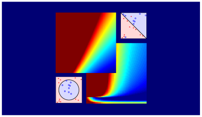
Machine Learning Foundations
(機器學習基石)



Lecture 4: Feasibility of Learning

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Roadmap

1. **When** Can Machines Learn?

Lecture 3: Types of Learning

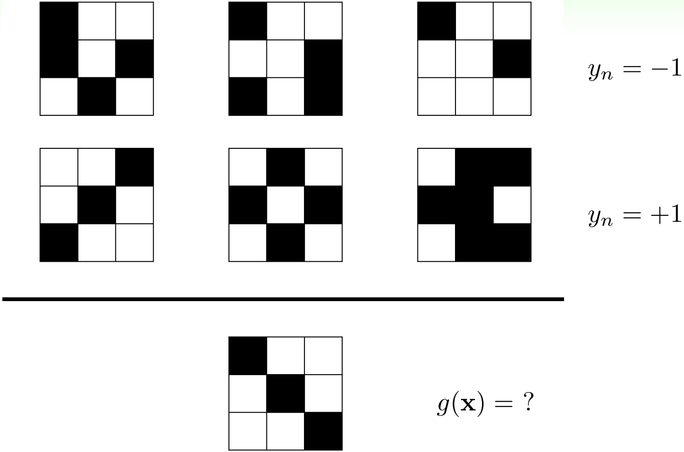
focus: **binary classification** or **regression** from a **batch** of **supervised** data with **concrete** features

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?

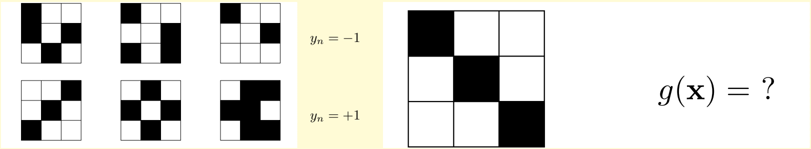
A Learning Puzzle



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

Two Controversial Answers

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



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	×

- $\mathcal{X} = \{0, 1\}^3$, $\mathcal{Y} = \{\circ, \times\}$, 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

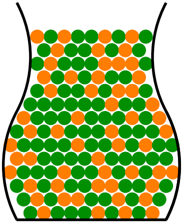
	$\mathbf{x}$	y	g	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8
$\mathcal{D}$	0 0 0	○	○	○	○	○	○	○	○	○	○
$\mathcal{D}$	0 0 1	×	×	×	×	×	×	×	×	×	×
$\mathcal{D}$	0 1 0	×	×	×	×	×	×	×	×	×	×
$\mathcal{D}$	0 1 1	○	○	○	○	○	○	○	○	○	○
$\mathcal{D}$	1 0 0	×	×	×	×	×	×	×	×	×	×
	1 0 1		?	○	○	○	○	×	×	×	×
	1 1 0		?	○	○	×	×	○	○	×	×
	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**. **:-(**

Inferring Something Unknown

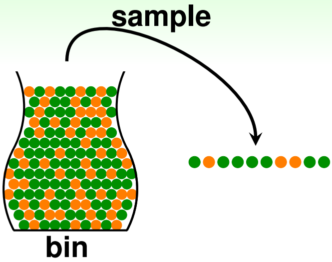
difficult to infer **unknown target f outside $\mathcal{D}$** in learning;
can we infer **something unknown** in **other scenarios**?



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

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

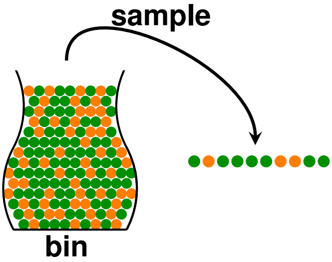
does **in-sample** ν say anything about out-of-sample μ?

No!

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

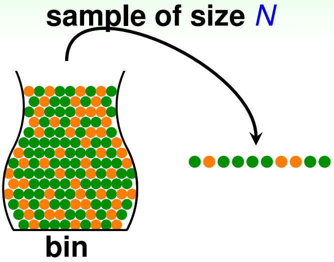
Yes!

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



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

Hoeffding's Inequality (1/2)



$\mu =$ orange
probability in bin

$\nu =$ orange
fraction in sample

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

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

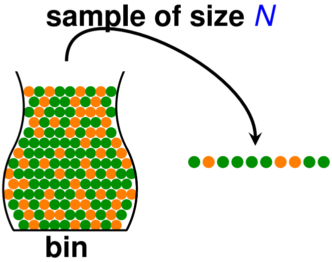
- called **Hoeffding's Inequality**, for marbles, coin, polling, ...

