

CSE 417T

# Introduction to Machine Learning

Lecture 4

Instructor: Chien-Ju (CJ) Ho

# Logistics: HW1

- Due: **Feb 19 (Friday), 2020**
  - <http://chienjuho.com/courses/cse417t/hw1.pdf>
  - Strongly encouraged to work on it before the drop deadline
  - Two submission links: Report and Code
    - 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.
- (Optional) Python session
  - See Piazza post

# Logistics: Office Hours

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

Monday	10:00 AM to 11:20 AM (Oliver)	02:30 PM to 03:50 PM (Guanghui)	
Tuesday	02:30 PM to 03:50 PM (Quentin)	05:00 PM to 06:20 PM (Victoria)	
Wednesday	04:30 PM to 05:50 PM (Amrit)	08:00 PM to 09:20 PM (Cecilia)	
Thursday	10:00 AM to 11:20 AM (Aaron)	02:30 PM to 03:50 PM (Matthew)	
Friday	08:00 AM to 09:20 AM (Shohaib)	12:00 PM-1:20 PM (Tong)	04:10 PM to 05:30 PM (Flora)

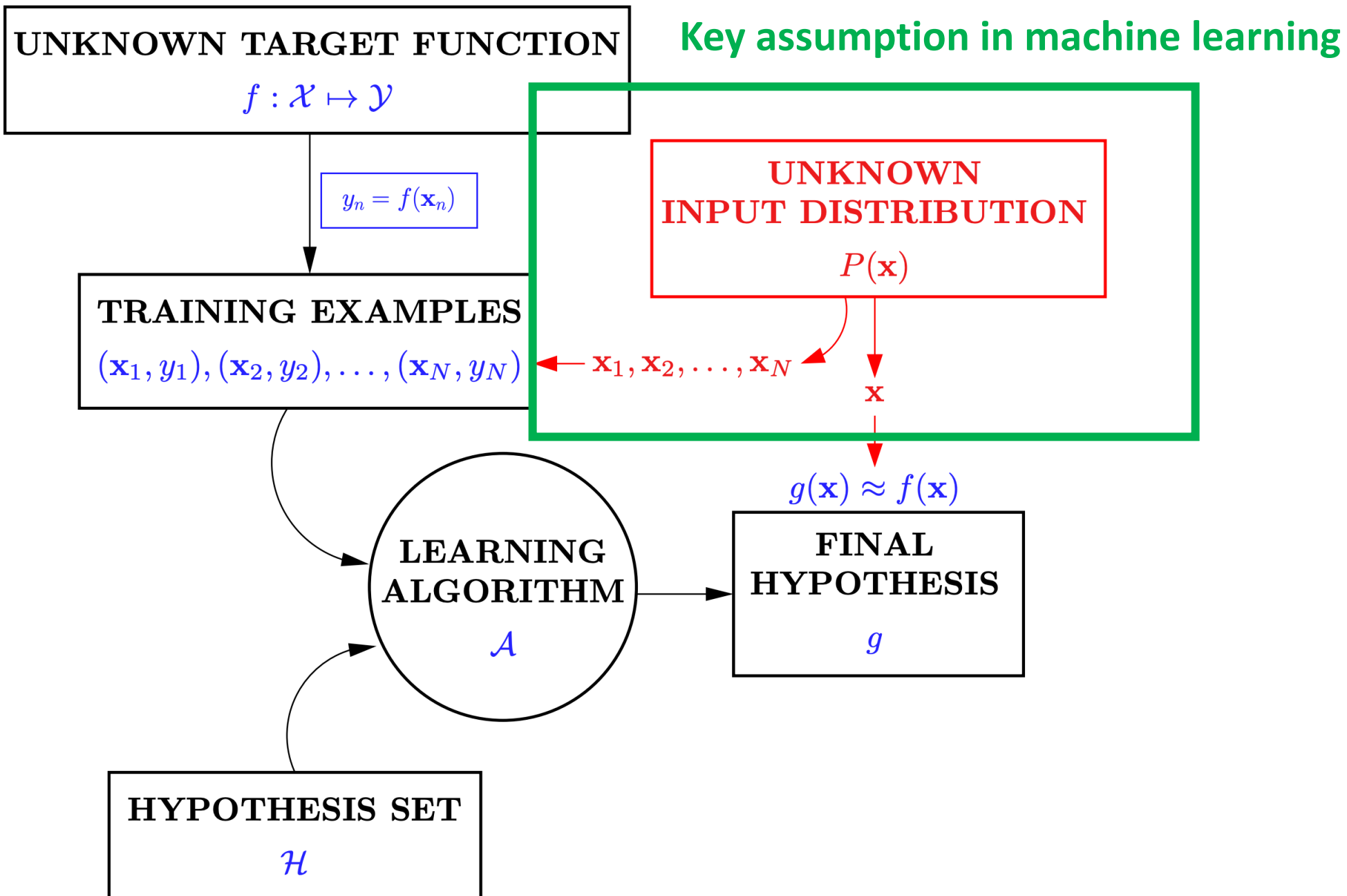
- Remote via Zoom
- Please follow **Piazza** for zoom links and potential updates
- Recommendation: Try to utilize the office hour early (way ahead of deadlines), you are likely to get more of TAs' time this way.

