CSE 417T
Introduction to Machine Learning

Lecture 3

Instructor: Chien-Ju (CJ) Ho

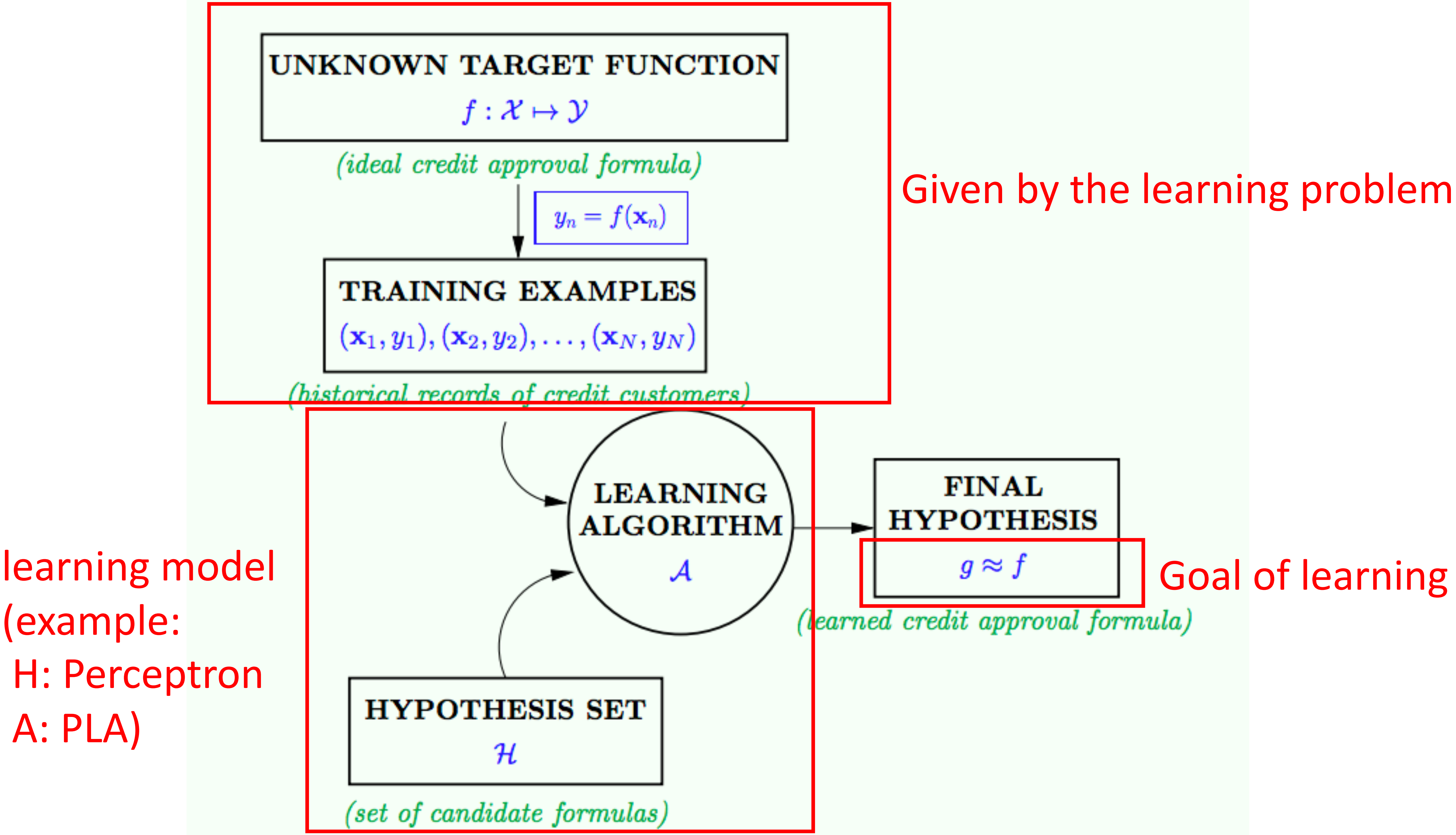
Logistics

- Course website and Piazza
  - Website: http://chienjuho.com/courses/cse417t/
  - Piazza: http://piazza.com/wustl/fall2022/cse417t
  - Make sure you follow both regularly

- Office hours
  - Will be announced later this week
  - Will start next week

- Homework 1
  - Will be announced later this week
  - A mixture of math questions and programming questions
    - Programming language: Python (We won't teach you how to program Python)

Recap


UNKNOWN TARGET FUNCTION
$f : \mathcal{X} \mapsto \mathcal{Y}$
(ideal credit approval formula)
$y_n = f(\mathbf{x}_n)$
TRAINING EXAMPLES
$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)$
(historical records of credit customers)
LEARNING ALGORITHM
$\mathcal{A}$
HYPOTHESIS SET
$\mathcal{H}$
(set of candidate formulas)
FINAL HYPOTHESIS
$g \approx f$
(learned credit approval formula)
Given by the learning problem
Goal of learning
learning model
(example:
H: Perceptron
A: PLA)

