

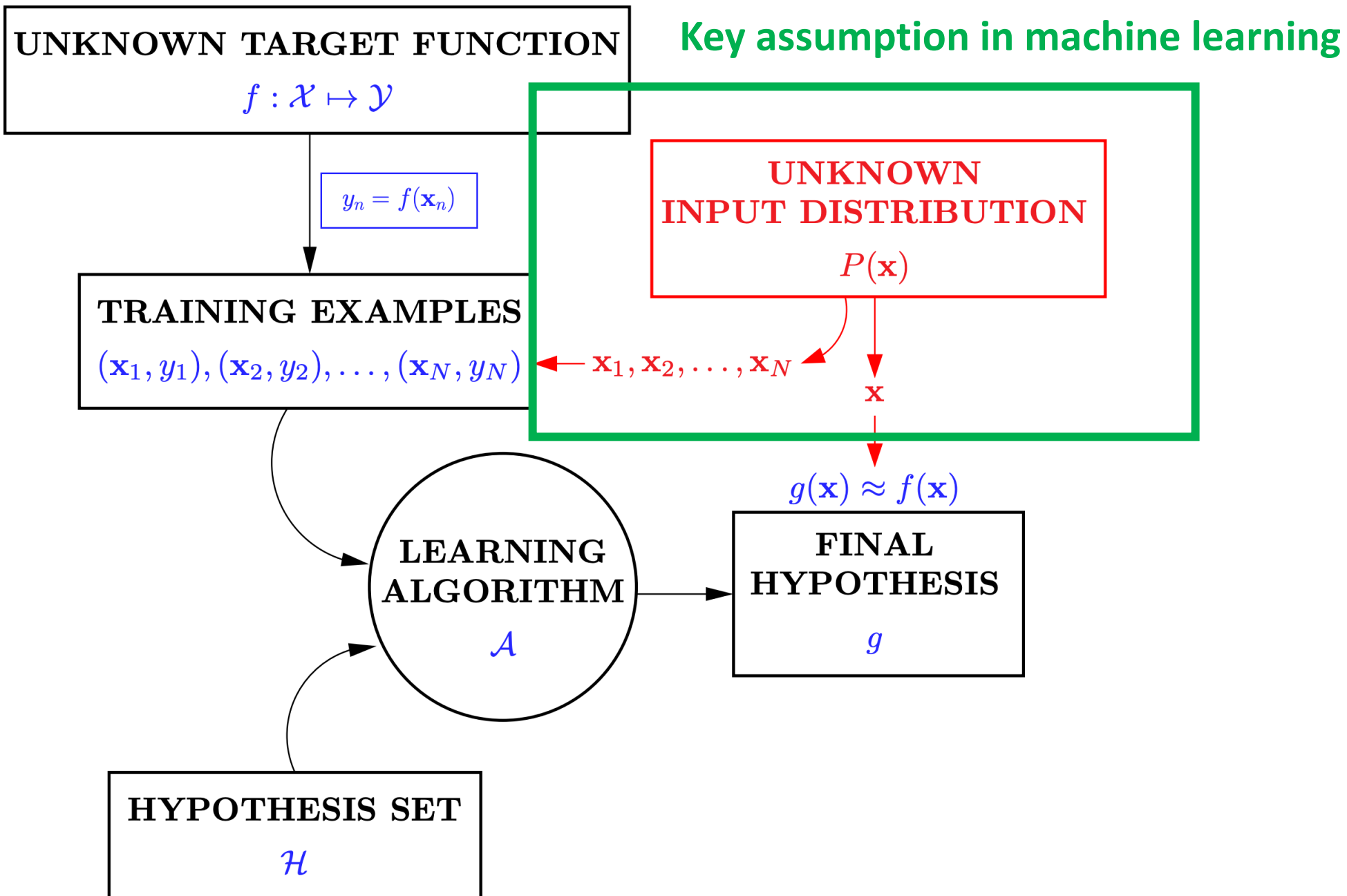
CSE 417T

# Introduction to Machine Learning

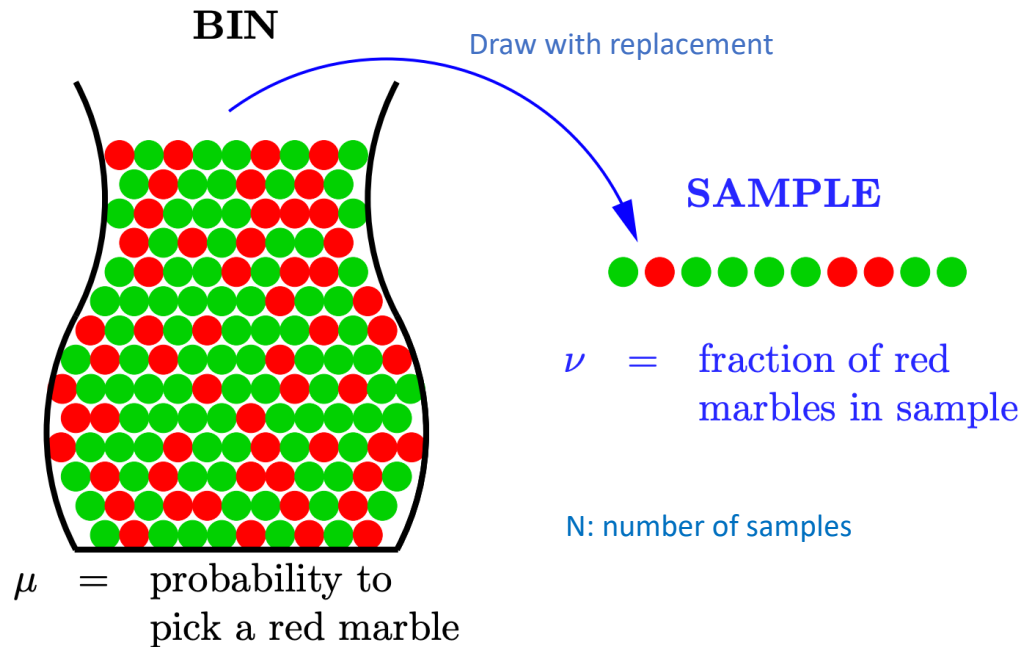
Lecture 4

Instructor: Chien-Ju (CJ) Ho

Recap



# Hoeffding's Inequality



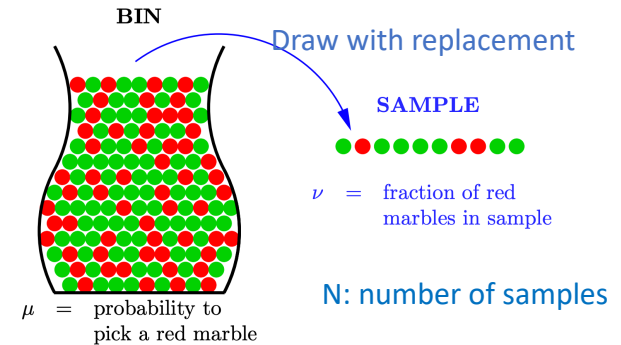
$$\Pr[|\mu - \nu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$$

