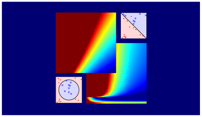
Machine Learning Foundations
(機器學習基石)



Lecture 4: Feasibility of Learning

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?

Lecture 3: Types of Learning

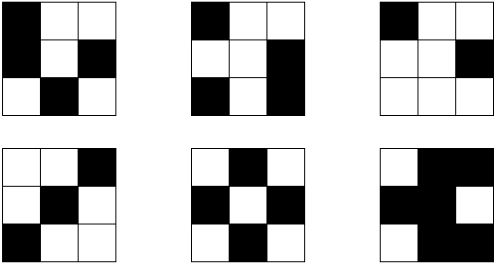
focus: **binary classification** or **regression** from a **batch** of **supervised** data with **concrete** features

Lecture 4: Feasibility of Learning

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

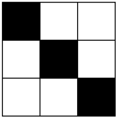
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn Better?

A Learning Puzzle



$y_n = -1$

$y_n = +1$

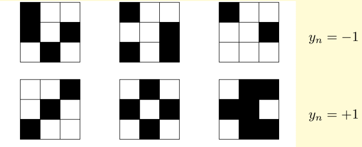


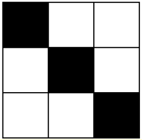
$g(\mathbf{x}) = ?$

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

Two Controversial Answers

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





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

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	$\circ$
0 0 1	$\times$
0 1 0	$\times$
0 1 1	$\circ$
1 0 0	$\times$

- $\mathcal{X} = \{0, 1\}^3$, $\mathcal{Y} = \{\circ, \times\}$, 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
	0 0 0	○	○	○	○	○	○	○	○	○	○
	0 0 1	×	×	×	×	×	×	×	×	×	×
$\mathcal{D}$	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!)

If we learned from D, it would be irrational to infer something that is outside from D.

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'.

$$(5, 3, 2) \to 151022, \qquad (7, 2, 5) \to \textbf{?}$$

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

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1. 151026
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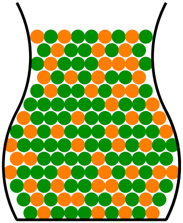
Reference Answer: 4 The answer from Internet is 2, but it's just one explanation.

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**?

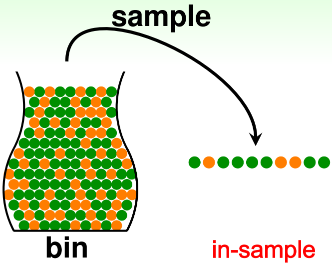


- consider a bin of many many orange and green marbles
- do we **know** the orange portion (probability)? **No!**

can you **infer** the orange probability?

by sample

Statistics 101: Inferring Orange Probability



out-of-sample

bin

assume

orange probability = μ,
green probability = $1 - \mu$,

with μ **unknown**

in-sample

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

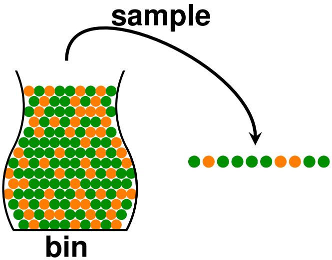
does **in-sample** ν say anything about out-of-sample μ?

No!

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

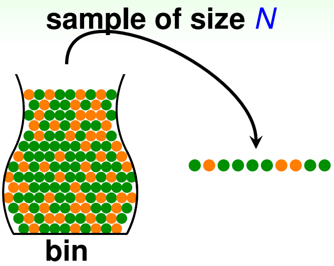
Yes!

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)

The probability of not being close

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

If sample size is very big, the probability of not being close is very small.

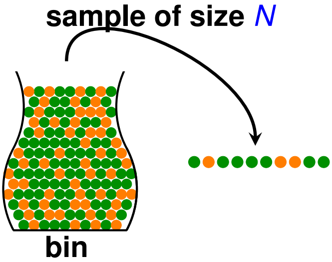
- called **Hoeffding's Inequality**, for marbles, coin, polling, ...