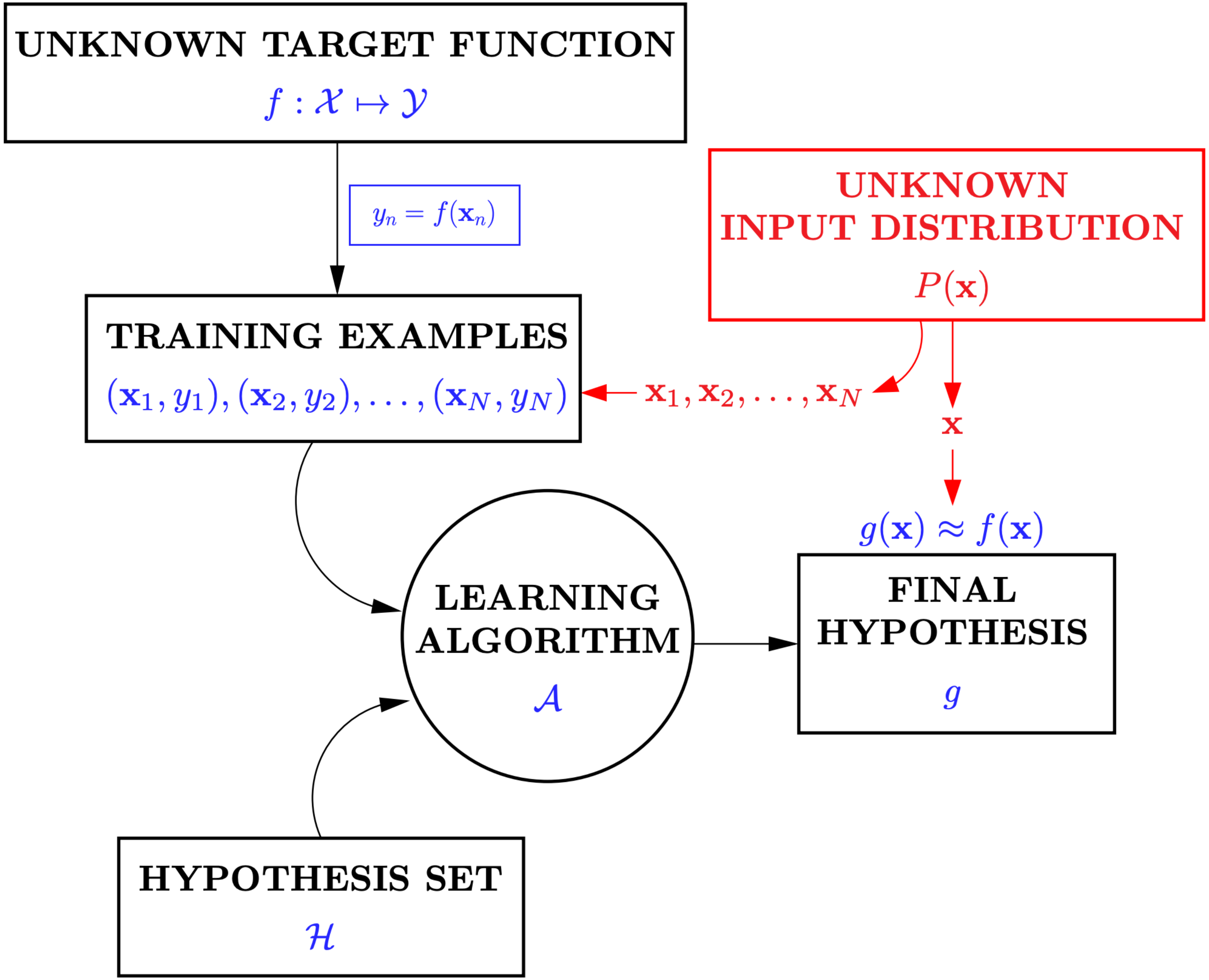
Goal of Learning: Generalization

- Given **training data**, find $g \approx f$ on the **unseen test data**.

- This goal is generally impossible without assumptions.

<u>Key assumption of ML</u>

Training data points and test data points are i.i.d. drawn from the same (unknown) distribution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$P(\mathbf{x})$
TRAINING EXAMPLES
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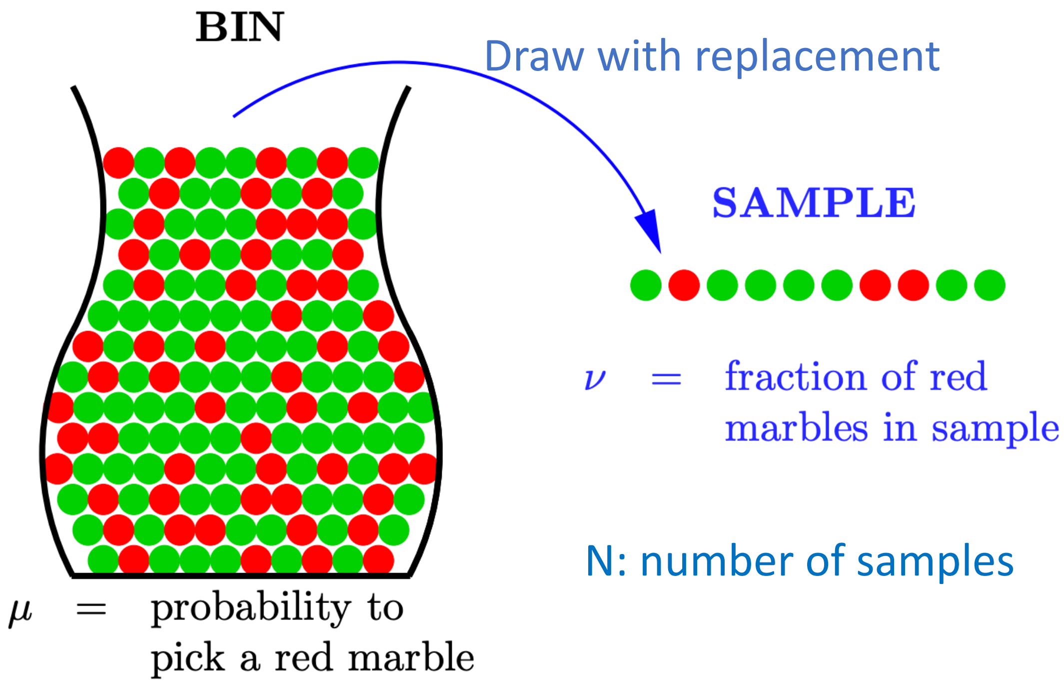
$\mathbf{x}$
$g(\mathbf{x}) \approx f(\mathbf{x})$
LEARNING
ALGORITHM
$\mathcal{A}$
FINAL
HYPOTHESIS
g
HYPOTHESIS SET
$\mathcal{H}$

A Thought Experiment about Probability



What can we say about μ from ν?

Law of large numbers

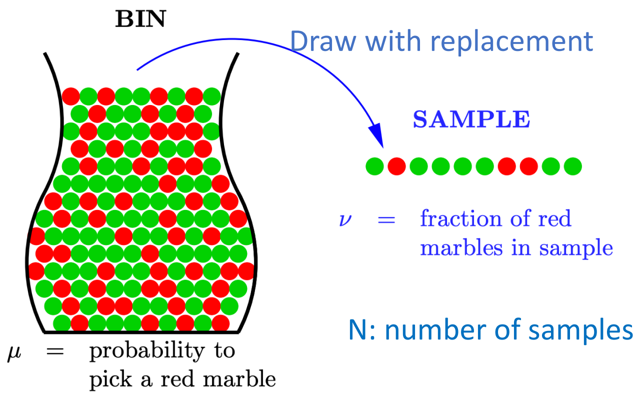
- When $N \to \infty$, $\nu \to \mu$

Hoeffding's Inequality

- $\mathbf{Pr}[|\mu - \nu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$ for any $\epsilon > 0$

