

Machine Learning Foundations

(機器學習基石)



Lecture 4: Feasibility of Learning

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Roadmap

① When Can Machines Learn?

Lecture 3: Types of Learning

focus: **binary classification** or **regression** from a **batch** of **supervised** data with **concrete** features

Lecture 4: Feasibility of Learning

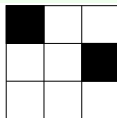
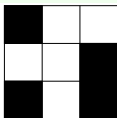
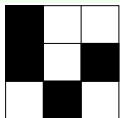
- Learning is Impossible?
- Probability to the Rescue
- Connection to Learning
- Connection to Real Learning

② Why Can Machines Learn?

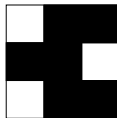
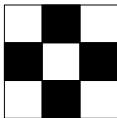
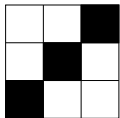
③ How Can Machines Learn?

④ How Can Machines Learn Better?

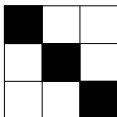
A Learning Puzzle



$$y_n = -1$$



$$y_n = +1$$



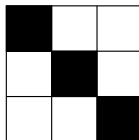
$$g(\mathbf{x}) = ?$$

**let's test your 'human learning'
with 6 examples :-)**

Two Controversial Answers

whatever you say about $g(\mathbf{x})$,


 $y_n = -1$

 $y_n = +1$

 $g(\mathbf{x}) = ?$

truth $f(\mathbf{x}) = +1$ because ...

- symmetry $\Leftrightarrow +1$
- (black or white count = 3) or (black count = 4 and middle-top black) $\Leftrightarrow +1$

truth $f(\mathbf{x}) = -1$ because ...

- left-top black $\Leftrightarrow -1$
- middle column contains at most 1 black and right-top white $\Leftrightarrow -1$

all valid reasons, your **adversarial teacher**
can always call you '**didn't learn**'. :-)

A 'Simple' Binary Classification Problem

\mathbf{x}_n	$y_n = f(\mathbf{x}_n)$
0 0 0	○
0 0 1	×
0 1 0	×
0 1 1	○
1 0 0	×

输入有8种，输出有2种情况，所以函数的数量
总共有 $2^8=256$ 种可能

- $\mathcal{X} = \{0, 1\}^3$, $\mathcal{Y} = \{\text{○}, \text{×}\}$, can enumerate all candidate f as \mathcal{H}

pick $g \in \mathcal{H}$ with all $g(\mathbf{x}_n) = y_n$ (like PLA),
does $g \approx f$?

No Free Lunch

\mathcal{D}

\mathbf{x}	y	g	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8
0 0 0	○	○	○	○	○	○	○	○	○	○
0 0 1	×	×	×	×	×	×	×	×	×	×
0 1 0	×	×	×	×	×	×	×	×	×	×
0 1 1	○	○	○	○	○	○	○	○	○	○
1 0 0	×	×	×	×	×	×	×	×	×	×
1 0 1		?	○	○	○	○	×	×	×	×
1 1 0		?	○	○	×	×	○	○	×	×
1 1 1		?	○	×	○	×	○	×	○	×

- $g \approx f$ inside \mathcal{D} : sure!
- $g \approx f$ outside \mathcal{D} : **No!** (but that's really what we want!)

learning from \mathcal{D} (to infer something outside \mathcal{D})
is doomed if **any 'unknown' f can happen.** :-)

Fun Time

This is a popular 'brain-storming' problem, with a claim that 2% of the world's cleverest population can crack its 'hidden pattern'.

$$(5, 3, 2) \rightarrow 151022, \quad (7, 2, 5) \rightarrow ?$$

It is like a 'learning problem' with $N = 1$, $\mathbf{x}_1 = (5, 3, 2)$, $y_1 = 151022$.
Learn a hypothesis from the one example to predict on $\mathbf{x} = (7, 2, 5)$.
What is your answer?

