CSE 417T
Introduction to Machine Learning

Lecture 4

Instructor: Chien-Ju (CJ) Ho

Logistics: Homework 1

- Due: **September 23 (Friday), 2022**
  - http://chienjuho.com/courses/cse417t/hw1.pdf
  - Two submission links: Report and Code (The links will be up over the weekend)
    - Report: Answer all questions, including the implementation question
      - **Grades are based on the report**
    - Code: Complete and submit **hw1.py** for Problem 2
      - The code will only be used for correctness checking (when in doubts) and plagiarism checking
  - Reserve time if you never used Gradescope.
    - Make sure to **specify the pages for each problem**. You **won't get points** otherwise

Logistics: Office Hours

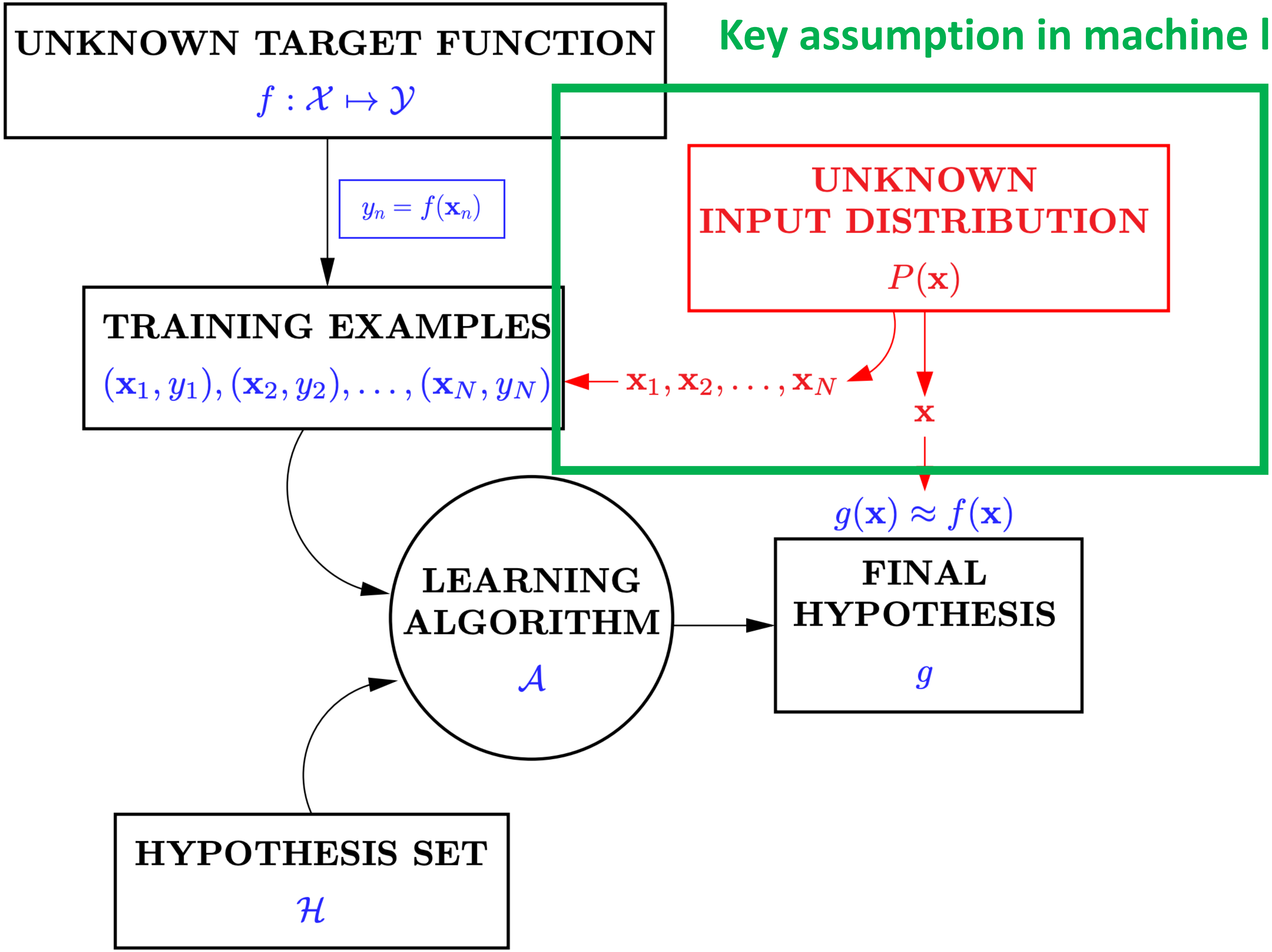
- Tentative schedule of TA office hours (starting next Monday)