Connection to Learning

- Let each marble represent a point $\vec{x}$, drawn from unknown $P(\vec{x})$
  - Dataset $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$
  - Recall that $y_n = f(\vec{x}_n)$ (will discuss noisy target function f later in the semester)
- "Fix" a hypothesis h
  - For each marble $\vec{x}$, color it as below
    - If $h(\vec{x}) = f(\vec{x})$, color it as green marble [h is correct on $\vec{x}$]
    - If $h(\vec{x}) \neq f(\vec{x})$, color it as red marble [h is wrong on $\vec{x}$]



- With the above coloring

$$\mu = \Pr_{\vec{x} \sim P(\vec{x})}[h(\vec{x}) \neq f(\vec{x})] \stackrel{\text{def}}{=} E_{out}(h)$$ **[Out-of-sample error of h]**

$$\nu = \frac{1}{N}\sum_{n=1}^{N} \mathbb{I}[h(\vec{x}_n) \neq f(\vec{x}_n)] \stackrel{\text{def}}{=} E_{in}(h)$$ **[in-sample error of h]**

Connection to Learning

- $\boldsymbol{E_{out}(h)}$: What we really want to know but unknown to us
- $\boldsymbol{E_{in}(h)}$: What we can calculate from dataset

- Fixed a h, What can we say about $E_{out}(h)$ from $E_{in}(h)$?

Hoeffding's Inequality

$\Pr[|E_{out}(h) - E_{in}(h)| > \epsilon] \leq 2e^{-2\epsilon^2 N}$ for any $\epsilon > 0$

- This is verification, not learning!

Verification vs. Learning

- Verification
  - I have a hypothesis h
  - I know $E_{in}(h)$, i.e., how well h performs in my dataset
  - I can infer what $E_{out}(h)$ (how well h will perform for unseen data) might be
- Learning
  - Given a dataset D and hypothesis set H
  - Apply some learning algorithm, that outputs a $g \in \mathrm{H}$
  - Know $E_{in}(g)$
  - Want to infer $E_{out}(g)$

Connection to "Real" Learning

- Given a finite hypothesis set $H = \{h_1, \dots, h_M\}$
  - Will discuss the infinite case in the next few lectures.

- Apply some learning algorithm on D, output a $g \in H$
  - For example, choosing the hypothesis that minimizes in-sample error
    - $g = argmin_{h \in H} E_{in}(h)$

- Can we apply Hoeffding's inequality and claim

$$\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2e^{-2\epsilon^2 N} \quad \text{for any } \epsilon > 0$$

- **No!**

Today’s Lecture

The notes are not intended to be comprehensive.

Let me know if you spot errors.

An Analogy

- Three fair coins, numbered by 1, 2, 3.
  - Flip each coin 10 times

- Question: (choosing from >5, =5, or <5)
  - Ans: = 5 For coin 1, what's the expected number of heads among 10 flips?
  - Ans: = 5 Randomly choose a coin, what's the expected number of heads for this coin?
  - Ans: >5 Look at the realized flips and choose the coin with the largest number of heads. What is the expected number of heads (on the already flipped results) for the coin?
  - Ans: = 5 Without observing the flips, choose the coin anyway you like, what is the expected number of heads of the 10 flips for this coin?

- You will simulate this process (with 1,000 coins) in HW1.

An Analogy

- Connects to learning
  - Coin -> Hypothesis
  - Coin flips -> Performance of hypothesis in training data D

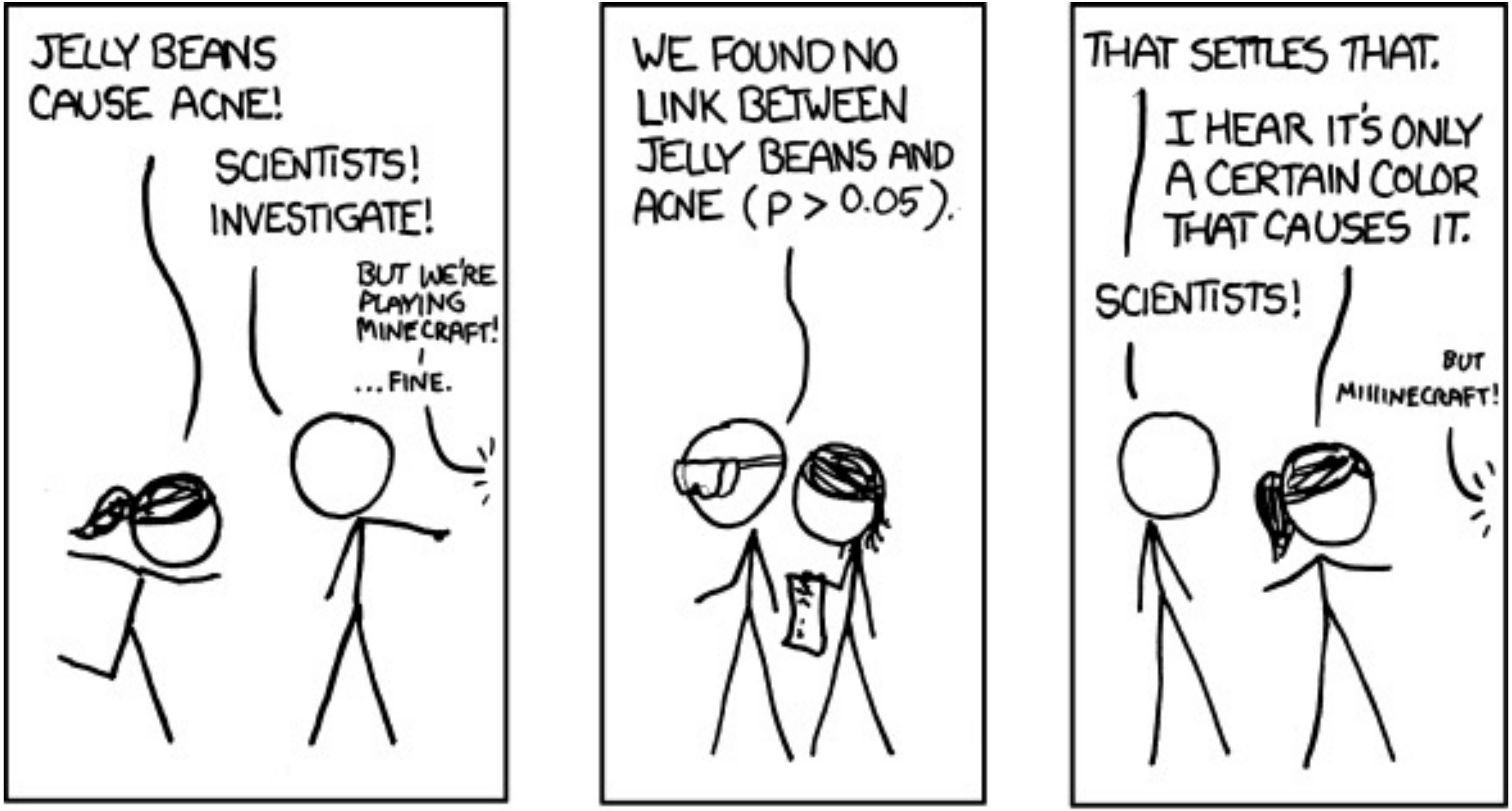
- Choosing the hypothesis “before” or “after” looking at the data (knowing the realization of the data drawing) makes a big difference!