- ① 151026
- ② 143547
- ③ I need more examples to get the correct answer
- ④ there is no 'correct' answer

Fun Time

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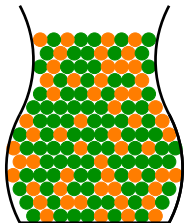
- ① 151026
- ② 143547
- ③ I need more examples to get the correct answer
- ④ there is no ‘correct’ answer

Reference Answer: ④

Following the same nature of the no-free-lunch problems discussed, we cannot hope to be correct under this ‘adversarial’ setting. BTW, ② is the designer’s answer: the first two digits = $x_1 \cdot x_2$; the next two digits = $x_1 \cdot x_3$; the last two digits = $(x_1 \cdot x_2 + x_1 \cdot x_3 - x_2)$.

Inferring Something Unknown

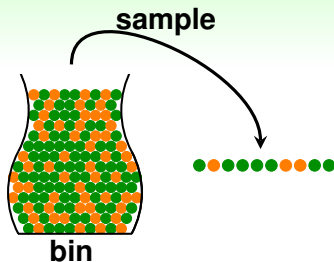
difficult to infer **unknown target f outside \mathcal{D}** in learning;
can we infer **something unknown** in **other scenarios**?



- consider a bin of many many **orange** and **green** marbles
- do we **know** the **orange** portion (probability)? **No!**

我们不知道橘色弹珠的比例，但我们可以去infer
估计，推断

can you **infer** the **orange** probability?

Statistics 101: Inferring **Orange** Probability**bin**

assume

orange probability = μ ,

green probability = $1 - \mu$,

with μ **unknown**

sample

N marbles sampled independently, with

orange fraction = ν ,

green fraction = $1 - \nu$,

now ν **known**

does **in-sample** ν say anything about
out-of-sample μ ?

Possible versus Probable

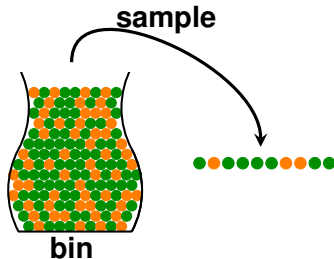
does **in-sample** ν say anything about out-of-sample μ ?

No!

possibly not: sample can be mostly **green** while bin is mostly **orange**

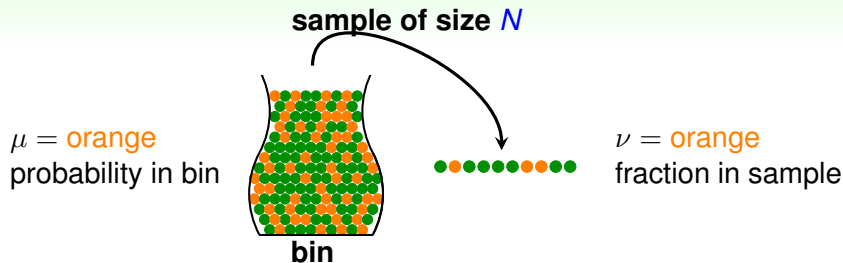
Yes!

probably yes: in-sample ν likely **close**
to unknown μ



formally, **what does** ν **say about** μ ?

Hoeffding's Inequality (1/2)



- in big sample (N large), ν is probably close to μ (within ϵ)

$$\mathbb{P} [|\nu - \mu| > \epsilon] \leq 2 \exp \left(-2\epsilon^2 N \right)$$

霍夫丁不等式 (Hoeffding's inequality)

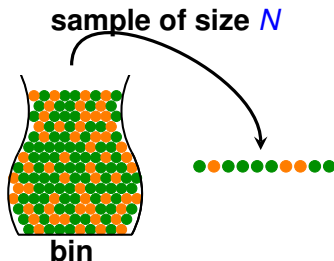
- called **Hoeffding's Inequality**, for marbles, coin, polling, ...

the statement ' $\nu = \mu$ ' is
probably approximately correct (PAC)

Hoeffding's Inequality (2/2)

$$\mathbb{P} [|\nu - \mu| > \epsilon] \leq 2 \exp(-2\epsilon^2 N)$$

- valid for all N and ϵ
- does not depend on μ ,
no need to 'know' μ
- larger sample size N or
looser gap ϵ
 \implies higher probability for ' $\nu \approx \mu$ '



if **large N** , can **probably** infer
unknown μ by known ν

Fun Time

Let $\mu = 0.4$. Use Hoeffding's Inequality

$$\mathbb{P} [|\nu - \mu| > \epsilon] \leq 2 \exp(-2\epsilon^2 N)$$

to bound the probability that a sample of 10 marbles will have $\nu \leq 0.1$. What bound do you get?