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  $\{h_1, \dots, h_M\}$

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

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

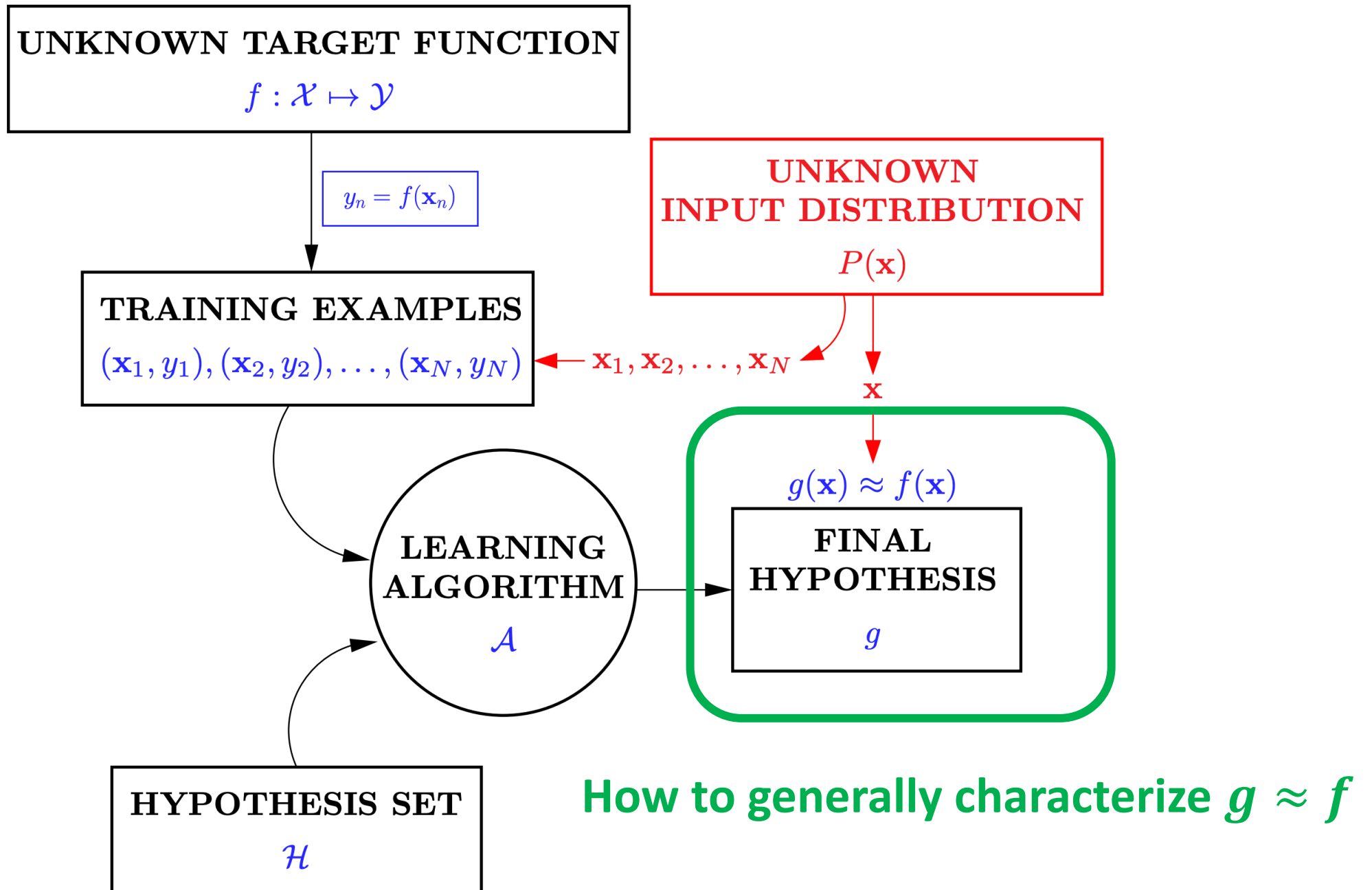
each of the  $\Pr[B(h_m)]$  follows Hoeffding's inequality