Monday	9:30am Asher Baraban	3pm Qihang Zhao	
Tuesday	10am Di Huang	1pm Andrew Ruttenberg	4pm Quinn Wai Wong
Wednesday	1pm Wenxuan Zhu	3pm William Sepesi	4:30pm Sylvia Tang
Thursday	11:30am Yuan Liu	4pm Elyse Tang	7pm Fankun Zen
Friday	11am Riggie Kong	3pm Nan Huang	5:30pm Weiwei Ma
Sunday	Noon Jonathan Ma	1:30pm Kenneth Li	

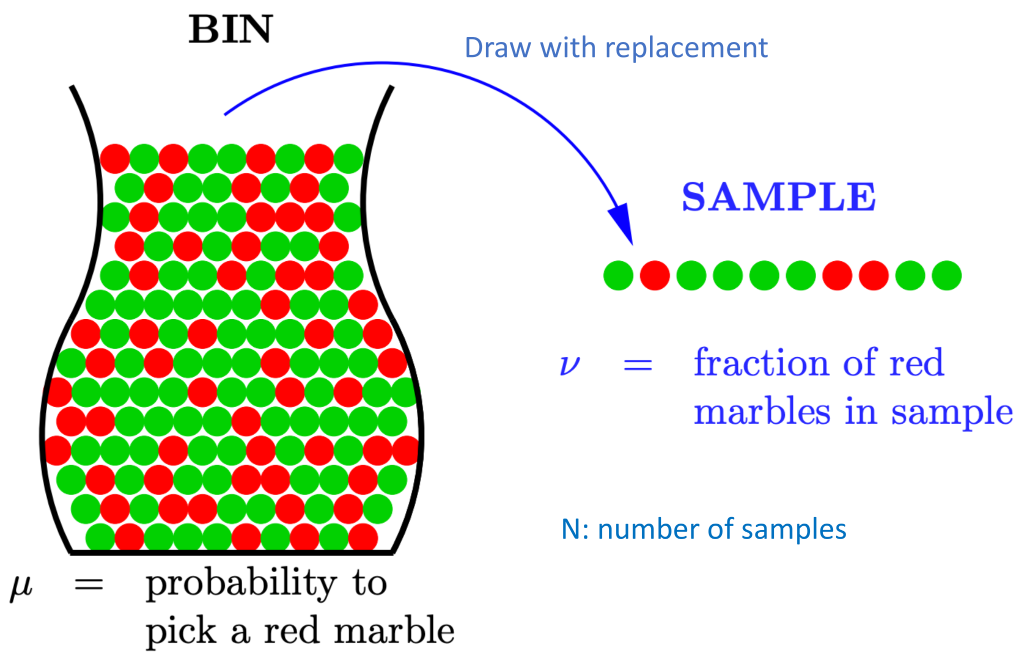
- 60 minutes per session; In-person office hours are highlighted in orange
- Please follow **Piazza** for additional information (location, zoom link, etc)
- Recommendation: Try to utilize the office hour early (way ahead of deadlines), you are likely to get more of TAs' time this way

Recap

Key assumption in machine learning



Hoeffding's Inequality



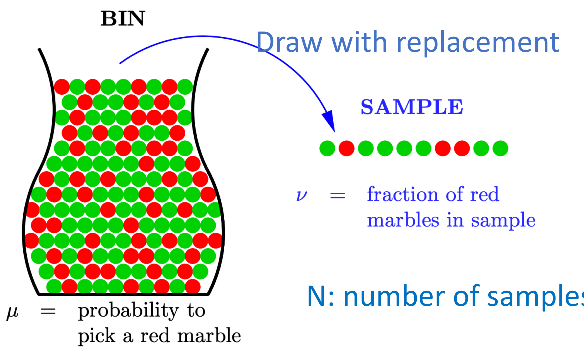
$$\Pr[|\mu - \nu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$$

Define $\delta = \Pr[|\mu - \nu| > \epsilon]$

- Fix δ, ϵ decreases as N increases
- Fix ϵ, δ decreases as N increases
- Fix N, δ decreases as ϵ increases

Informal intuitions of notations
N: # sample
δ: probability of "bad" event
ϵ: error of estimation

Connection to Learning



N: number of samples

- Given dataset $D = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_N, y_N)\}$.
- Fix a hypothesis h
  - $\boldsymbol{E_{in}(h)} \stackrel{\text{def}}{=} \frac{1}{N}\sum_{n=1}^{N} \mathbb{I}[h(\vec{x}_n) \neq f(\vec{x}_n)]$ [In-sample error, analogy to ν]
  - $\boldsymbol{E_{out}(h)} \stackrel{\text{def}}{=} \Pr_{\vec{x}\sim P(\vec{x})}[h(\vec{x}) \neq f(\vec{x})]$ [Out-of-sample error, analogy to μ]
- Apply Hoeffding's inequality

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

- This is *verification*, not *learning*

Connection to "Real" Learning

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

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

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

Intuitions:

1. Bad event $B(g) \subseteq B(h_1) \cup B(h_2) \dots \cup B(h_M)$

   g is selected within $\{h_1, \dots, h_M\}$

   => bad event of g is within the union of the bad events of $h_1, \dots, h_M$

2. $\Pr[B(g)] \leq \Pr[B(h_1)] + \cdots + \Pr[B(h_M)]$

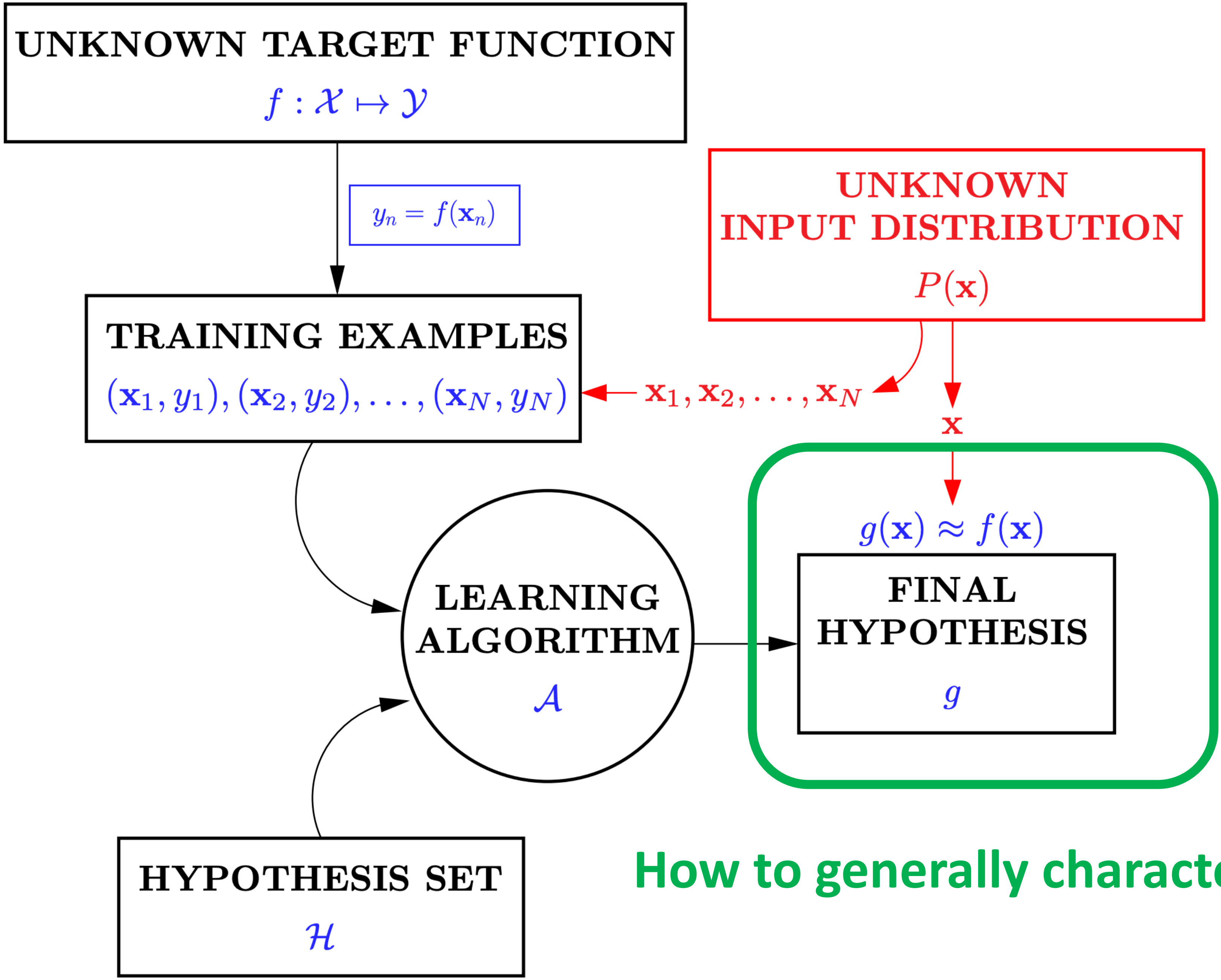
   each of the $\Pr[B(h_m)]$ follows Hoeffding's inequality

Today’s Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

Let me know if you spot errors.

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 $g = \underset{h \in \mathcal{H}}{\operatorname{argmin}} E(h, f)$
- A major component of ML is optimization
- 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): $e(h(\vec{x}), f(\vec{x})) = \left(f(\vec{x}) - h(\vec{x})\right)^2$

$E_{in}(h) = \frac{1}{N}\sum_{n=1}^{N} e(h(\vec{x}_n), f(\vec{x}_n))$
$E_{out}(h) = \mathbb{E}_{\vec{x}}[e(h(\vec{x}), f(\vec{x}))]$

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 algorithms are essentially performing optimization (finding g with smallest error)

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

  - Choose the error that is “easier” to optimize
    - e.g., if the error function is continuous, differentiable, and convex, we usually have efficient algorithms