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

Hoeffding's Inequality (2/2)

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

- 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

Fun Time

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

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

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

1. 0.67
2. 0.40
3. 0.33
4. 0.05

Fun Time

v ≤ 0.1 and we take 10 marbles, it means the probability of taking 1 green marble ($\nu = 0.1$) and taking zero green ball ($\nu = 0$)

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

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

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

$C^{10}_{1} \cdot 0.4^{1} \cdot C^{9}_{9} \cdot 0.6^{9}$

$+$

$\underbrace{C^{10}_{0} \cdot 0.4^{0}}_{\text{orange}} \cdot \underbrace{C^{10}_{10} \cdot 0.6^{10}}_{\text{green}}$

$=$

0.04636

1. 0.67
2. 0.40
3. 0.33
4. 0.05

overestimate (because it's upper bound)

⇗

∵ μ = 0.4 and $\nu \le 0.1$
∴ We can set ϵ to 0.3

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.

$2e^{-2\cdot(0.3)^2\cdot 10} \approx 0.33$

Connection to Learning

unknown

bin

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

  of i.i.d. marbles

learning

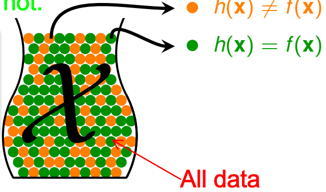
- fixed hypothesis $h(\mathbf{x}) \stackrel{?}{=}$ target $f(\mathbf{x})$
- $\mathbf{x} \in \mathcal{X}$
- h is wrong $\Leftrightarrow h(\mathbf{x}) \neq f(\mathbf{x})$
- h is right $\Leftrightarrow h(\mathbf{x}) = f(\mathbf{x})$
- check h on $\boxed{\mathcal{D} = \{(\mathbf{x}_n, \underbrace{y_n}_{f(\mathbf{x}_n)})\}}$

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

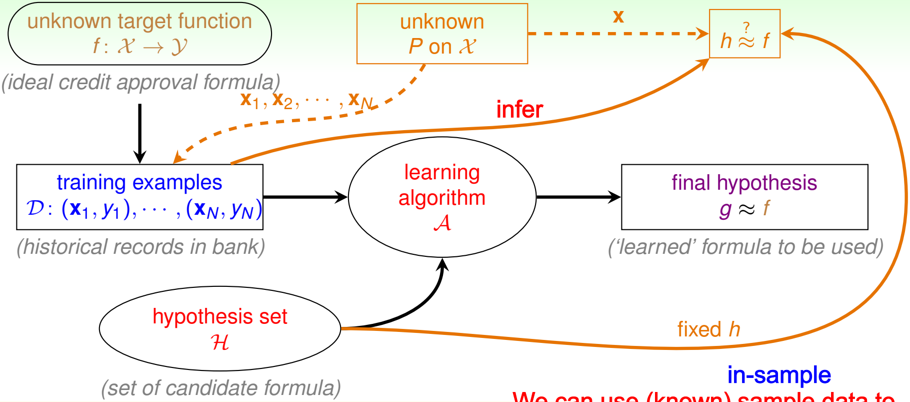
sample
(training data)

All marbles mean all data, and the vase means the h we chose.
The color of marble means the result of h(x) is correct or not.

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



Added Components



for any fixed h, can probably infer

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

by

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

in-sample

We can use (known) sample data to infer (unknown) the whole data.

out-of-sample

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)

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

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)**

We have a model with good results.

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

This model should also do well on unseen data.

Verification of One h

for any fixed h, when data large enough,

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

h: one model in H
g: a well-trained model in H

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

E_{in}(h) needs to be very small.

Yes!

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

No!