- ① 0.67
- ② 0.40
- ③ 0.33
- ④ 0.05

Fun Time

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- ① 0.67
- ② 0.40
- ③ 0.33
- ④ 0.05

Reference Answer: ③

Set $N = 10$ and $\epsilon = 0.3$ and you get the answer. BTW, ④ is the actual probability and Hoeffding gives only an upper bound to that.

Connection to Learning

bin

- unknown **orange** prob. μ
- marble $\bullet \in \text{bin}$
- **orange** \bullet
- **green** \bullet
- size- N sample from bin

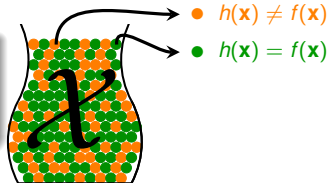
of i.i.d. marbles

learning

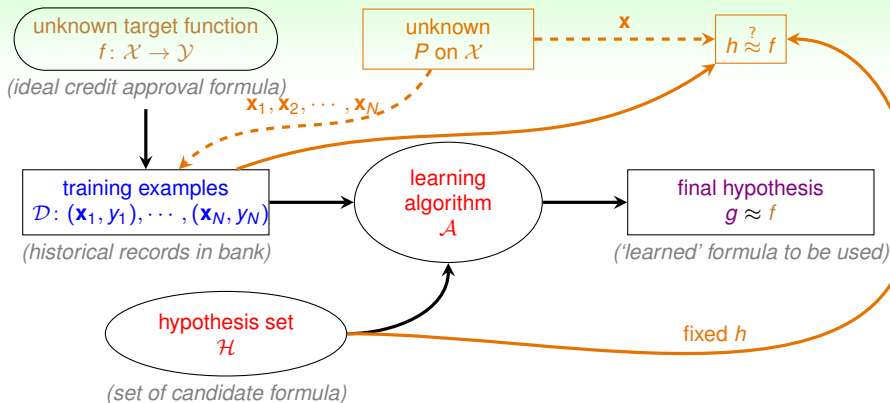
- fixed hypothesis $h(\mathbf{x}) \stackrel{?}{=} \text{target } f(\mathbf{x})$
- $\mathbf{x} \in \mathcal{X}$
- h is **wrong** $\Leftrightarrow h(\mathbf{x}) \neq f(\mathbf{x})$
- h is **right** $\Leftrightarrow h(\mathbf{x}) = f(\mathbf{x})$
- check h on $\mathcal{D} = \{(\mathbf{x}_n, \underbrace{y_n}_{f(\mathbf{x}_n)})\}$

with i.i.d. \mathbf{x}_n

if **large** N & **i.i.d.** \mathbf{x}_n , can **probably** infer
unknown $\llbracket h(\mathbf{x}) \neq f(\mathbf{x}) \rrbracket$ probability
by known $\llbracket h(\mathbf{x}_n) \neq y_n \rrbracket$ fraction



Added Components



for any fixed h , can probably infer

$$\text{unknown } E_{\text{out}}(\mathbf{h}) = \mathcal{E}_{\mathbf{x} \sim P} \llbracket h(\mathbf{x}) \neq f(\mathbf{x}) \rrbracket$$

$$\text{by known } E_{\text{in}}(\mathbf{h}) = \frac{1}{N} \sum_{n=1}^N \llbracket h(\mathbf{x}_n) \neq y_n \rrbracket.$$

The Formal Guarantee

for any fixed h , in ‘big’ data (N large),

in-sample error $E_{\text{in}}(h)$ is probably close to

out-of-sample error $E_{\text{out}}(h)$ (within ϵ)

$$\mathbb{P} [|E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon] \leq 2 \exp(-2\epsilon^2 N)$$

same as the ‘bin’ analogy . . .