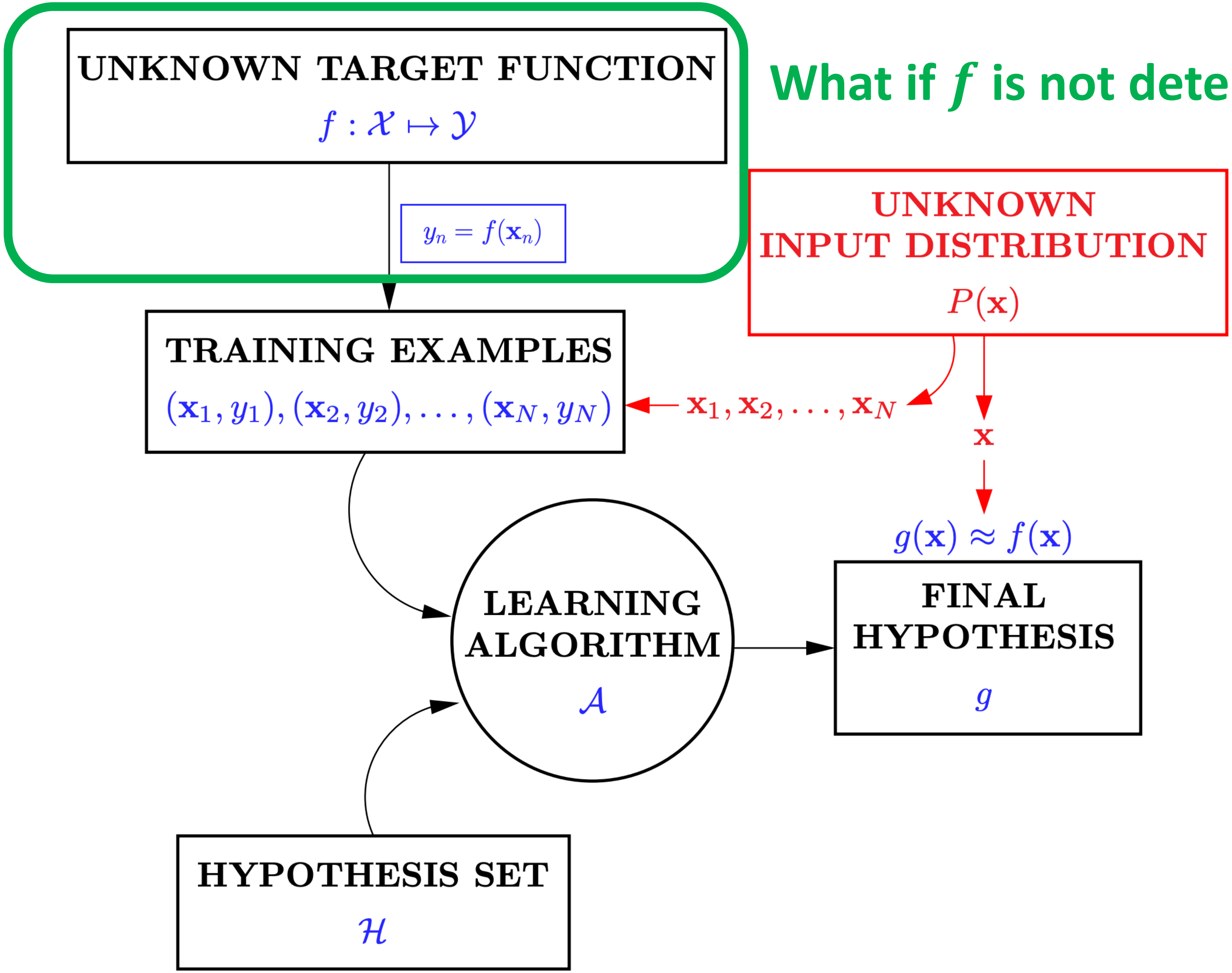
How to choose the error function?

- 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

What if f is not deterministic?