An Analogy

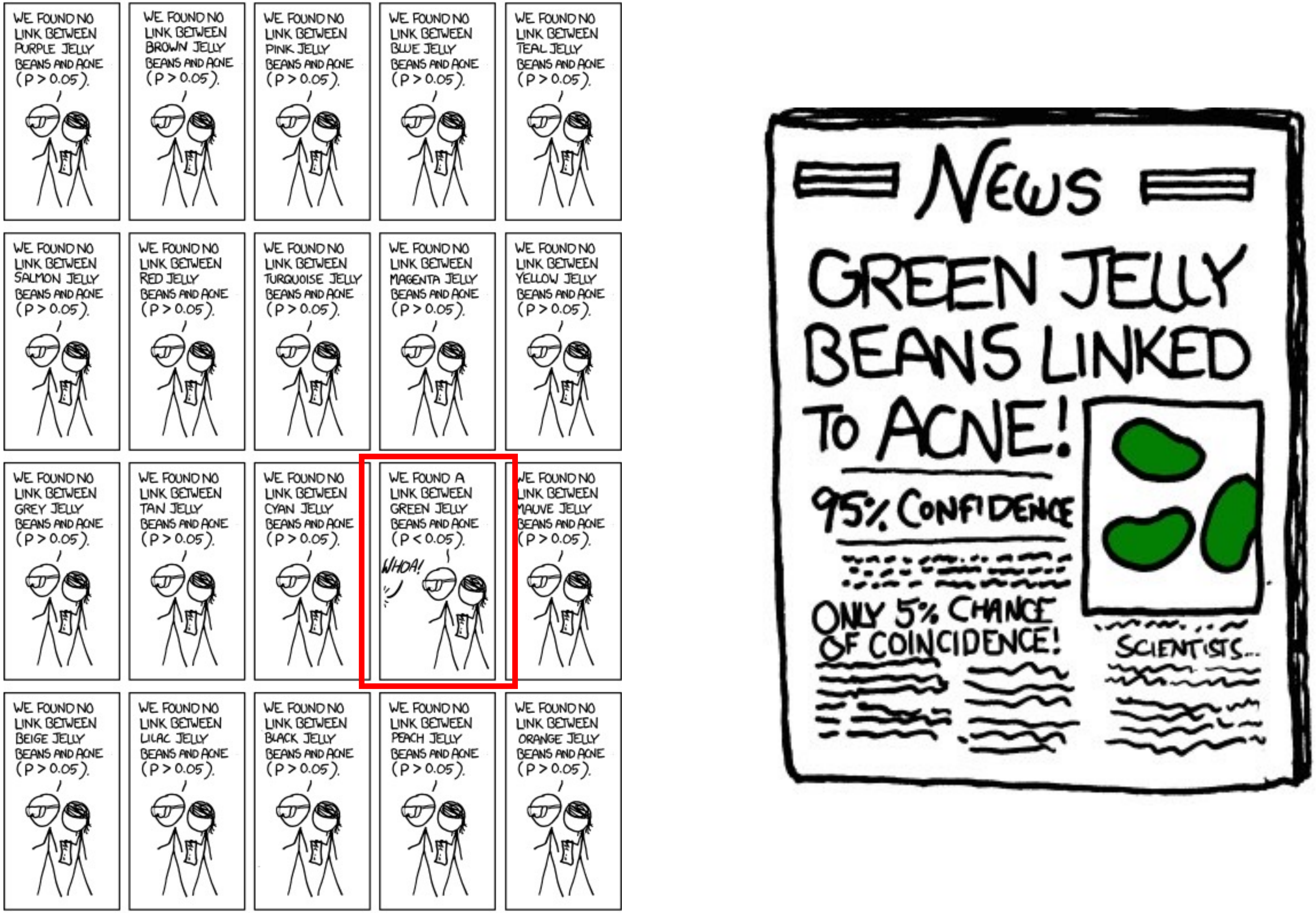
<u>Hoeffding's Inequality</u>

- $\mathbf{Pr}[|\boldsymbol{\mu} - \boldsymbol{\nu}| > \boldsymbol{\epsilon}] \leq \mathbf{2}\boldsymbol{e}^{-\mathbf{2}\boldsymbol{\epsilon}^{\mathbf{2}}\boldsymbol{N}}$ for any $\boldsymbol{\epsilon} > \mathbf{0}$

- Some graphical explanations



From xkcd, by Randall Munroe: http://xkcd.com/882



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What Can We Do?

Connection to "Real" Learning

- Given a finite hypothesis set $H = \{h_1, \dots, h_M\}$
- Apply some learning algorithm on D, output a $g \in H$
  - For example, choosing the hypothesis that minimizes in-sample error
    - $g = argmin_{h \in H} E_{in}(h)$

- Question: What can we say about $E_{out}(g)$ from $E_{in}(g)$?

Derivations

- Define ”bad event of h” $B(h)$ as $|E_{out}(h) - E_{in}(h)| > \epsilon$
  - Informally, you can interpret “bad event of h” as the event that we draw a “unrepresentative dataset D” that makes the in-sample errors of h to be far away from out-of-sample error of h

For each fixed $h \in H$, we have $\Pr[B(h)] \leq 2e^{-2\epsilon^2 N}$

- Recall g is selected from H (it could be any $h \in H$)
- What can we say about $\Pr[B(g)]$?

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For each fixed $h \in H$, we have $\Pr[B(h)] \leq 2e^{-2\epsilon^2 N}$

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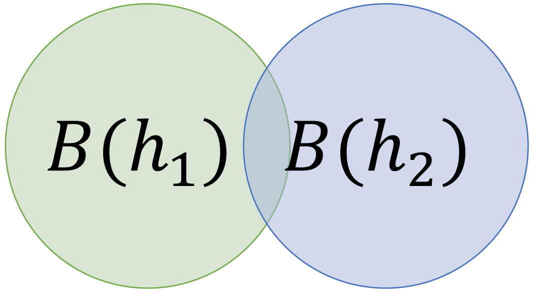
- What can we say about $\Pr[B(g)]$?

