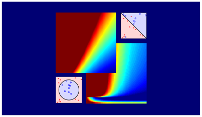
Machine Learning Foundations
(機器學習基石)



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

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

	$B(N,k)$	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 $\cancel{N \geq 2,}$ $k \geq 3$

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

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 $d_{\mathrm{VC}}(\mathcal{H})$ is

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

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

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

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

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

The Four VC Dimensions

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

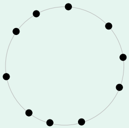
  $d_{\mathrm{VC}} = 1$

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

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

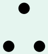
- convex sets: $m_{\mathcal{H}}(N) = 2^N$

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



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

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

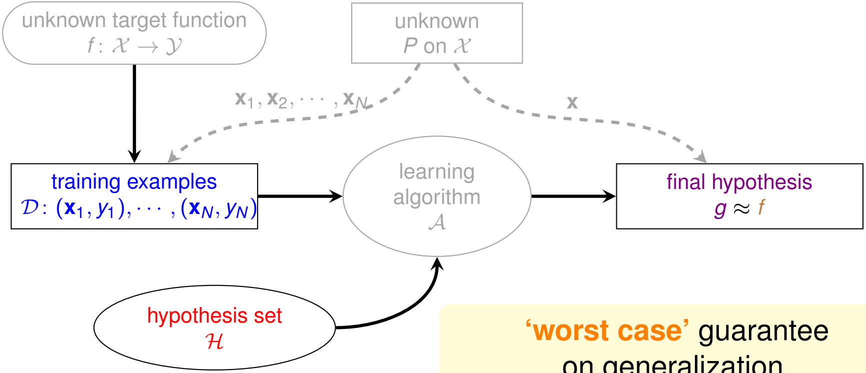


good: **finite** d_{VC}

VC Dimension and Learning

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

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



'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

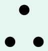
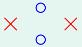
linearly separable $\mathcal{D}$ $\downarrow$ PLA can converge $\xrightarrow{T \text{ large}}$ $E_{\text{in}}(g) = 0$

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

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

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

VC Dimension of Perceptrons

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

two steps:

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

Extra Fun Time

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

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

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

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

- some 'trivial' inputs:

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

- visually in 2D: 

note: **X invertible!**

Can We Shatter X?

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

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 $d_{\mathrm{VC}} \leq d + 1$?

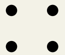
1. There are some $d + 1$ inputs we can shatter.
2. We can shatter any set of $d + 1$ inputs.
3. There are some $d + 2$ inputs we cannot shatter.
4. We cannot shatter any set of $d + 2$ inputs.

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

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

A 2D Special Case



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

$$\begin{array}{cc} \circ & \mathbf{?} \\ \times & \circ \end{array}$$

? cannot be $\times$

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

linear dependence **restricts dichotomy**

$d_{\mathrm{VC}} \le d + 1$ (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 $(\mathrm{sign}(a_1), \mathrm{sign}(a_2), \ldots, \mathrm{sign}(a_{d+1}), \times)$? if so, what $\mathbf{w}$?

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

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

Fun Time

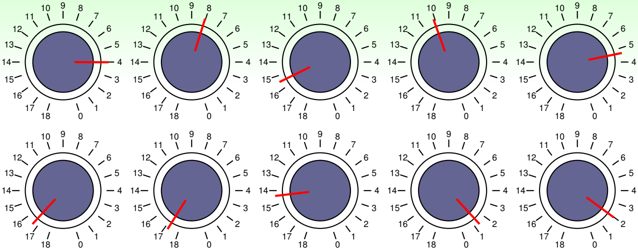
Based on the proof above, what is d_{VC} of 1126-D perceptrons?

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

Reference Answer: 3

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

Degrees of Freedom



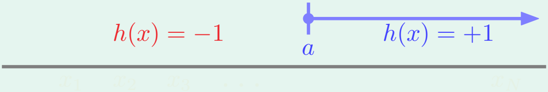
(modified from the work of Hugues Vermeiren on `http://www.texample.net`)

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

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

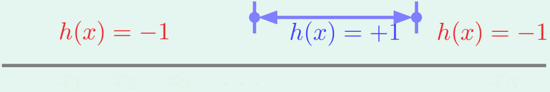
Two Old Friends

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



free parameters: a

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



free parameters: ℓ, r

practical rule of thumb:

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

M and d_{VC}

copied from Lecture 5 :-)

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

small M

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

large M

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

small d_{VC}

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

large d_{VC}

1. No!, $\mathbb{P}[\textbf{BAD}] \leq 4 \cdot (2N)^{d_{\text{VC}}} \cdot \exp(\ldots)$
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 ~~$N \geq 2$,~~ $d_{\text{VC}} \geq 2$

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

Rephrase

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

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

VC Bound Rephrase: Penalty for Model Complexity

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

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

Rephrase

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

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

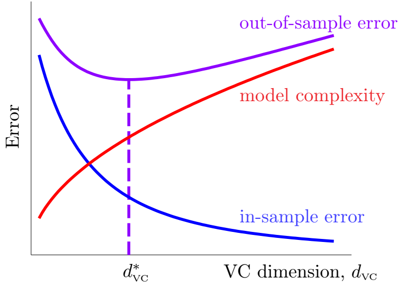
$$E_{\mathrm{in}}(g) - \sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right)} \quad \leq \quad E_{\mathrm{out}}(g) \quad \leq \quad E_{\mathrm{in}}(g) + \sqrt{\frac{8}{N} \ln\left(\frac{4(2N)^{d_{\mathrm{VC}}}}{\delta}\right)}$$

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

THE VC Message

with a high probability,

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



- $d_{\text{VC}} \uparrow$: $E_{\text{in}} \downarrow$ 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 ~~$N \geq 2$,~~ $d_{\text{VC}} \geq 2$

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

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

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

practical rule of thumb:

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

Looseness of VC Bound

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

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

Why?

- 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?

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

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
  $d_{\mathrm{VC}}(\mathcal{H}) = d + 1$
- Physical Intuition of VC Dimension
  $d_{\mathrm{VC}} \approx \#$**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?