Recap

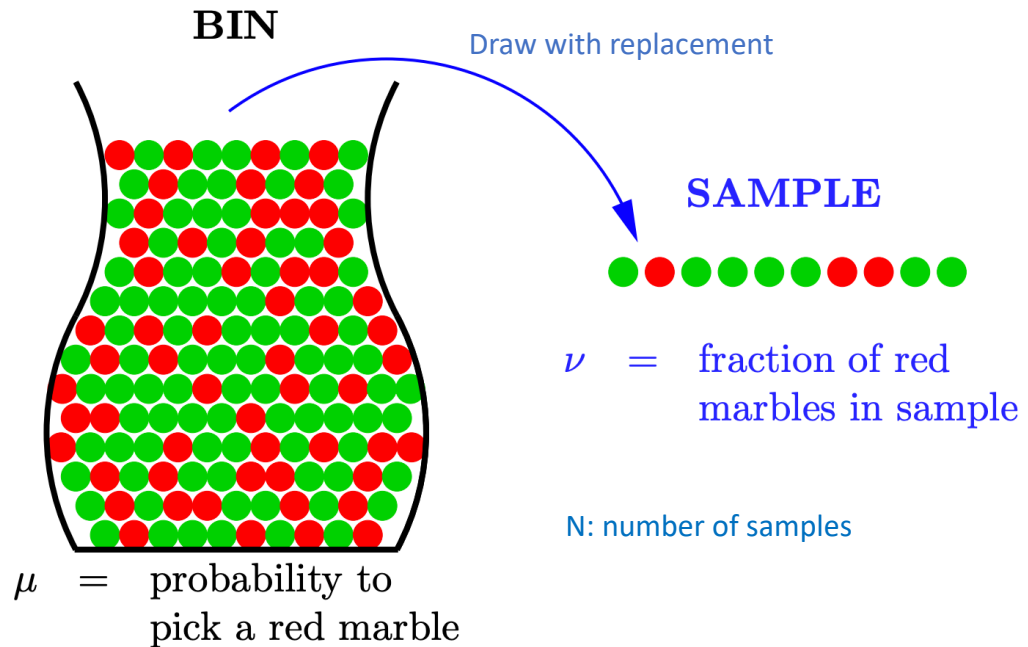
# Common Notations

- Data point with augmented  $x_0$ :  $\vec{x} = (x_0, \dots, x_d)$ 
  - We often use  $d$  to specify the dimensions of data points
  - We augment  $x_0 = 1$  for each data point (Check Lecture 1 for the reasoning)
- Dataset:  $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$ 
  - We often use  $N$  to specify the number of data points in the dataset
- Hypothesis set  $H$ 
  - We use  $h \in H$  to specify an arbitrary hypothesis
  - We use  $g \in H$  to specify the hypothesis output by the learning algorithm
- Indicator variable:
  - $\mathbb{I}[\text{event}] = \begin{cases} 1 & \text{if event is true} \\ 0 & \text{if event is false} \end{cases}$

Example:  $\mathbb{I}[h(\vec{x}) \neq f(\vec{x})] = \begin{cases} 1 & \text{if } h(\vec{x}) \neq f(\vec{x}) \\ 0 & \text{if } h(\vec{x}) = f(\vec{x}) \end{cases}$



# Hoeffding's Inequality



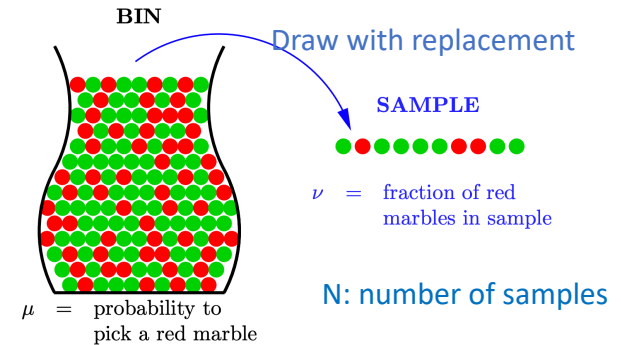
$$\Pr[|\mu - \nu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$$