# 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 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

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

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

# How to choose the error function?

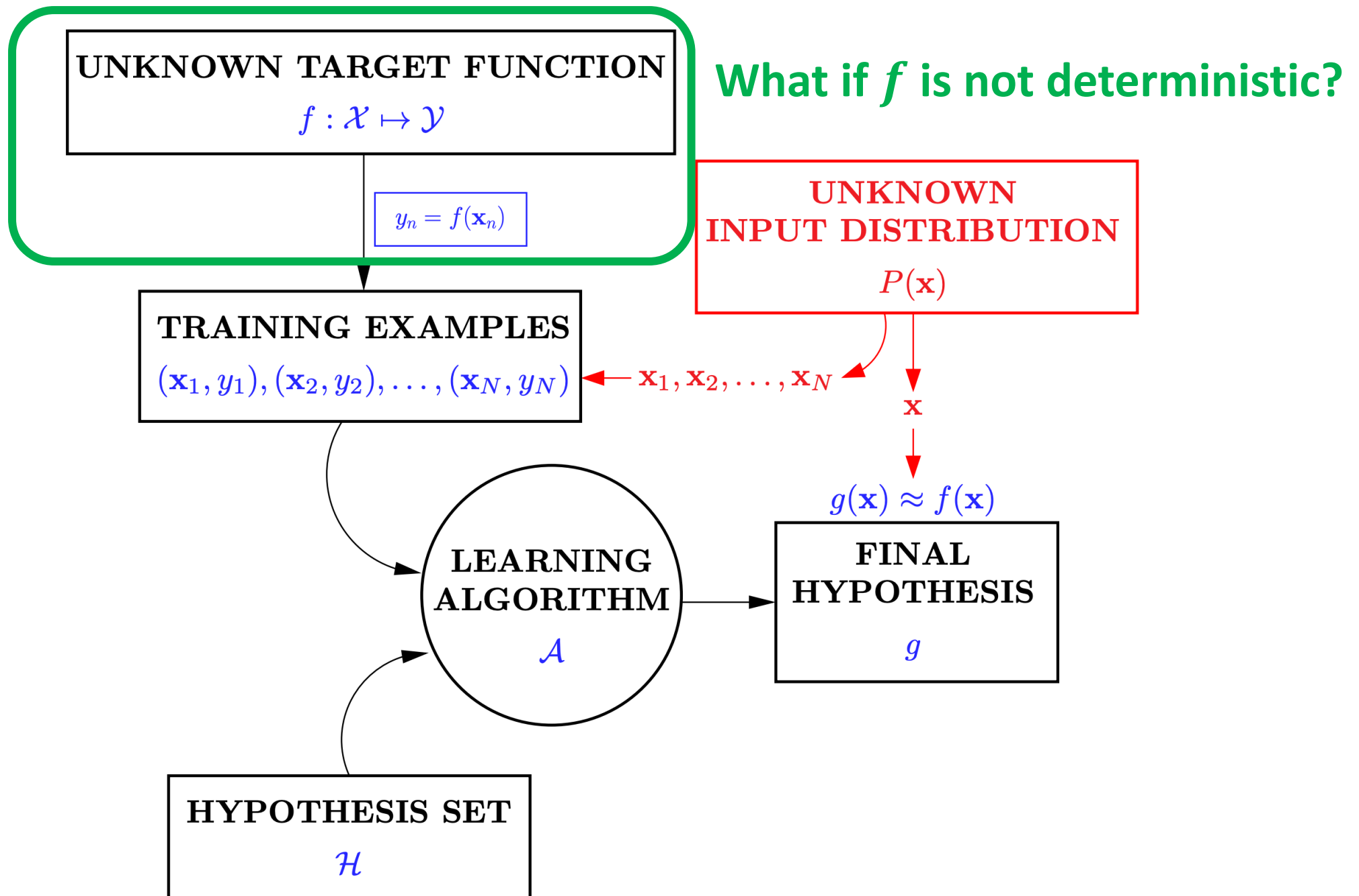
- Consideration 1: Properties of application problems
- Consideration 2: Computation
  - ML algorithms are essentially performing **optimization** (finding  $g$  with smallest error)