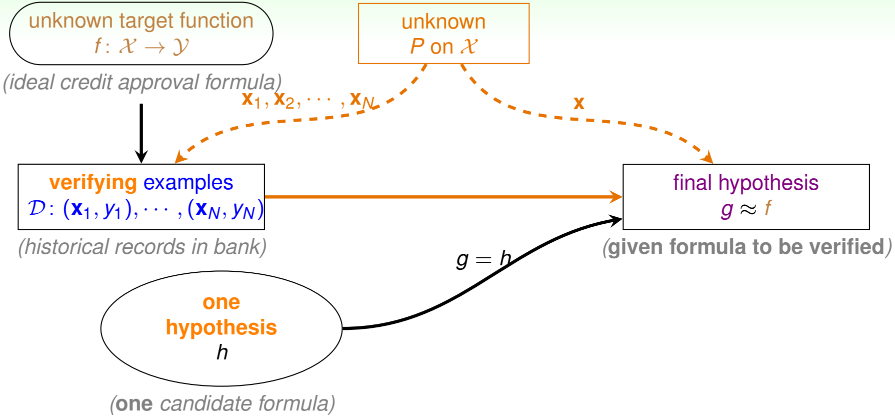
if $\mathcal{A}$ **forced to pick THE** h **as** g
$\Longrightarrow$ $E_{\text{in}}(h)$ **almost always not small**
$\Longrightarrow$ '$g \neq f$' PAC!

If algorithm A always gives us the same h regardless of different sample data, it is NOT machine "learning"!

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

Given h (≡ we don't have A to choose the g from H), we can verify this h's performance.

⇒ This is not learning but verification.

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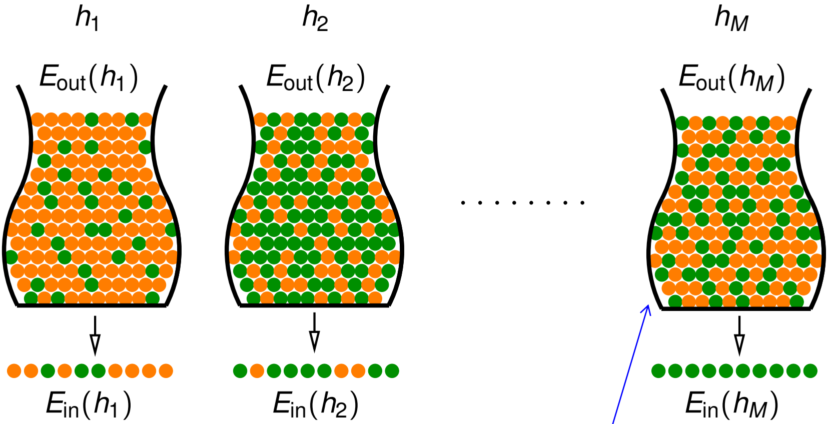
3. You'll likely be rich by exploiting the 'best rule' from 20 more friends in the next 100 days.
4. You'd definitely have been rich if you had exploited the rule in the past 10 years.

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.

Multiple h

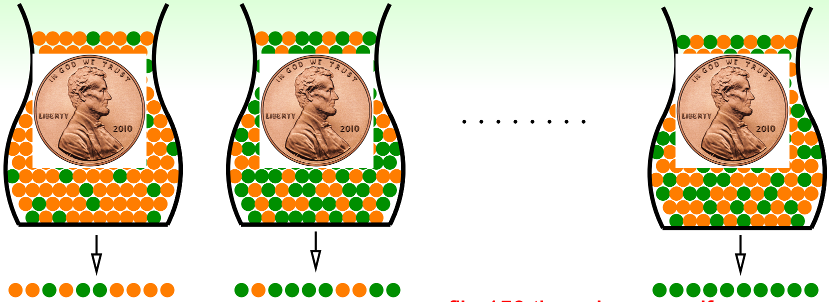
orange: wrong
green: correct



real learning (say like PLA):
BINGO when getting ●●●●●●●●●●?

It's actually a bad hypothesis.

Coin Game



or flip 150 times by yourself

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 $1 - \left(\frac{31}{32}\right)^{150} > 99\%$.