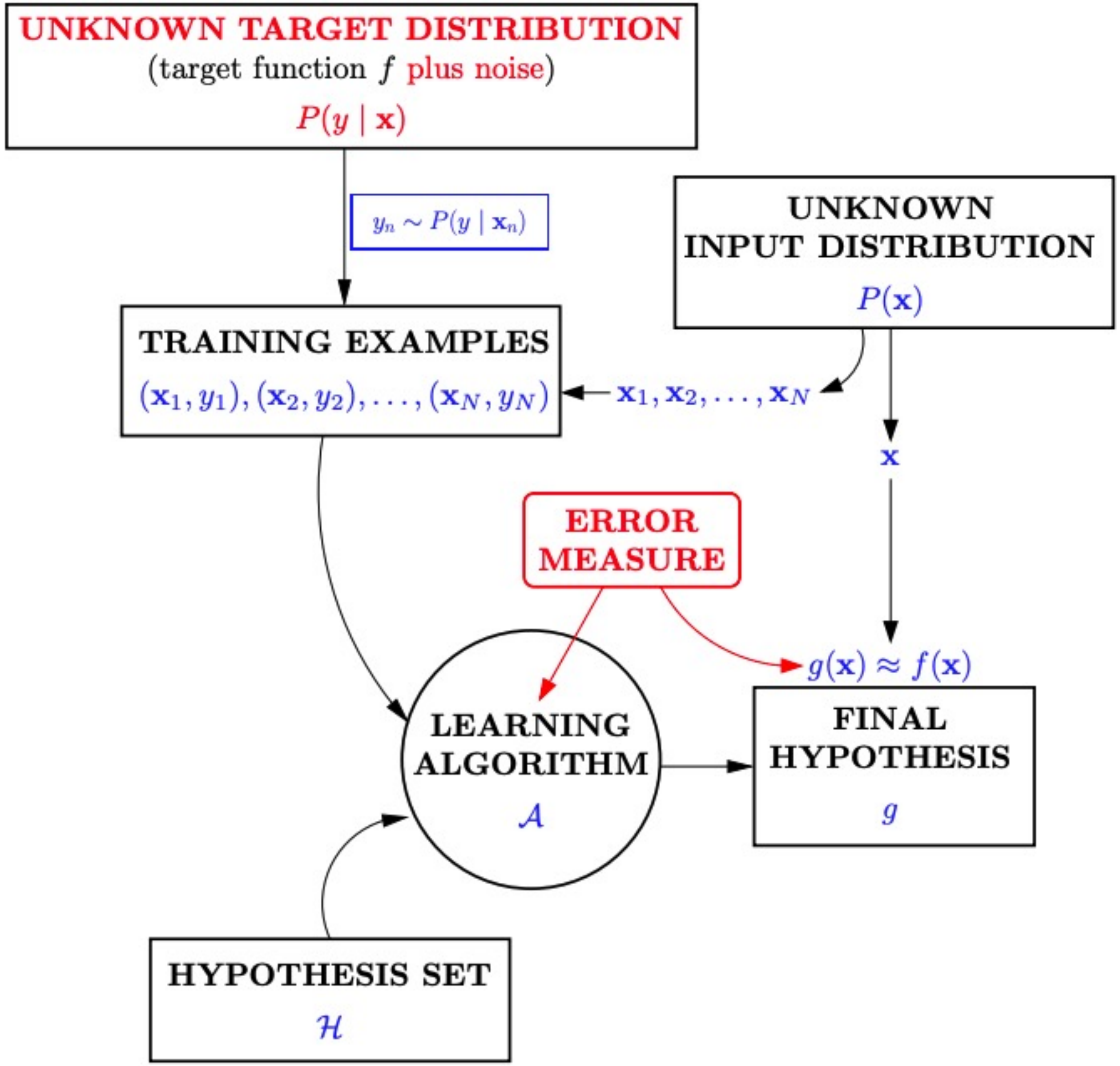
Noisy Target

- What if there doesn't exist f such that $y = f(\vec{x})$?
  - f is stochastic instead of deterministic
  - (even if two customers have exactly the same attributes, one might be a good customer for bank, and the other might not be)

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

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

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

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

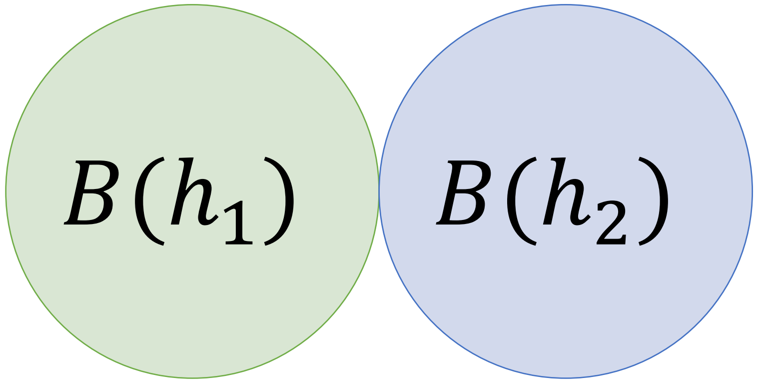
What if M is infinite?

$Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$ 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 $\{h_1, h_2\}$
  - $B(g) \subseteq B(h_1) \cup B(h_2)$
  - $\Pr[B(g)] \leq \Pr[B(h_1) \text{ or } B(h_2)]$