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

- Fix  $\delta$ ,  $\epsilon$  decreases as  $N$  increases
- Fix  $\epsilon$ ,  $\delta$  decreases as  $N$  increases
- Fix  $N$ ,  $\delta$  decreases as  $\epsilon$  increases

Informal intuitions of notations  
 $N$ : # sample  
 $\delta$ : probability of "bad" event  
 $\epsilon$ : error of estimation

# Connection to Learning



- Given dataset  $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$ .
- Fix a hypothesis  $h$

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

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

- Apply Hoeffding's inequality

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

- 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  $E_{in}(g)$ ?

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

## 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  $h_1, \dots, h_M$

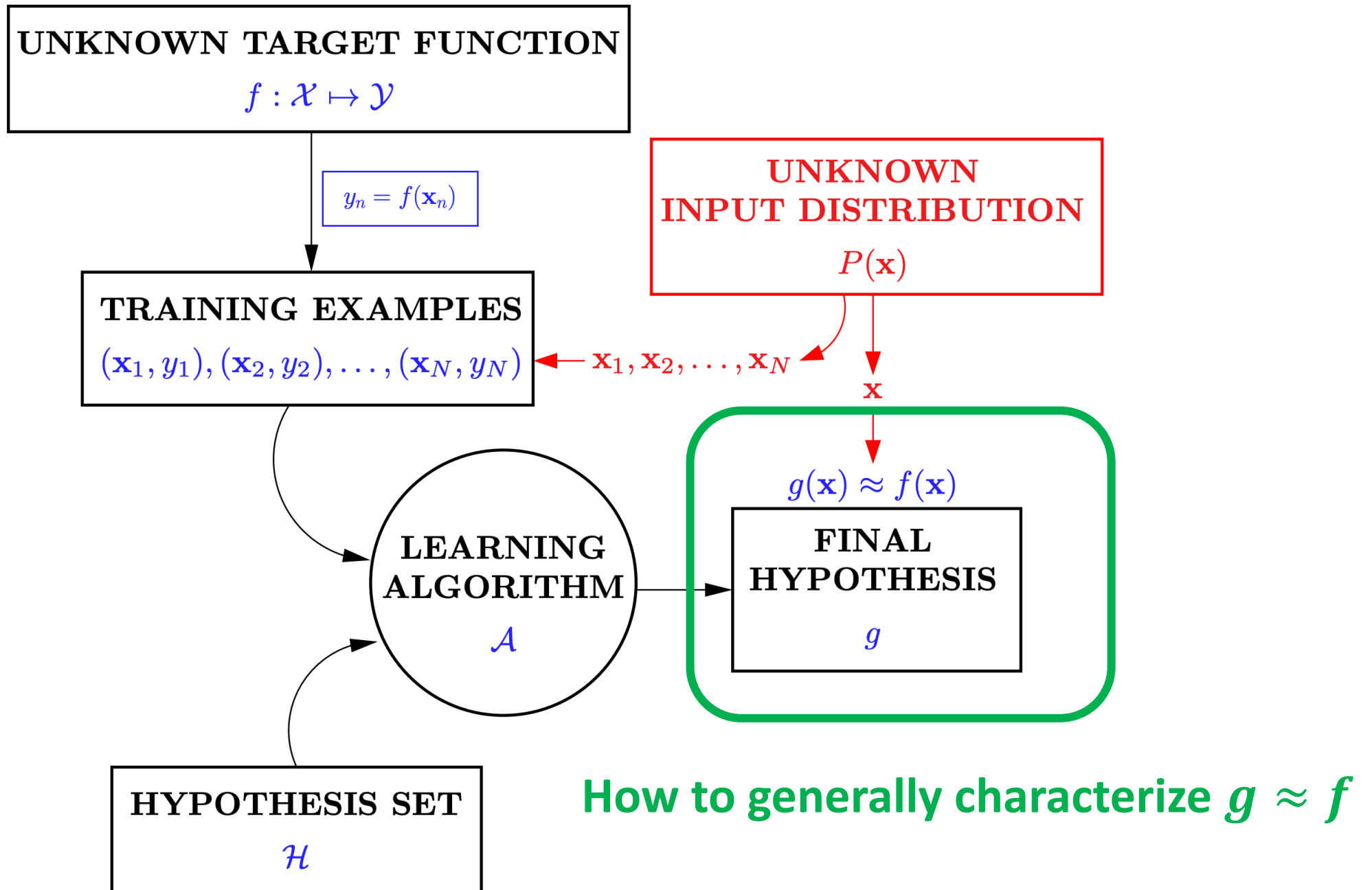
2.  $\Pr[B(g)] \leq \Pr[B(h_1)] + \dots + \Pr[B(h_M)]$