If we had so many vases (h), the possibility of getting a "E_{in} that is a very small one" is very high.

extremely low possibility

in average!

BAD sample: E_{in} and E_{out} far away

—can get worse when involving 'choice'

Toss 1 time

↓

Toss 150 times

The possibility of getting a bad sample becomes way more larger.

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)

one bundle of data

	$\mathcal{D}_1$	$\mathcal{D}_2$	...	$\mathcal{D}_{1126}$	...	$\mathcal{D}_{5678}$	...	Hoeffding
h	**BAD**	GOOD		GOOD		**BAD**	GOOD	$\mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D} \text{ for } h] \le \ldots$

When we grab a small amount of data every time, the chance of catching a handful of bad data is very small.

Hoeffding: small

For one h

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

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

Hoeffding

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

Good data

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

For D_i :
all = h_1 or h_2 or … or h_m

Bound of BAD Data

$$
\begin{aligned}
& \mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D}] \\
= \; & \mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D} \text{ for } h_1 \textbf{ or } \textbf{BAD } \mathcal{D} \text{ for } h_2 \textbf{ or } \ldots \textbf{ or } \textbf{BAD } \mathcal{D} \text{ for } h_M] \\
\leq \; & \mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D} \text{ for } h_1] + \mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D} \text{ for } h_2] + \ldots + \mathbb{P}_{\mathcal{D}}[\textbf{BAD } \mathcal{D} \text{ for } h_M] \\
& \text{(union bound)} \quad \text{worse case: not over-lapping} \\
\leq \; & 2\exp\left(-2\epsilon^2 N\right) + 2\exp\left(-2\epsilon^2 N\right) + \ldots + 2\exp\left(-2\epsilon^2 N\right) \\
= \; & 2M\exp\left(-2\epsilon^2 N\right) \qquad \text{M}\searrow, \text{N}\nearrow \Rightarrow \text{P}\searrow
\end{aligned}
$$

- 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** $\mathcal{A}$

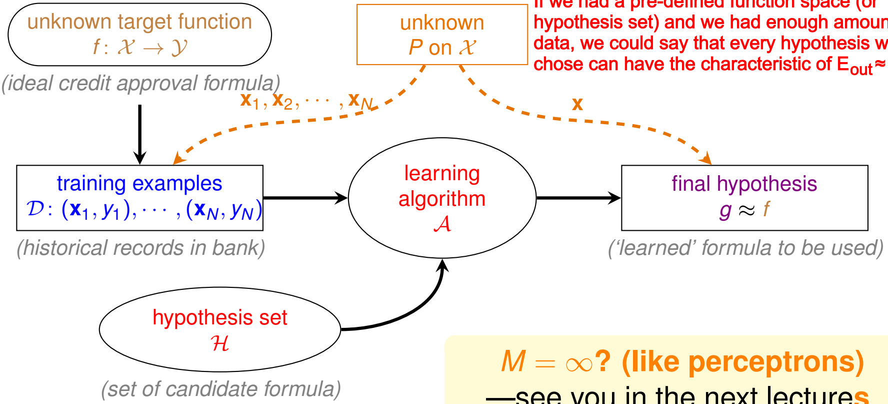
'most reasonable' $\mathcal{A}$ (like PLA/pocket):
pick the h_m with **lowest** $E_{\text{in}}(h_m)$ as g

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 :-)**

If we had a pre-defined function space (or hypothesis set) and we had enough amount of data, we could say that every hypothesis we chose can have the characteristic of $E_{out} \approx E_{in}$.



$M = \infty$? (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. $\mathbb{P}_{\mathcal{D}}[\textbf{BAD} \text{ for some } h_k] \le 8 \exp\left(-2\epsilon^2 N\right)$
4. $\mathbb{P}_{\mathcal{D}}[\textbf{BAD} \text{ for some } h_k] \le 4 \exp\left(-2\epsilon^2 N\right)$

Fun Time

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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?