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

Hoeffding's Inequality (2/2)

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

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



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

Connection to Learning

bin

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

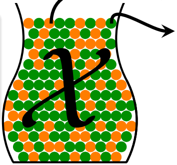
  of i.i.d. marbles

learning

- fixed hypothesis $h(\mathbf{x}) \stackrel{?}{=}$ 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 $\mathcal{D} = \{(\mathbf{x}_n, \underbrace{y_n}_{f(\mathbf{x}_n)})\}$

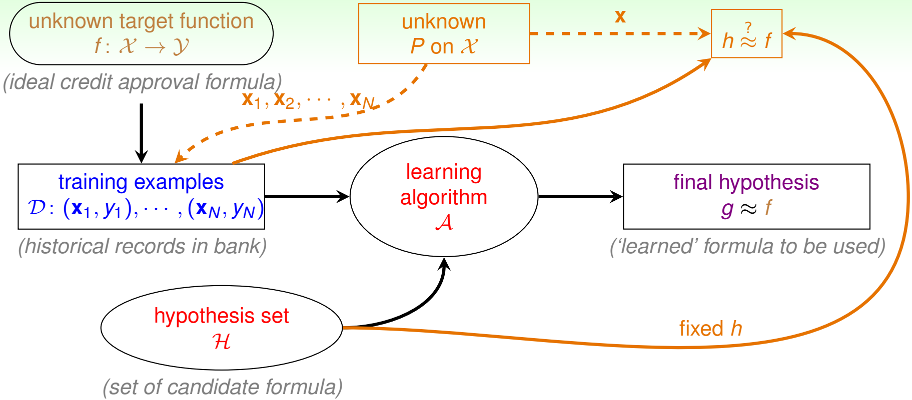
  with i.i.d. $\mathbf{x}_n$

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



- $h(\mathbf{x}) \neq f(\mathbf{x})$
- $h(\mathbf{x}) = f(\mathbf{x})$

Added Components



for any fixed h, can probably infer

$$\textbf{unknown } E_{\text{out}}(\mathbf{h}) = \underset{\mathbf{x} \sim P}{\mathcal{E}} [\![h(\mathbf{x}) \neq f(\mathbf{x})]\!]$$

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

The Formal Guarantee

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

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

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

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

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**'
$\Longrightarrow E_{\text{out}}(h)$ small $\Longrightarrow h \approx f$ 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!

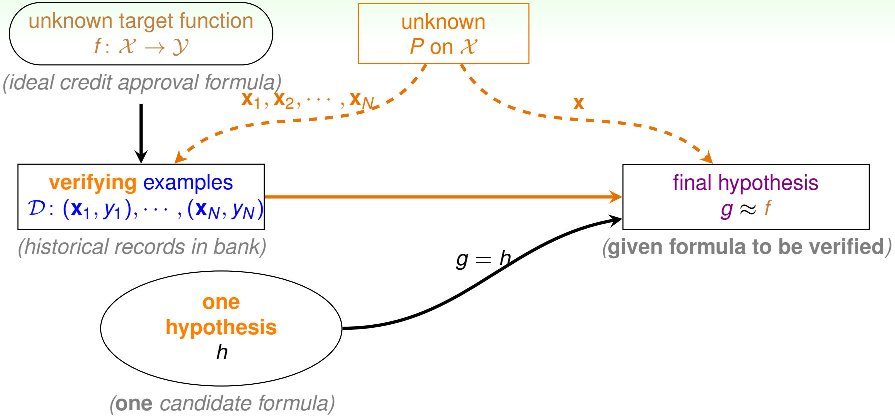
if $E_{\text{in}}(h)$ **small for the fixed** h
and $\mathcal{A}$ **pick the** h **as** g
$\Longrightarrow$ '$g = f$' PAC

No!

if $\mathcal{A}$ **forced to pick THE** h **as** g
$\Longrightarrow$ $E_{\text{in}}(h)$ **almost always not small**
$\Longrightarrow$ '$g \neq f$' 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.

Fun Time

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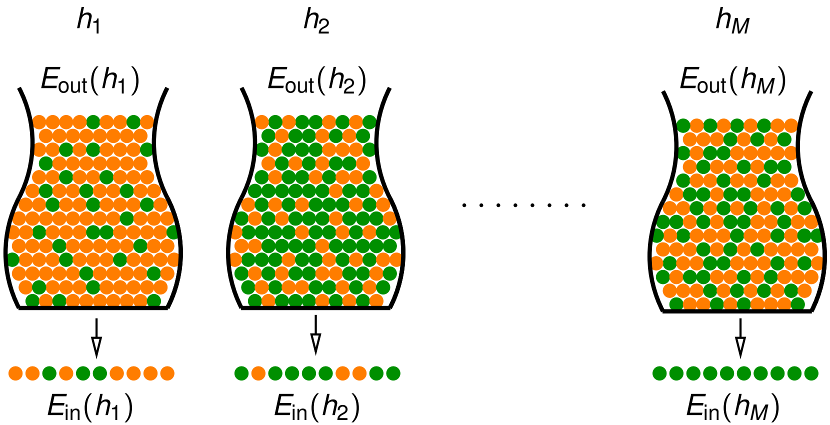
Reference Answer: 2

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.