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



# 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):  $e(h(\vec{x}), f(\vec{x})) = (f(\vec{x}) - h(\vec{x}))^2$

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

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

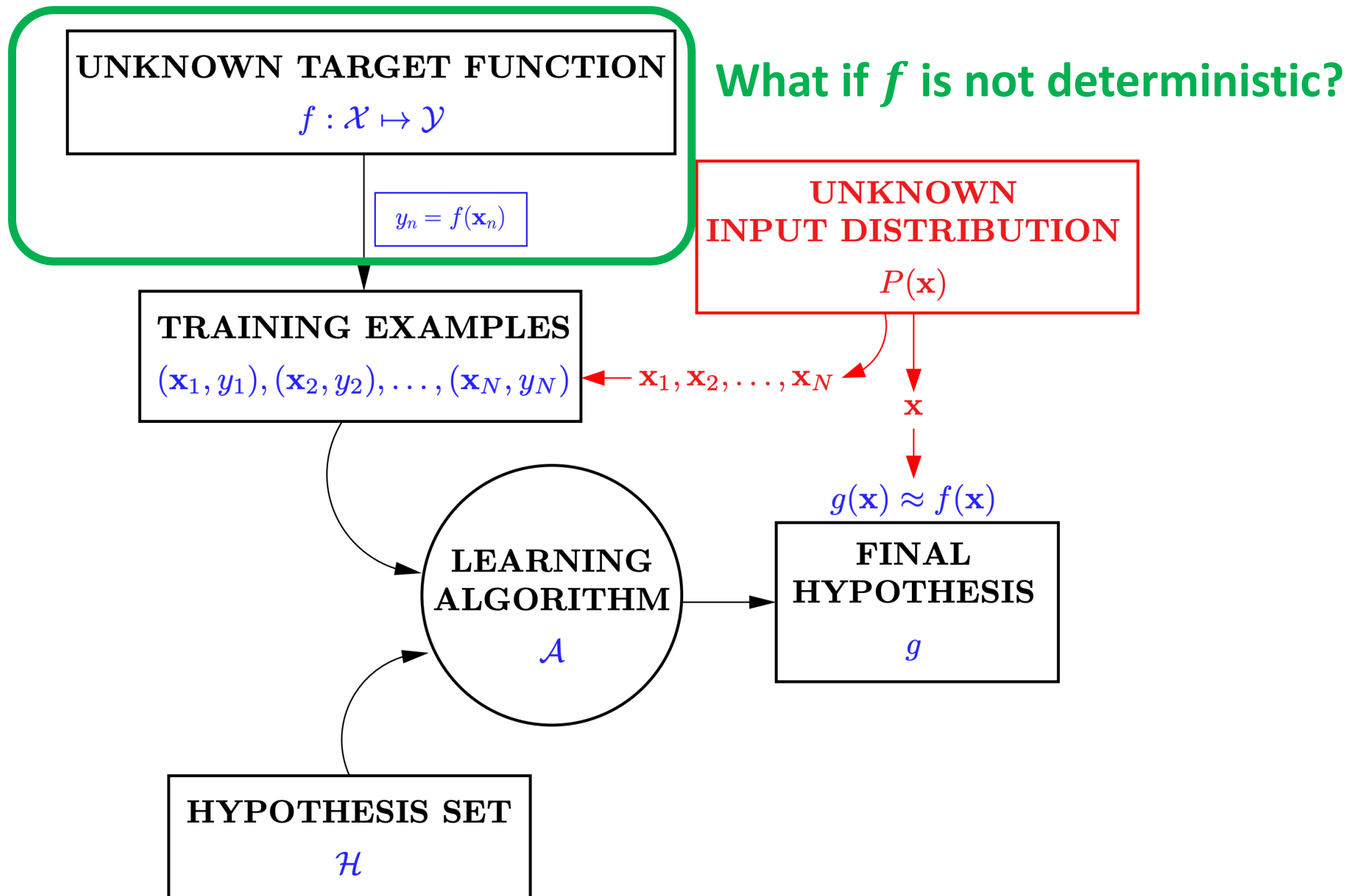
# How to Choose Error Function

- Depending on domain application

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

- Make it “easier” to **optimize**
  - One natural ML algorithm:  $g = \operatorname{argmin}_{h \in \mathcal{H}} E_{in}(h)$
  - (e.g., if  $E_{in}$  is convex, continuous, differentiable, we usually have efficient algorithms.)