If g is selected from $\{h_1, h_2\}$



$B(g) \subseteq B(h_1) \cup B(h_2)$

$$\Pr[B(g)] \leq \Pr[B(h_1) \text{ or } B(h_2)]$$
$$\leq \Pr[B(h_1)] + \Pr[B(h_2)]$$

(Union Bound)

Derivations

- Define "bad event of h" $B(h)$ *as* $|E_{out}(h) - E_{in}(h)| > \epsilon$
  - Informally, you can interpret "bad event of h" as the event that we draw a "unrepresentative dataset D" that makes the in-sample errors of h to be far away from out-of-sample error of h

For each fixed $h \in H$, we have $\Pr[B(h)] \leq 2e^{-2\epsilon^2 N}$

- Recall g is selected from H (it could be any $h \in H$)
- What can we say about $\Pr[B(g)]$?

$$\begin{aligned}\Pr[B(g)] &\leq \Pr[B(h_1) \text{ } or \text{ } B(h_2) \text{ } or \text{ } \ldots or \text{ } B(h_M)] \\ &\leq \Pr[B(h_1)] + \Pr[B(h_2)] + \cdots + \Pr[B(h_M)] \\ &\leq M \, 2e^{-2\epsilon^2 N}\end{aligned}$$

Connection to "Real" Learning

- Given a finite hypothesis set $H = \{h_1, \dots, h_M\}$
- Apply some learning algorithm on D, output a $g \in H$

- Question: What can we say about $E_{out}(g)$ from $E_{in}(g)$?

$$\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \le 2\boldsymbol{M}e^{-2\epsilon^2 N} \quad \text{for any } \epsilon > 0$$

- *M* can be considered as a proxy of the "complexity" of the hypothesis set
  - Will talk about what happens when $M \to \infty$ in the next few lectures

Interpreting $\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$

Interpreting $\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$

- Playing around with the math
  - Define $\delta = \Pr[|E_{out}(g) - E_{in}(g)| > \epsilon]$
  - We have $\delta \leq 2Me^{-2\epsilon^2 N}$ => $\epsilon \leq \sqrt{\frac{1}{2N} \ln \frac{2M}{\delta}}$

Interpreting $\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2\color{red}{M}e^{-2\epsilon^2 N}$

- Playing around with the math
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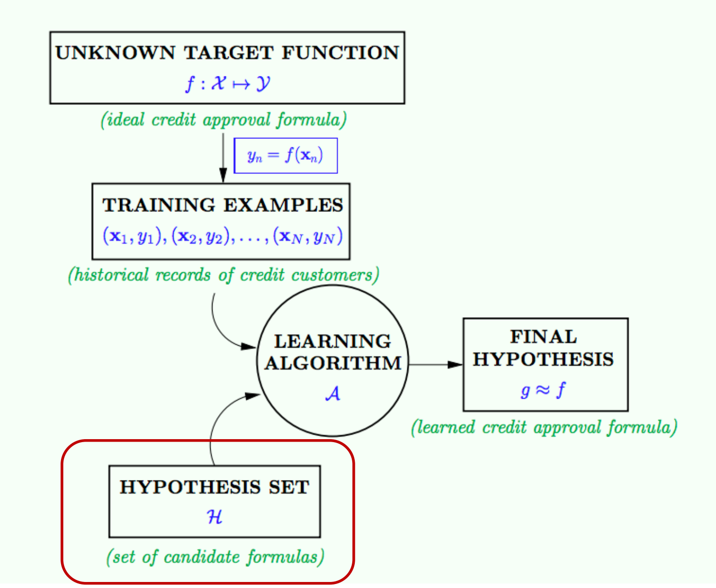
  - We have $\delta \leq 2Me^{-2\epsilon^2 N}$ => $\epsilon \leq \sqrt{\frac{1}{2N}\ln\frac{2M}{\delta}}$

- This means, with probability $1 - \delta$
  - $E_{out}(g) \leq E_{in}(g) + \epsilon \leq E_{in}(g) + \sqrt{\frac{1}{2N}\ln\frac{2M}{\delta}}$