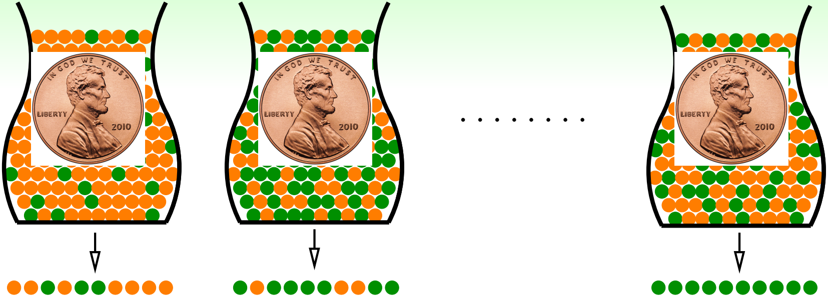
Multiple h



real learning (say like PLA):

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**		$\mathbb{P}_{\mathcal{D}}$ [**BAD** $\mathcal{D}$ for h] $\leq \ldots$

Hoeffding: small

$$\mathbb{P}_{\mathcal{D}}\left[\textbf{BAD } \mathcal{D}\right] = \sum_{\text{all possible}\mathcal{D}} \mathbb{P}(\mathcal{D}) \cdot [\![\textbf{BAD } \mathcal{D}]\!]$$

BAD Data for Many h

BAD data for many h
$\Longleftrightarrow$ **no 'freedom of choice'** by $\mathcal{A}$
$\Longleftrightarrow$ **there exists some h such that** $E_{\text{out}}(h)$ and $E_{\text{in}}(h)$ far away

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

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

Bound of BAD Data

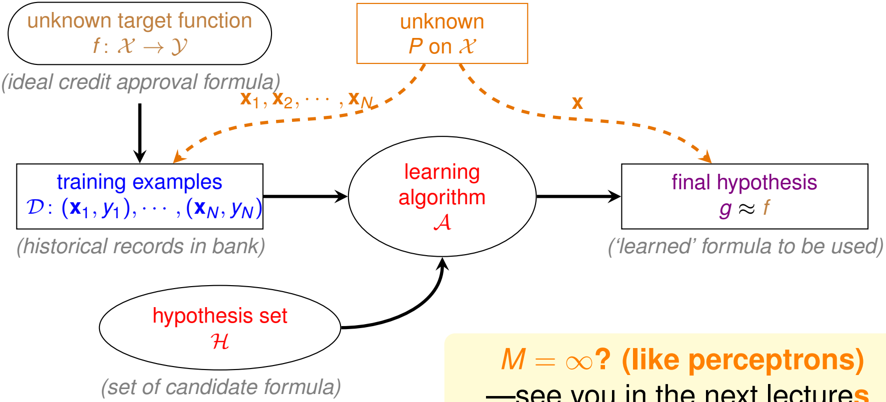
$$
\begin{aligned}
& \mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D}] \\
= \quad & \mathbb{P}_{\mathcal{D}}\,[\textbf{BAD } \mathcal{D} \text{ for } h_1 \textbf{ or } \textbf{BAD } \mathcal{D} \text{ for } h_2 \textbf{ or } \ldots \textbf{ or } \textbf{BAD } \mathcal{D} \text{ for } h_M] \\
\leq \quad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

- 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

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 $E_{\text{out}}(g) \approx 0 \Longrightarrow$ **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. $\mathbb{P}_{\mathcal{D}}$[**BAD** for some h_k] $\leq 8 \exp\left(-2\epsilon^2 N\right)$
4. $\mathbb{P}_{\mathcal{D}}$[**BAD** for some h_k] $\leq 4 \exp\left(-2\epsilon^2 N\right)$

Fun Time

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3. $\mathbb{P}_{\mathcal{D}}[$**BAD** for some $h_k] \leq 8 \exp\left(-2\epsilon^2 N\right)$
4. $\mathbb{P}_{\mathcal{D}}[$**BAD** for some $h_k] \leq 4 \exp\left(-2\epsilon^2 N\right)$

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?