- valid for all N and ϵ
- does not depend on $E_{\text{out}}(h)$, **no need to ‘know’** $E_{\text{out}}(h)$
— f and P can stay unknown
- ‘ $E_{\text{in}}(h) = E_{\text{out}}(h)$ ’ is **probably approximately correct (PAC)**

if ‘ $E_{\text{in}}(h) \approx E_{\text{out}}(h)$ ’ and ‘ $E_{\text{in}}(h)$ **small**’
 $\implies E_{\text{out}}(h)$ small $\implies h \approx f$ with respect to P

Verification of One h

for any fixed h , when data large enough,

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

Can we claim ‘good learning’ ($g \approx f$)?

Yes!

if $E_{\text{in}}(h)$ **small for the fixed h**
and \mathcal{A} **pick the h as g**
 \implies ‘ $g = f$ ’ PAC

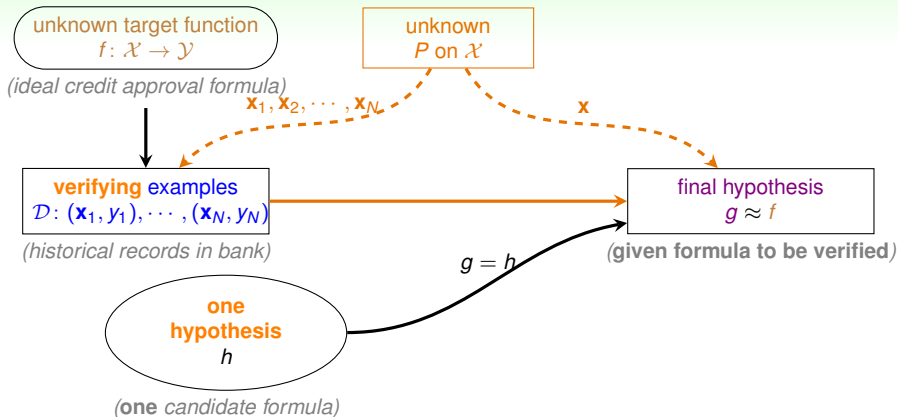
No!

if \mathcal{A} **forced to pick THE h as g**
 $\implies E_{\text{in}}(h)$ **almost always not small**
 \implies ‘ $g \neq f$ ’ PAC!

real learning:

\mathcal{A} shall **make choices** $\in \mathcal{H}$ (like PLA)
rather than **being forced to pick one h** . :-)

The 'Verification' Flow



can now use 'historical records' (data) to
verify 'one candidate formula' h

Fun Time

Your friend tells you her secret rule in investing in a particular stock: 'Whenever the stock goes down in the morning, it will go up in the afternoon; vice versa.' **To verify the rule, you chose 100 days uniformly at random from the past 10 years of stock data, and found that 80 of them satisfy the rule.** What is the best guarantee that you can get from the verification?

- 1 You'll definitely be rich by exploiting the rule in the next 100 days.
- 2 You'll likely be rich by exploiting the rule in the next 100 days, if the market behaves similarly to the last 10 years.
- 3 You'll likely be rich by exploiting the 'best rule' from 20 more friends in the next 100 days.
- 4 You'd definitely have been rich if you had exploited the rule in the past 10 years.



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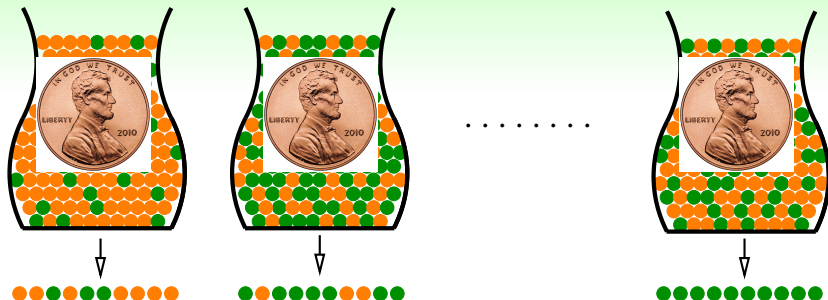
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- ③ You'll likely be rich by exploiting the 'best rule' from 20 more friends in the next 100 days.
- ④ You'd definitely have been rich if you had exploited the rule in the past 10 years.