More Discussion



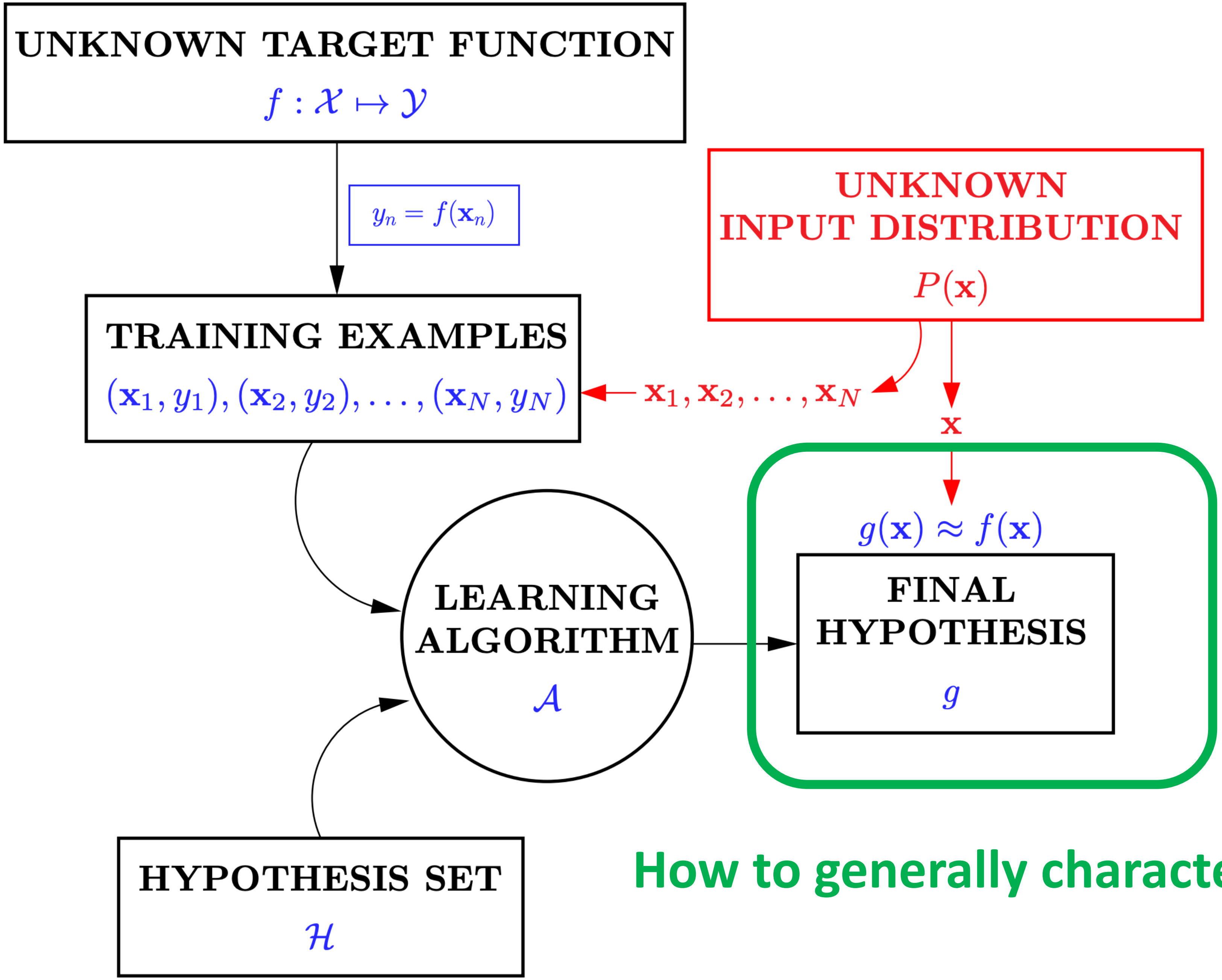
- With probability $1 - \delta$

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{1}{2N} \ln \frac{2M}{\delta}}$$

Consider M as a proxy measure on the "complexity" of H

- Our ultimate goal is to have a small $E_{out}(g)$
  - There is a tradeoff of choosing M (what "learning model" to use)
    - Increase M -> Smaller $E_{in}(g)$ (more hypothesis to "fit" the training data)
    - Increase M -> Larger ϵ
  - It also depends on N, the number of data points you have
    - A small number of data points => use simple models (e.g., linear models)
    - Complex models (e.g., deep learning) work when you have a lot of data

Revisit the Learning Problem



How to generally characterize $g \approx f$

Goal: $g \approx f$

- A general approach:
  - Define an error function $E(h, f)$ that quantify how far away h is to f
  - choose $g = \underset{h \in \mathcal{H}}{\operatorname{argmin}} E(h, f)$

- E is usually defined in terms of a pointwise error function $e(h(\vec{x}), f(\vec{x}))$
  - Binary error (classification): $e(h(\vec{x}), f(\vec{x})) = \mathbb{I}[h(\vec{x}_n) \neq f(\vec{x}_n)]$
  - Squared error (regression): $e(h(\vec{x}), f(\vec{x})) = \big(f(\vec{x}) - h(\vec{x})\big)^2$

$E_{in}(h) = \frac{1}{N} \sum_{n=1}^{N} e(h(\vec{x}_n), f(\vec{x}_n))$

$E_{out}(h) = \mathbb{E}_{\vec{x}}[e(h(\vec{x}), f(\vec{x}))]$

The discussion on the Hoeffding's inequality applies for general (bounded) error functions.

How to choose the error function?

- Consideration 1: Properties of domain applications
- Example: Fingerprint recognition
  - Input: fingerprints
  - Outputs: whether the person is authorized

		$f(\vec{x})$	
		+1	-1
$h(\vec{x})$	+1	No error	False positive
	-1	False negative	No error

Supermarket

		$f(\vec{x})$	
		$+1$	-1
$h(\vec{x})$	$+1$	0	Small
	-1	Large	0

FBI

		$f(\vec{x})$	
		$+1$	-1
$h(\vec{x})$	$+1$	0	Large
	-1	Small	0

How to choose the error function?

- Consideration 1: Properties of application problems

- Consideration 2: Computation
  - ML Algorithm is essentially doing optimization (finding g with smallest error)

$$g = \operatorname*{argmin}_{h \in \mathcal{H}} E(h, f)$$

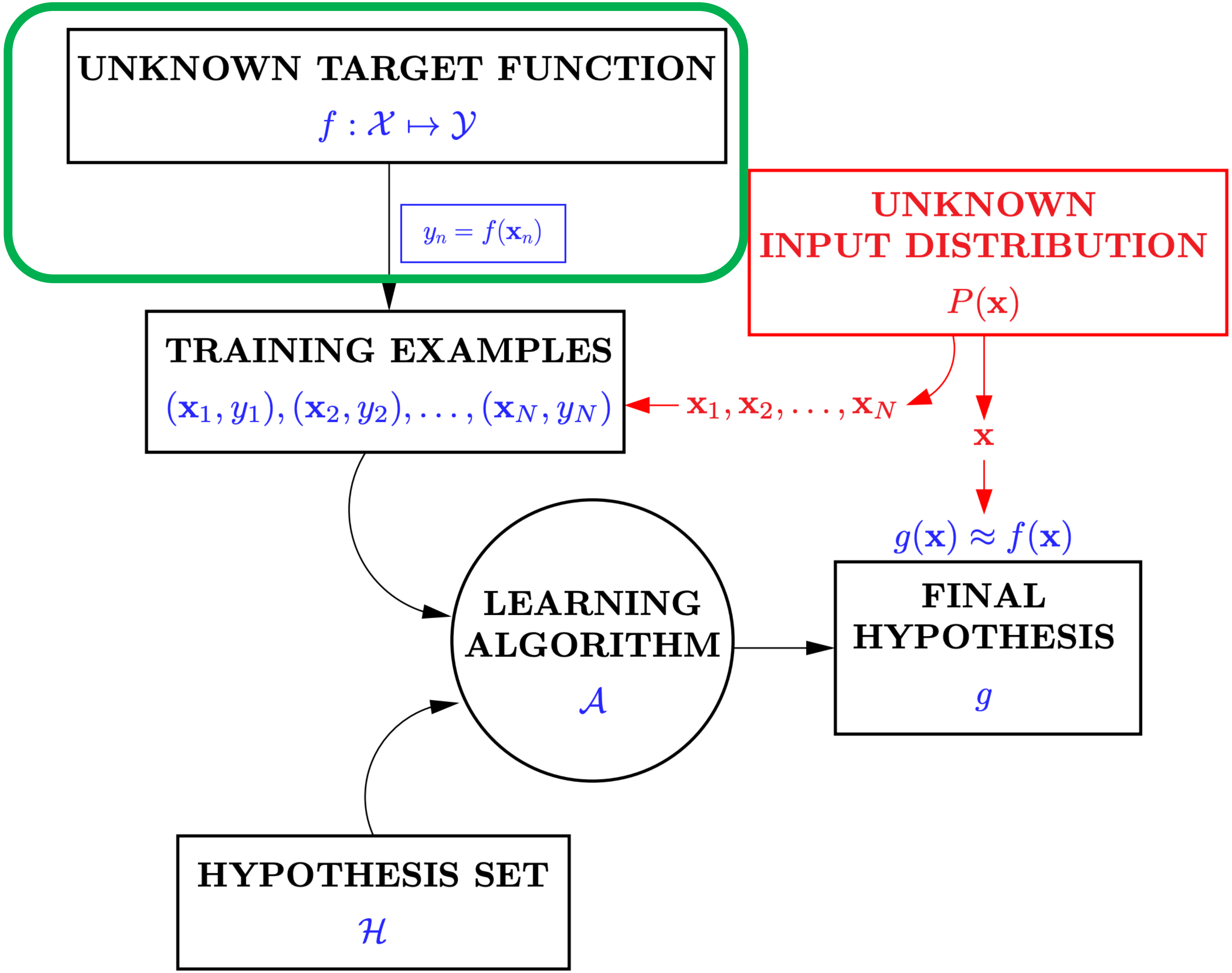
  - Choosing the error that is "easier" to optimize
    - e.g., if the error function is convex, continuous, differentiable, we usually have efficient algorithms