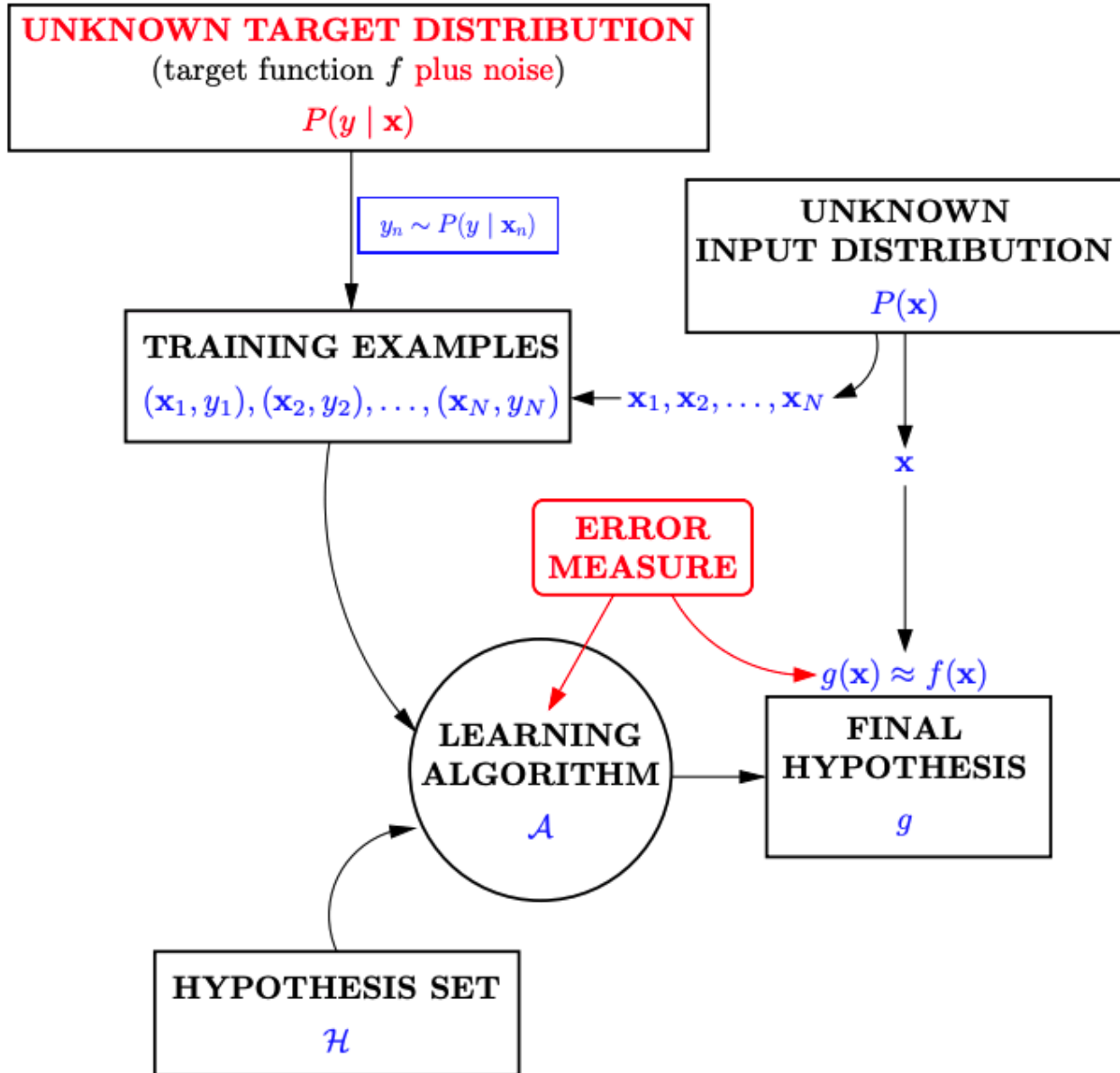
# Noisy Target

- 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
    - $\epsilon$  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  $H = \{h_1, \dots, h_M\}$
- Apply some learning algorithm on  $D$ , output a  $g \in H$
- What can we say about  $E_{out}(g)$  from  $E_{in}(g)$ ?