Reference Answer: ②

①: no free lunch; ③: no 'learning' guarantee in verification; ④: verifying with only 100 days, possible that the rule is mostly wrong for whole 10 years.

BINGO when getting ●●●●●●●●?

Coin Game



Q: if everyone in size-150 NTU ML class flips a coin 5 times, and **one of the students gets 5 heads for her coin 'g'**. Is 'g' really magical?

A: No. Even if all coins are fair, the probability that **one of the coins** results in **5 heads** is $1 - \left(\frac{31}{32}\right)^{150} > 99\%$.

BAD sample: E_{in} and E_{out} far away
—can get worse when involving 'choice'

BAD Sample and BAD Data

BAD Sample

e.g., $E_{\text{out}} = \frac{1}{2}$, but getting all heads ($E_{\text{in}} = 0$)!

BAD Data for One h

$E_{\text{out}}(h)$ and $E_{\text{in}}(h)$ far away:

e.g., E_{out} big (far from f), but E_{in} small (correct on most examples)

	\mathcal{D}_1	\mathcal{D}_2	...	\mathcal{D}_{1126}	...	\mathcal{D}_{5678}	...	Hoeffding
h	BAD					BAD		$\mathbb{P}_{\mathcal{D}} [\text{BAD } \mathcal{D} \text{ for } h] \leq \dots$

Hoeffding: small

$$\mathbb{P}_{\mathcal{D}} [\text{BAD } \mathcal{D}] = \sum_{\text{all possible } \mathcal{D}} \mathbb{P}(\mathcal{D}) \cdot \llbracket \text{BAD } \mathcal{D} \rrbracket$$

BAD Data for Many h

BAD data for many h

\iff **no 'freedom of choice'** by \mathcal{A}

\iff **there exists some h such that $E_{\text{out}}(h)$ and $E_{\text{in}}(h)$ far away**

	\mathcal{D}_1	\mathcal{D}_2	...	\mathcal{D}_{1126}	...	\mathcal{D}_{5678}	Hoeffding
h_1	BAD					BAD	$\mathbb{P}_{\mathcal{D}} [\text{BAD } \mathcal{D} \text{ for } h_1] \leq \dots$
h_2		BAD					$\mathbb{P}_{\mathcal{D}} [\text{BAD } \mathcal{D} \text{ for } h_2] \leq \dots$
h_3	BAD	BAD				BAD	$\mathbb{P}_{\mathcal{D}} [\text{BAD } \mathcal{D} \text{ for } h_3] \leq \dots$
...							
h_M	BAD					BAD	$\mathbb{P}_{\mathcal{D}} [\text{BAD } \mathcal{D} \text{ for } h_M] \leq \dots$
all	BAD	BAD				BAD	?

for M hypotheses, bound of $\mathbb{P}_{\mathcal{D}}[\text{BAD } \mathcal{D}]$?

Bound of BAD Data

$$\begin{aligned}
& \mathbb{P}_{\mathcal{D}}[\text{BAD } \mathcal{D}] \\
&= \mathbb{P}_{\mathcal{D}}[\text{BAD } \mathcal{D} \text{ for } h_1 \text{ or BAD } \mathcal{D} \text{ for } h_2 \text{ or } \dots \text{ or BAD } \mathcal{D} \text{ for } h_M] \\
&\leq \mathbb{P}_{\mathcal{D}}[\text{BAD } \mathcal{D} \text{ for } h_1] + \mathbb{P}_{\mathcal{D}}[\text{BAD } \mathcal{D} \text{ for } h_2] + \dots + \mathbb{P}_{\mathcal{D}}[\text{BAD } \mathcal{D} \text{ for } h_M] \\
&\quad \text{(union bound)} \\
&\leq 2 \exp(-2\epsilon^2 N) + 2 \exp(-2\epsilon^2 N) + \dots + 2 \exp(-2\epsilon^2 N) \\
&= 2M \exp(-2\epsilon^2 N)
\end{aligned}$$