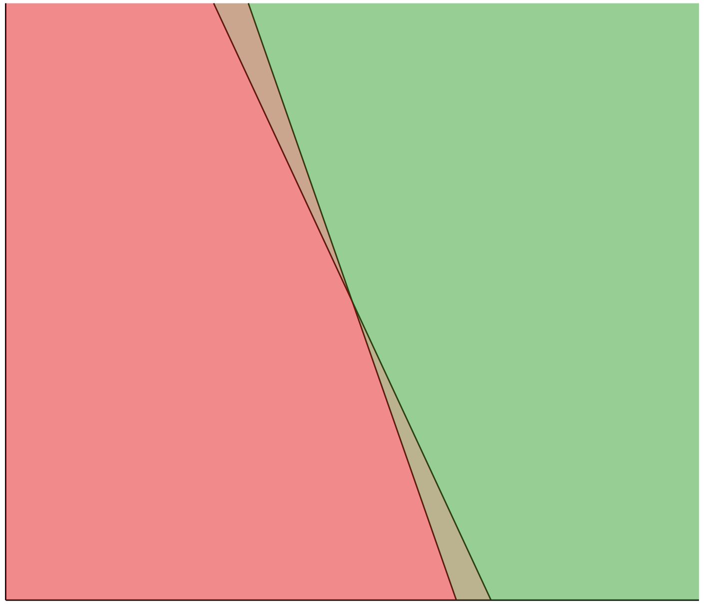
$$\leq \Pr[B(h_1)] + \Pr[B(h_2)]$$ (Union Bound)



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

Do Bad Events Overlap?

- Oftentimes, they overlap a lot!



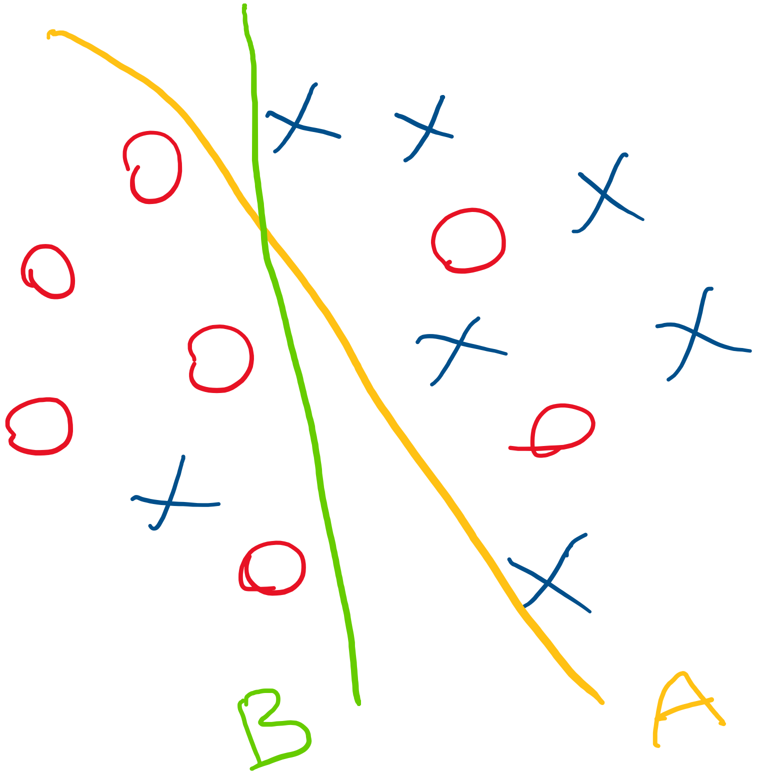
The two linear separators on the left make the same predictions for most points.

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

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

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?



For this dataset,
any difference between A and B?

For this dataset, probably no difference.

They make the same prediction 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 $h: X \rightarrow \{-1, +1\}$
- A dichotomy for a set of data points $(\vec{x}_1, \dots, \vec{x}_N)$:
  - 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

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

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

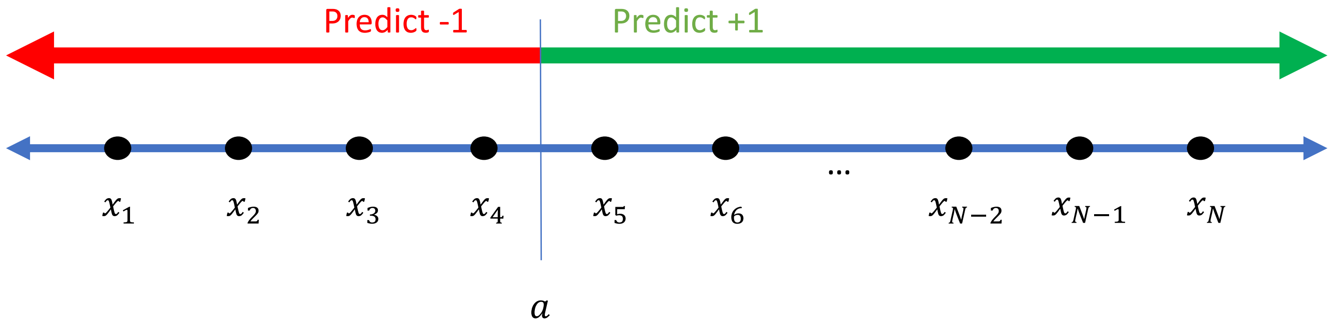
  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \dots, \vec{x}_N$

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

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

Example: H = Positive Rays

- Data points are in one-dimensional space
- Positive rays: $h(x) = sign(x - a)$



- What is $H(\vec{x}_1, \dots, \vec{x}_N)$?
- What is $m_H(N)$?

