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

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

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

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

d -D General Case

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

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

Fun Time

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

- ① 1024
- ② 1126
- ③ 1127
- ④ 6211

Fun Time

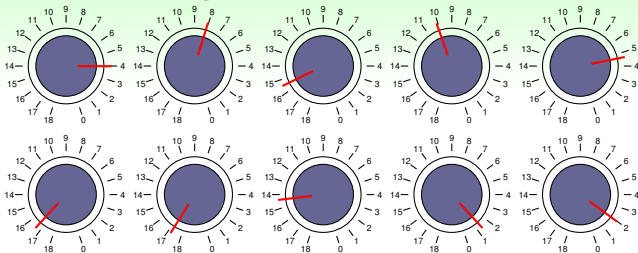
Based on the proof above, what is d_{VC} of 1126-D perceptrons?

- ① 1024
- ② 1126
- ③ 1127
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Reference Answer: ③

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

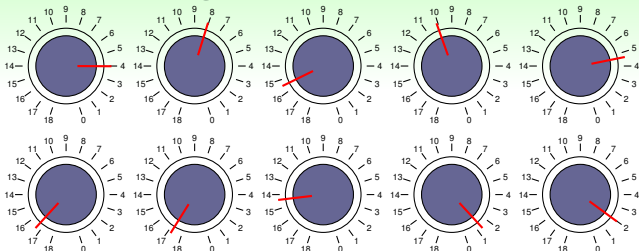
Degrees of Freedom



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

- hypothesis parameters $\mathbf{w} = (w_0, w_1, \dots, w_d)$:
creates degrees of freedom

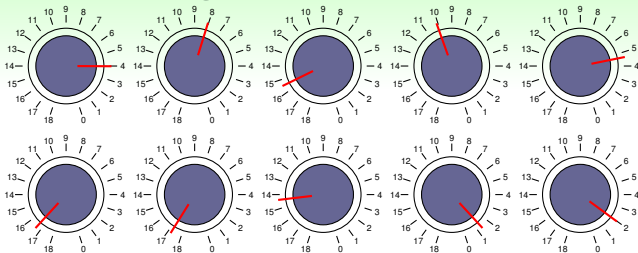
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- hypothesis quantity $M = |\mathcal{H}|$:
'analog' degrees of freedom

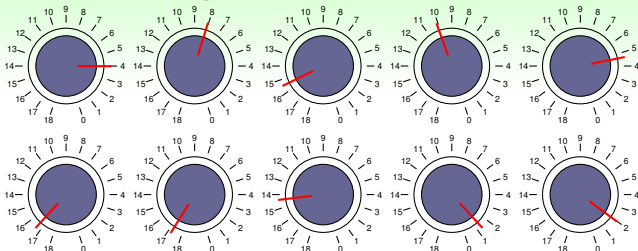
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- hypothesis 'power' $d_{VC} = d + 1$:
effective 'binary' degrees of freedom

Degrees of Freedom



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- hypothesis quantity $M = |\mathcal{H}|$:
'analog' degrees of freedom
- hypothesis 'power' $d_{VC} = d + 1$:
effective 'binary' degrees of freedom

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

Two Old Friends

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

free parameters: a

Two Old Friends

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

$$h(x) = -1 \quad a \quad h(x) = +1$$

free parameters: a

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

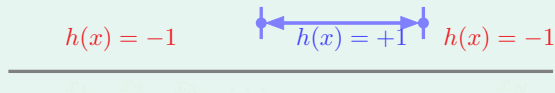
$$h(x) = -1 \quad l \quad h(x) = +1 \quad r \quad h(x) = -1$$

free parameters: l, r

Two Old Friends

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

free parameters: a

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

free parameters: l, r

practical rule of thumb:

$d_{VC} \approx$ #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!,
 $\mathbb{P}[\mathbf{BAD}] \leq 2 \cdot M \cdot \exp(\dots)$
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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
- d
- $d + 1$
- ∞

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
- d
- $d + 1$
- ∞

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 $N \geq 2, d_{VC} \geq 2$

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

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Rephrase

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

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

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

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Rephrase

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

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

VC Bound Rephrase: Penalty for Model Complexity

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

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

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

VC Bound Rephrase: Penalty for Model Complexity

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

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Rephrase

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

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

VC Bound Rephrase: Penalty for Model Complexity

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Rephrase

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

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

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

THE VC Message

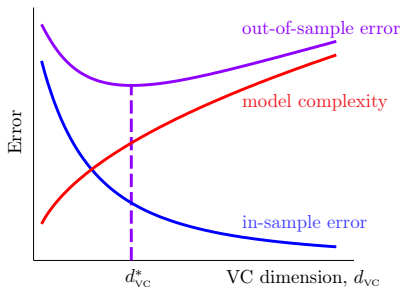
with a high probability,

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

THE VC Message

with a high probability,

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

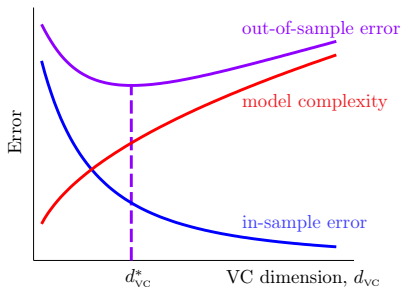


- $d_{\text{VC}} \uparrow$: $E_{\text{in}} \downarrow$ but $\Omega \uparrow$

THE VC Message

with a high probability,

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

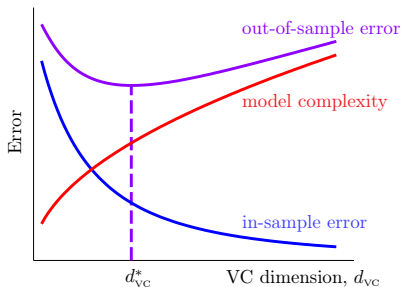


- $d_{\text{VC}} \uparrow$: $E_{\text{in}} \downarrow$ but $\Omega \uparrow$
- $d_{\text{VC}} \downarrow$: $\Omega \downarrow$ but $E_{\text{in}} \uparrow$

THE VC Message

with a high probability,

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

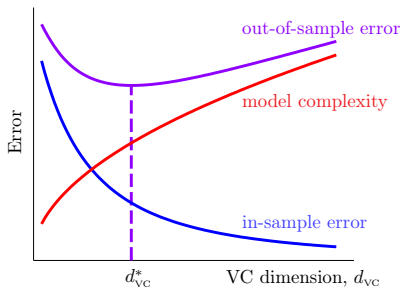


- $d_{\text{VC}} \uparrow$: $E_{\text{in}} \downarrow$ but $\Omega \uparrow$
- $d_{\text{VC}} \downarrow$: $\Omega \downarrow$ but $E_{\text{in}} \uparrow$
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powerful \mathcal{H} not always good!

VC Bound Rephrase: Sample Complexity

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

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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

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N	bound	
100	2.82×10^7	
1,000	9.17×10^9	sample complexity:
10,000	1.19×10^8	need $N \approx 10,000d_{VC}$ in theory
100,000	1.65×10^{-38}	
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practical rule of thumb:

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

Looseness of VC Bound

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

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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?

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- 2 increase data size N a lot
- 3 increase generalization error tolerance ϵ
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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?