How to choose the error function?

- Consideration 1: Properties of application problems

- Consideration 2: Computation

- Specifying the error function is part of setting up the learning problem
  - It impacts what you eventually learn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$g(\mathbf{x}) \approx f(\mathbf{x})$
LEARNING
ALGORITHM
$\mathcal{A}$
FINAL
HYPOTHESIS
g
HYPOTHESIS SET
$\mathcal{H}$

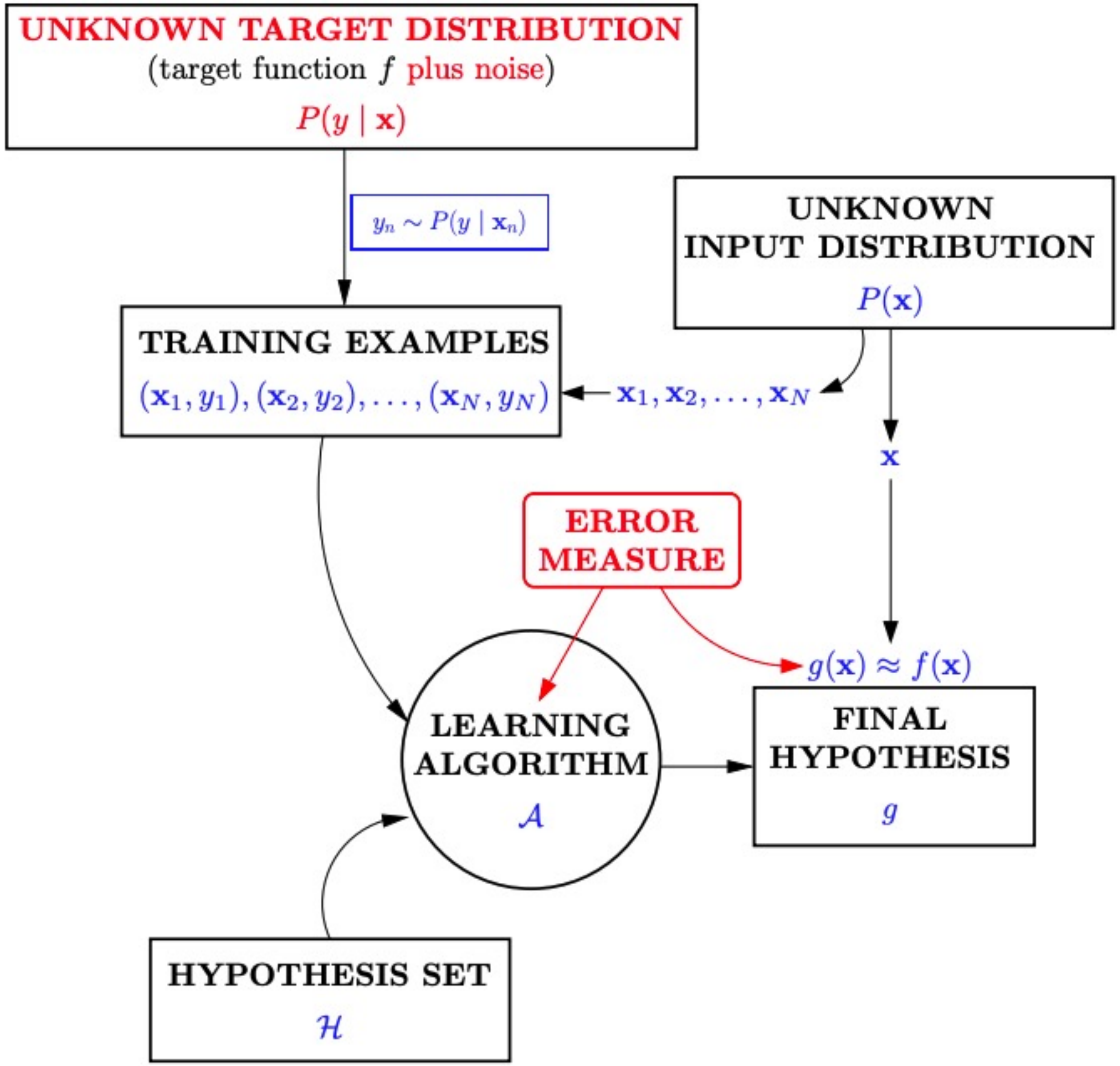
Noisy Target

- What if there doesn't exist f such that $y = f(\vec{x})$?
  - f is stochastic instead of deterministic

- Common approach
  - Instead of a target function, define a target **distribution**
  - Instead of $y = f(\vec{x})$, y is drawn from a conditional distribution $P(y|\vec{x})$
  - $y = f(\vec{x}) + \epsilon$ where ϵ is zero-mean noise

The discussion on the Hoeffding's inequality applies for noisy targets.