- <u>Dichotomies</u>
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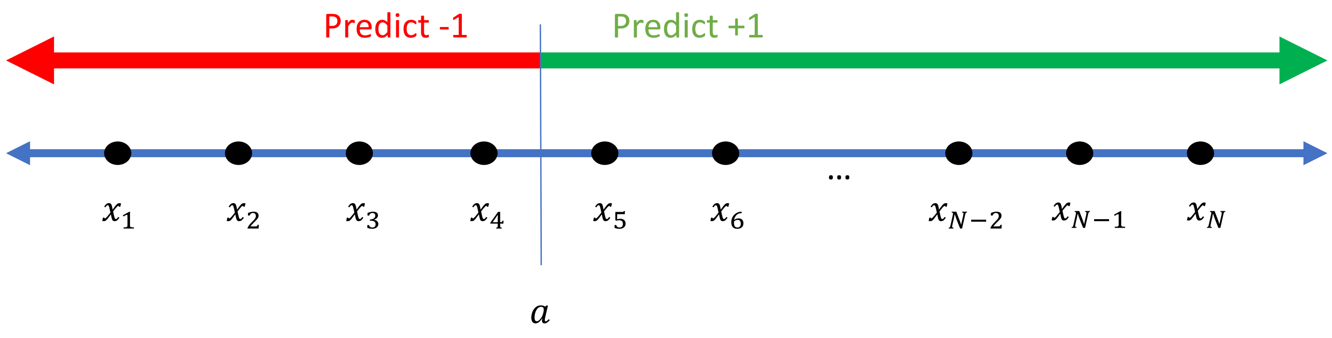

- What is $H(\vec{x}_1, \dots, \vec{x}_N)$?

$$H(\vec{x}_1, \dots, \vec{x}_N) = \{(+1, +1, \dots, +1), \\ (-1, +1, \dots, +1), \\ \dots \\ (-1, -1, \dots, -1)\}$$

- What is $m_H(N)$?

$$m_H(N) = N + 1$$

What is $m_H(N)$?

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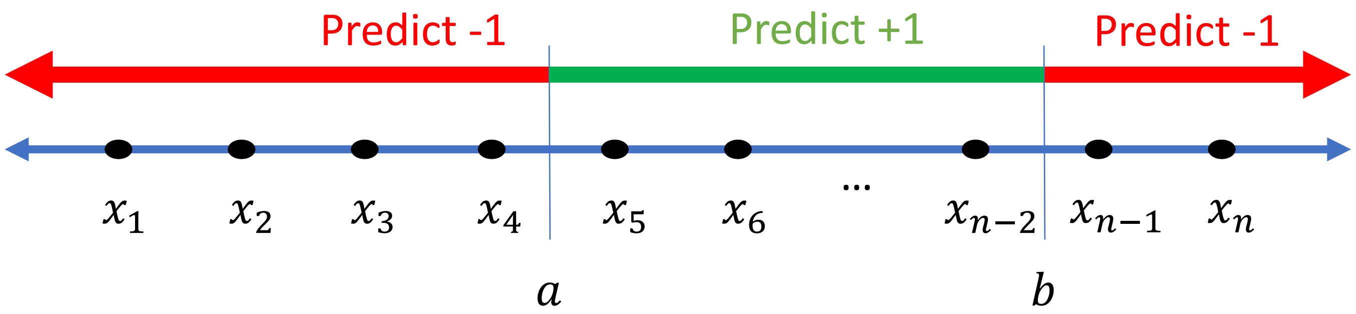
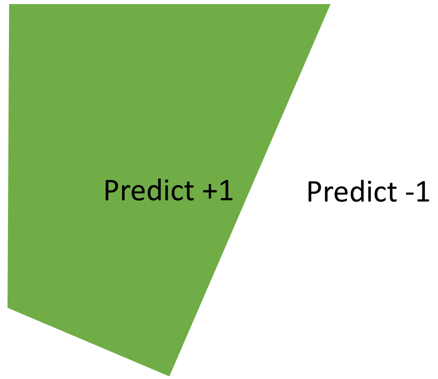
$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