- **finite-bin** version of Hoeffding, valid for all M , N and ϵ
- does not depend on any $E_{\text{out}}(h_m)$, **no need to 'know'** $E_{\text{out}}(h_m)$
— f and P can stay unknown
- ' $E_{\text{in}}(g) = E_{\text{out}}(g)$ ' is **PAC**, **regardless of** \mathcal{A}

'most reasonable' \mathcal{A} (like PLA/pocket):
pick the h_m with **lowest** $E_{\text{in}}(h_m)$ as g

有限个假设的情况

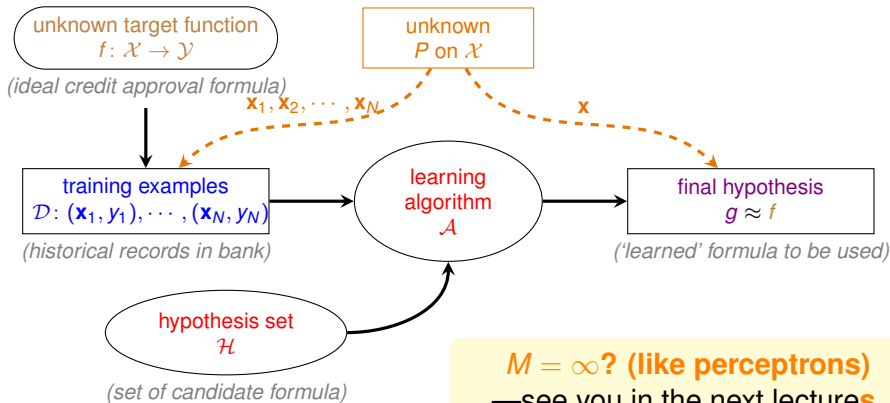
The 'Statistical' Learning Flow

if $|\mathcal{H}| = M$ finite, N large enough,

for whatever g picked by \mathcal{A} , $E_{\text{out}}(g) \approx E_{\text{in}}(g)$

if \mathcal{A} finds one g with $E_{\text{in}}(g) \approx 0$,

PAC guarantee for $E_{\text{out}}(g) \approx 0 \implies$ **learning possible :-)**



$M = \infty?$ (like perceptrons)
—see you in the next lectures

Fun Time

Consider 4 hypotheses.

$$h_1(\mathbf{x}) = \text{sign}(x_1), \quad h_2(\mathbf{x}) = \text{sign}(x_2),$$

$$h_3(\mathbf{x}) = \text{sign}(-x_1), \quad h_4(\mathbf{x}) = \text{sign}(-x_2).$$

For any N and ϵ , which of the following statement is not true?

- ① the **BAD** data of h_1 and the **BAD** data of h_2 are exactly the same
- ② the **BAD** data of h_1 and the **BAD** data of h_3 are exactly the same
- ③ $\mathbb{P}_{\mathcal{D}}[\text{BAD for some } h_k] \leq 8 \exp(-2\epsilon^2 N)$
- ④ $\mathbb{P}_{\mathcal{D}}[\text{BAD for some } h_k] \leq 4 \exp(-2\epsilon^2 N)$



Fun Time

Consider 4 hypotheses.

$$h_1(\mathbf{x}) = \text{sign}(x_1), \quad h_2(\mathbf{x}) = \text{sign}(x_2),$$

$$h_3(\mathbf{x}) = \text{sign}(-x_1), \quad h_4(\mathbf{x}) = \text{sign}(-x_2).$$

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Reference Answer: ①

The important thing is to note that ② is true, which implies that ④ is true if you revisit the union bound. Similar ideas will be used to conquer the $M = \infty$ case.

Summary

1 When Can Machines Learn?

Lecture 3: Types of Learning

Lecture 4: Feasibility of Learning

- Learning is Impossible?
absolutely no free lunch outside \mathcal{D}
- Probability to the Rescue
probably approximately correct outside \mathcal{D}
- Connection to Learning
verification possible if $E_{\text{in}}(h)$ small for fixed h
- Connection to Real Learning
learning possible if $|\mathcal{H}|$ finite and $E_{\text{in}}(g)$ small

2 Why Can Machines Learn?

- **next: what if $|\mathcal{H}| = \infty$?**

3 How Can Machines Learn?

4 How Can Machines Learn Better?