General Setup of (Supervised) Learning



Theory of Generalization

Revisit the "Multi-Hypothesis" Bound

- Given a finite hypothesis set $H = \{h_1, \ldots, h_M\}$
- Apply some learning algorithm on D, output a $g \in H$

- What can we say about $E_{out}(g)$ from $E_{in}(g)$?

$$\boldsymbol{Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}} \quad \text{for any } \boldsymbol{\epsilon > 0}$$

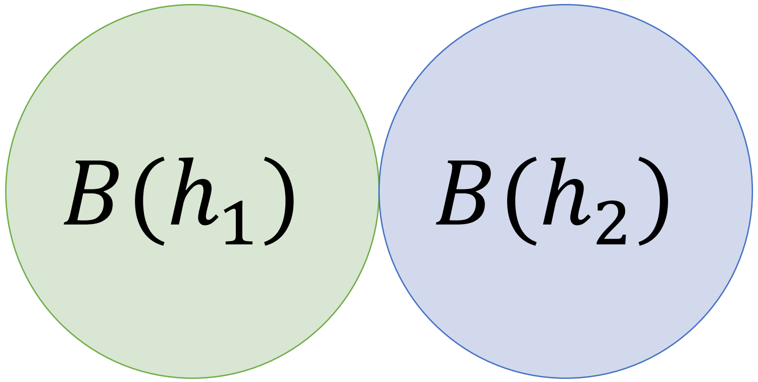
What if M is infinite?

$Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$ don't seem to carry any meanings

Key Intuitions in the Multi-Hypothesis Analysis

- Define "bad event of h" $B(h)\ as\ |E_{out}(h) - E_{in}(h)| > \epsilon$
- If g is selected from $\{h_1, h_2\}$
  - $B(g) \subseteq B(h_1) \cup B(h_2)$
  - $\Pr[B(g)] \leq \Pr[B(h_1) \text{ or } B(h_2)]$

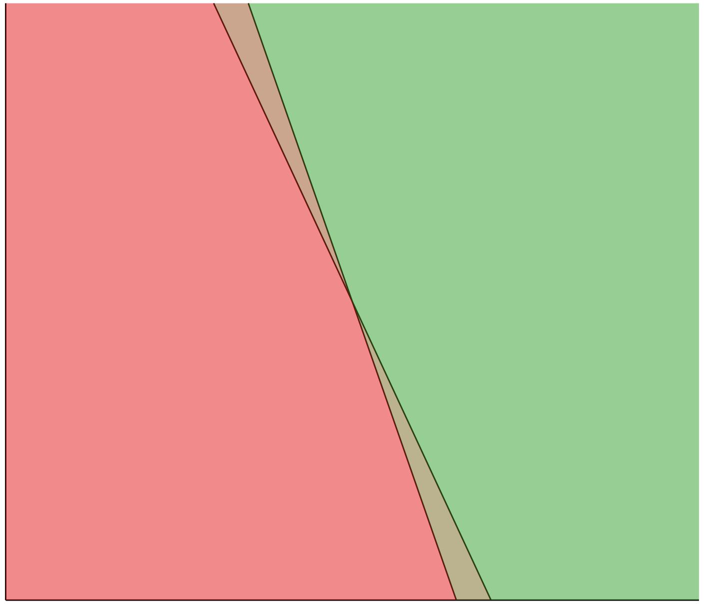
$$\leq \Pr[B(h_1)] + \Pr[B(h_2)]$$ (Union Bound)



- Union bound considers the worst case: Bad events don't overlap

Do Bad Events Overlap?

- Oftentimes, they overlap a lot!



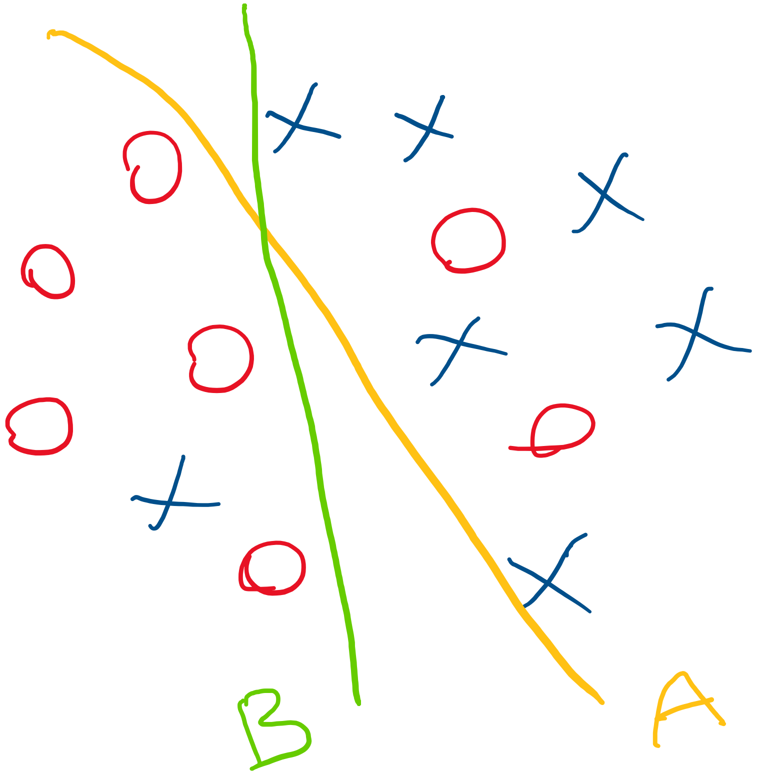
The two linear separators on the left make the same predictions for most points.

If it's a bad event for one, it's likely to be a bad event for the other.

"bad event of h" $B(h)$: $|E_{out}(h) - E_{in}(h)| > \epsilon$

Recall: Informally, you can interpret "bad event of h" as the event that we draw a "unrepresentative dataset D" that makes the in-sample errors of h to be far away from out-of-sample error of h

What Can We Do?



Any difference between A and B?

For this dataset, probably not.

They make the same predictions for every data point in this dataset.

What Can We Do?

- Let’s define “data-dependent” hypothesis, call it dichotomy.

> di·chot·o·my
> /dīˈkädəmē/
>
> *noun*
>
> a division or contrast between two things that are or are represented as being opposed or entirely different.
> "a rigid **dichotomy between** science and mysticism"

- A hypothesis $h: X \to \{-1, +1\}$
- A dichotomy for a set of data points $(\vec{x}_1, \ldots, \vec{x}_N)$:
  - Assign either +1 or -1 for each of the data points (divide the data points into two groups)

- Why dichotomies?
  - It helps us count “effective number of hypothesis” (to replace M)

More Formal Definitions

- Dichotomies
  - Informally, consider a dichotomy as “data-dependent” hypothesis
  - Characterized by both hypothesis set H and N data points $(\vec{x}_1, \dots, \vec{x}_N)$

$$H(\vec{x}_1, \dots \vec{x}_N) = \{h(\vec{x}_1), \dots, h(\vec{x}_N) | h \in H\}$$

  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \dots, \vec{x}_N$

- Growth function
  - Largest number of dichotomies H can induce across all possible data sets of size N

$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$