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

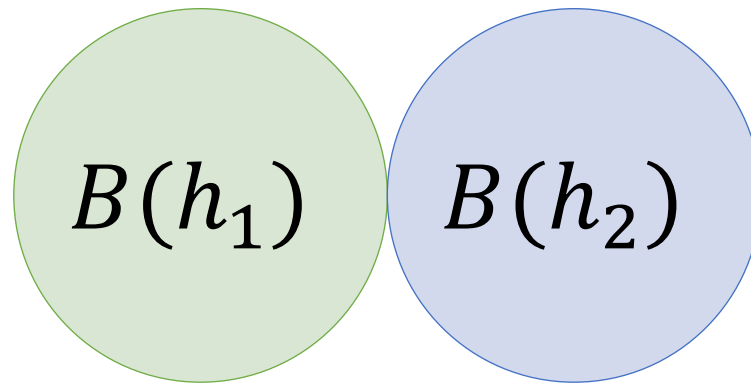
What if  $M$  is infinite?

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

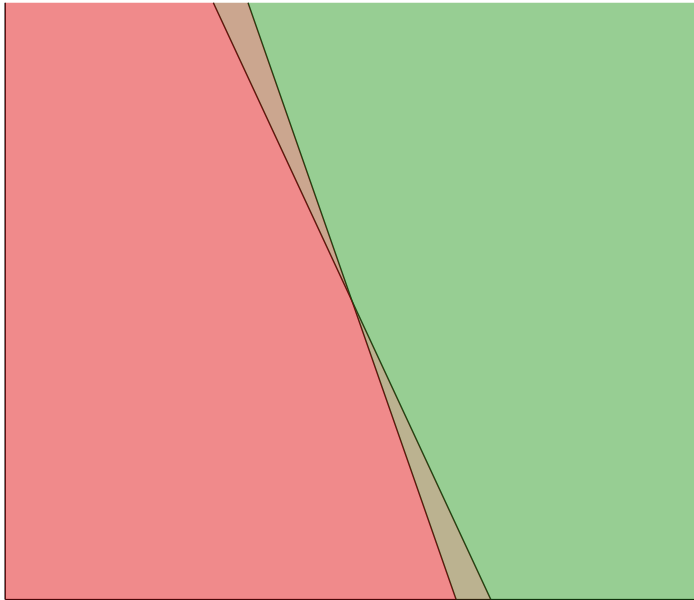
$$\leq \Pr[B(h_1)] + \Pr[B(h_2)] \quad (\text{Union Bound})$$



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

# Do Bad Events Overlap?

- Oftentimes, they overlap a lot!



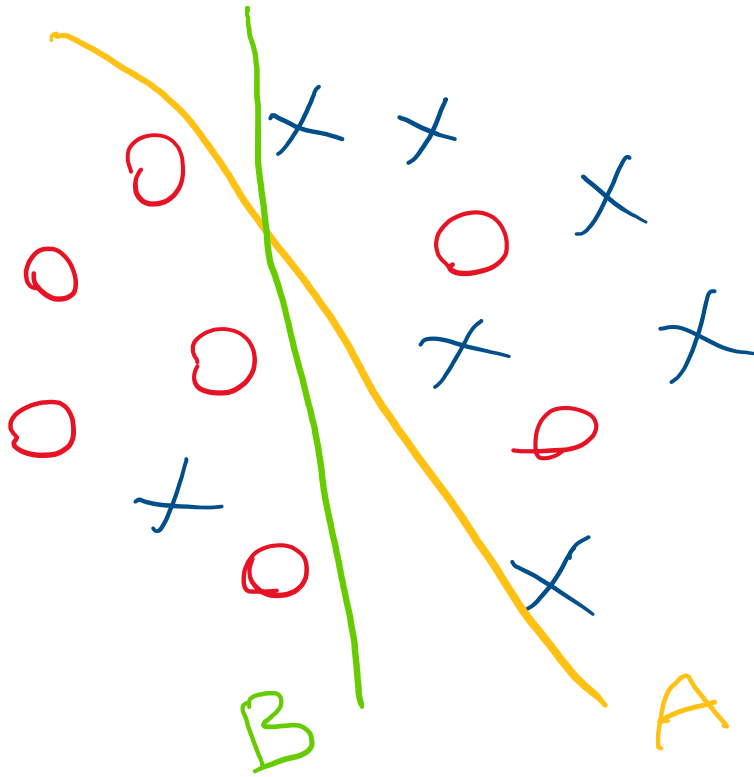
The two linear separators on the left make the same predictions for most points.