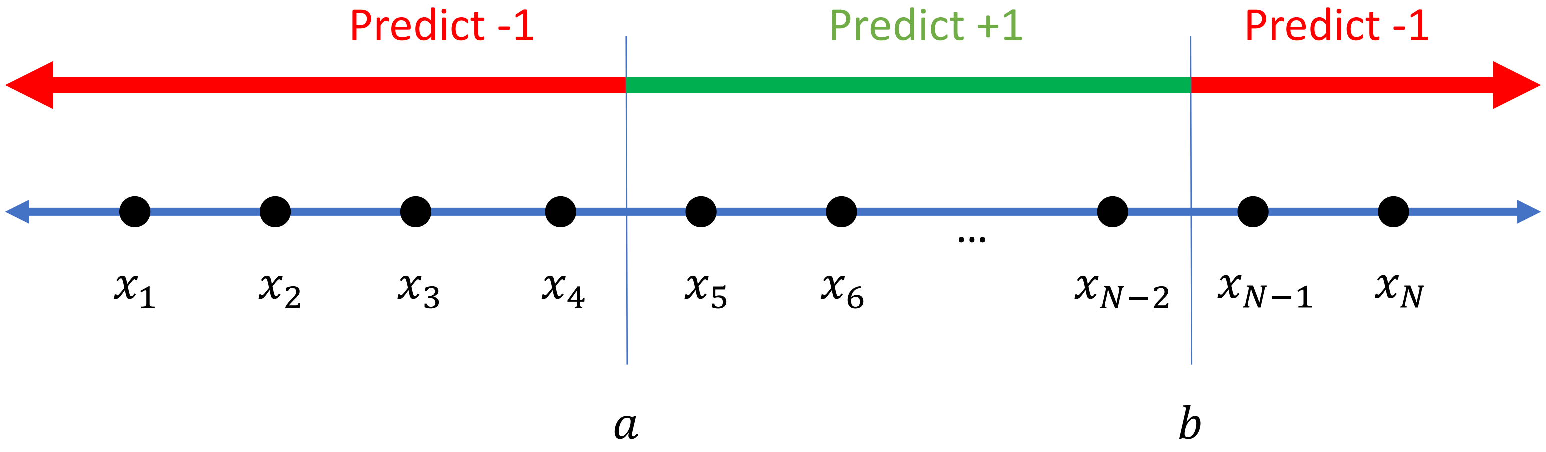
- H = Positive Intervals
  - Data points are in one-dimensional space
  - Choose two thresholds. Predict +1 within the interval, -1 outside



- H = Convex Sets
  - Data points are in 2-dimensional space
  - Hypothesis is represented by a convex set

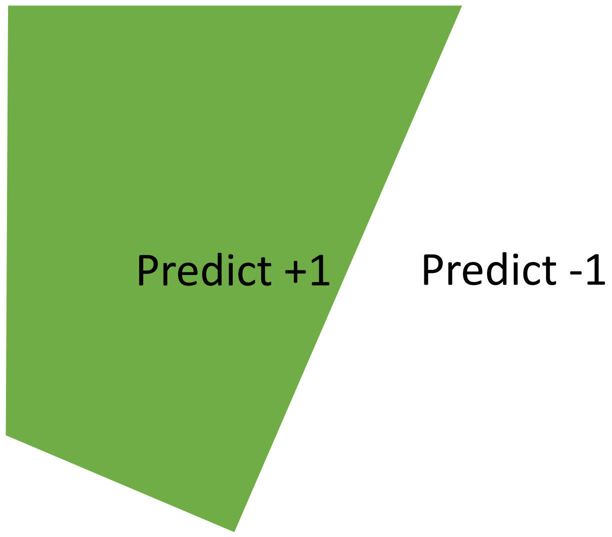


Example: H = Positive Intervals



- What is $m_H(N)$?
  - $m_H(N) = \binom{N+1}{2} + 1 = \frac{N^2}{2} + \frac{N}{2} + 1$

Example: H = Convex Sets



- What is $m_H(N)$?
  - $m_H(N) = 2^N$

Note:
$m_H(N) \leq 2^N$ for all H and all N
(There are only 2^N possible label combinations for N $points$)

Why Growth Function?

- Growth function $m_H(N)$
  - Largest number of "effective" hypothesis H can induce on N data points
  - A more precise "complexity" measure for H
  - Goal: Replace M in finite-hypothesis analysis with $m_H(N)$
    - With prob $1-\delta, E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{1}{2N} ln \frac{2M}{\delta}}$

- Theorem: VC Inequality (1971)

  With prob $1-\delta$

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4m_H(2N)}{\delta}}$$

Growth Functions for Other H

- H = 2-D Perceptron
  - What is $m_H(3)$
  - What is $m_H(4)$

- <u>Dichotomies</u>
  - Informally, consider a dichotomy as a "data-dependent" hypothesis
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$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

- Exactly calculating the growth function is generally hard!

- Goal: "bound" the growth function using some proxy

Bounding Growth Function

- More definitions….
  - Shatter:
    - H **shatters** $(\vec{x}_1, \dots, \vec{x}_N)$ if $|H(\vec{x}_1, \dots, \vec{x}_N)| = 2^N$
    - H can induce all label combinations for $(\vec{x}_1, \dots, \vec{x}_N)$
  - Break point
    - k is a **break point** for H if no data set of size k can be shattered by H
- A peek at the key result (take this as a fact for now)
  - If there are no break points for H, $m_H(N) = 2^N$
  - If k is a break point for H, $m_H(N)$ is polynomial in N.

    In particular, $m_H(N) = O(N^{k-1})$

A bit more accurately:

- $m_H(N) \leq \sum_{i=1}^{k-1} \binom{N}{i}$, or
- $m_H(N) \leq N^{k-1} + 1$