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

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

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  
*/dī'kädəmə/*  
*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

- 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  $\vec{x}_1, \dots, \vec{x}_N$

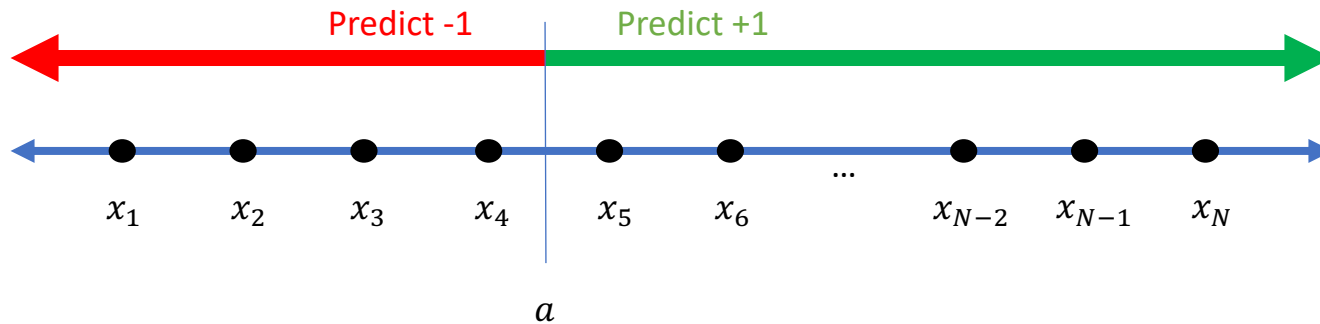
- Growth function

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

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

# Example: $H$ = Positive Rays

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



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

- What is  $m_H(N)$ ?

## • 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  $\vec{x}_1, \dots, \vec{x}_N$

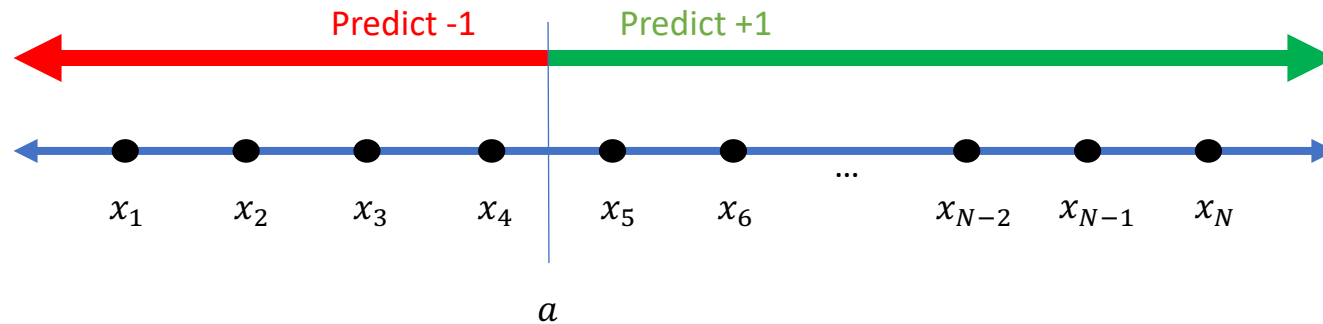
## • Growth function

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

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

# Example: $H$ = Positive Rays

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



- 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  $m_H(N)$ ?

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

## • 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

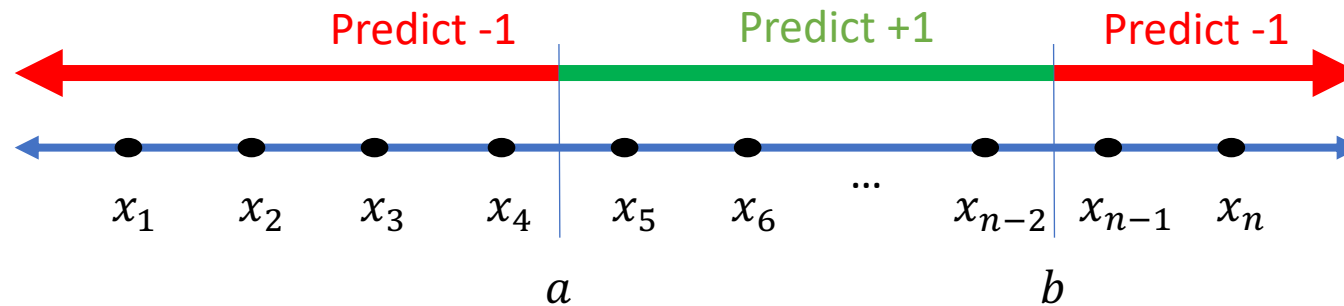
- Largest number of dichotomies  $H$  can induce across all possible data sets of size  $N$

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

# What is $m_H(N)$ ?

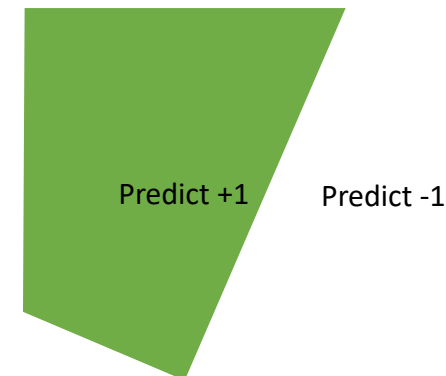
- $H$  = Positive Intervals

- 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



- Dichotomies

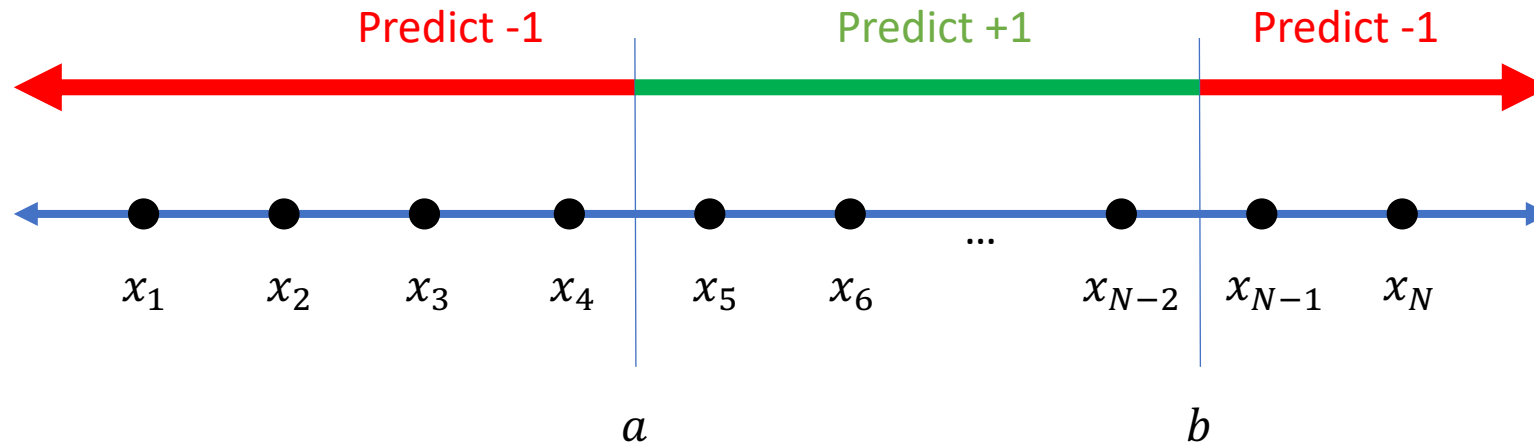
- Informally, consider a dichotomy as “data-dependent” hypothesis
- Characterized by both hypothesis set  $H$  and  $N$  data points  $(\vec{x}_1, \dots, \vec{x}_N)$ 
$$H(\vec{x}_1, \dots, \vec{x}_N) = \{h(\vec{x}_1), \dots, h(\vec{x}_N) | h \in H\}$$
- The set of possible prediction combinations  $h \in H$  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  $N$

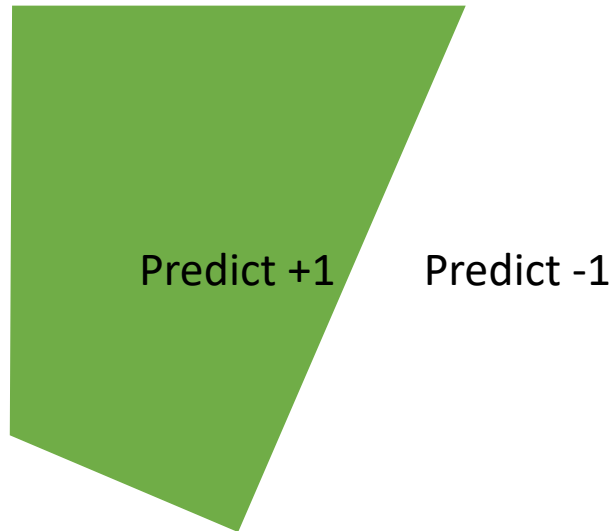
$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

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

- Theorem: VC Inequality (1971)

With prob at least  $1 - \delta$

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

- 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  $N$

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

# Growth Functions for Other $H$

- $H = 2\text{-D Perceptron}$ 
  - What is  $m_H(3)$
  - What is  $m_H(4)$

- 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  $N$

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



# Growth Functions for Other $H$

- $H = 2\text{-D Perceptron}$

- What is  $m_H(3)$
- What is  $m_H(4)$

- 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  $N$

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

- Exactly calculate growth function is generally hard!
- Next lecture
  - Discuss how we can “bound” the growth function
  - Introduce the notion of VC dimension