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

- 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

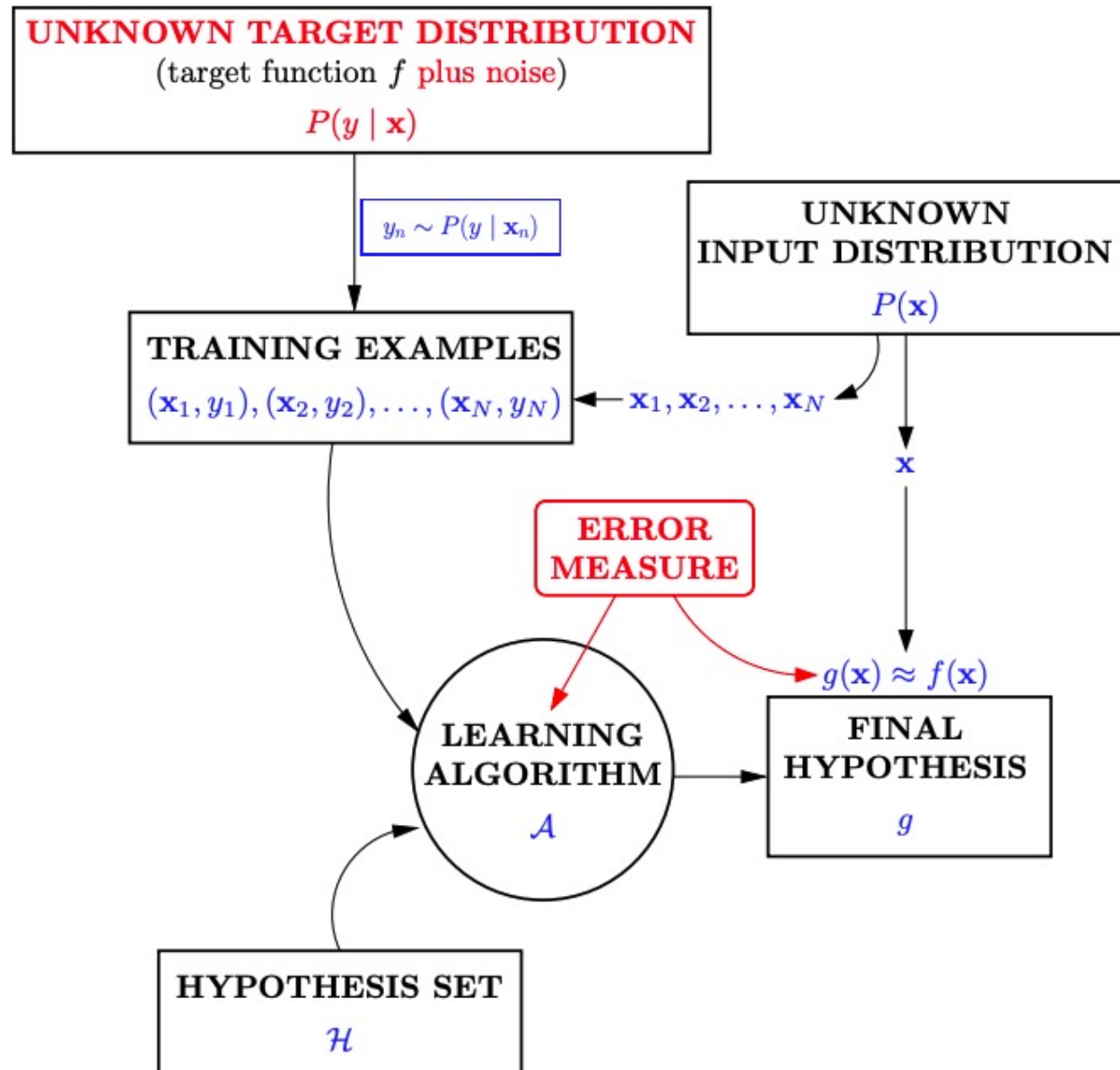


# Noisy Target

- 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  $\mathbb{E}[y|\vec{x}]$
    - $\epsilon$  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  $E_{in}(g)$ ?

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

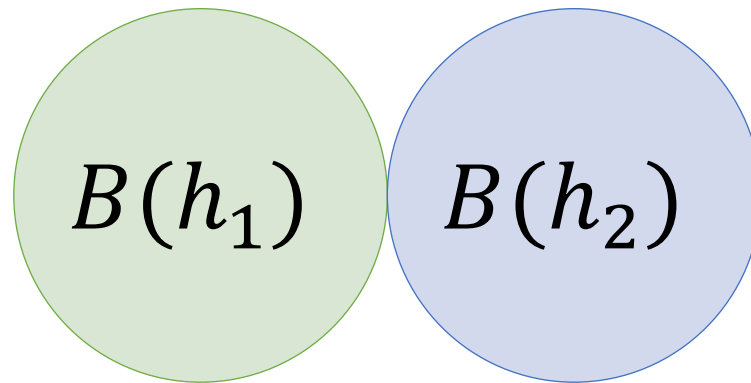
What if  $M$  is infinite?

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

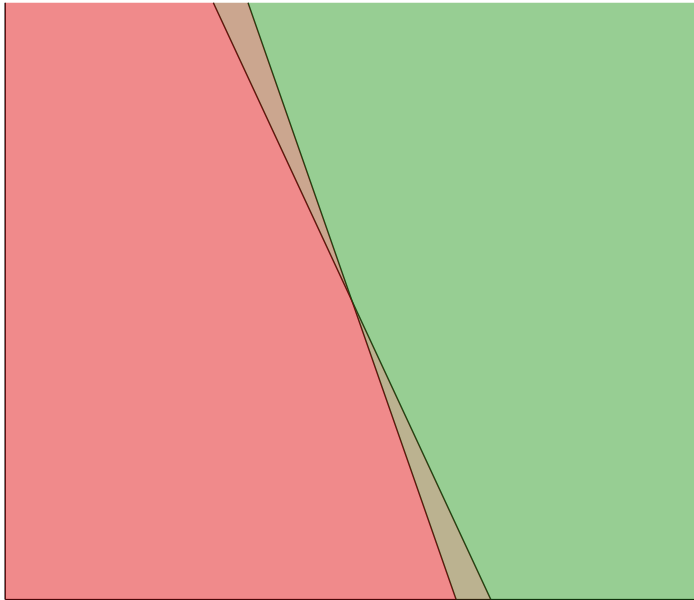
$$\leq \Pr[B(h_1)] + \Pr[B(h_2)] \quad (\text{Union Bound})$$



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

# Do Bad Events Overlap?

- Oftentimes, they overlap a lot!



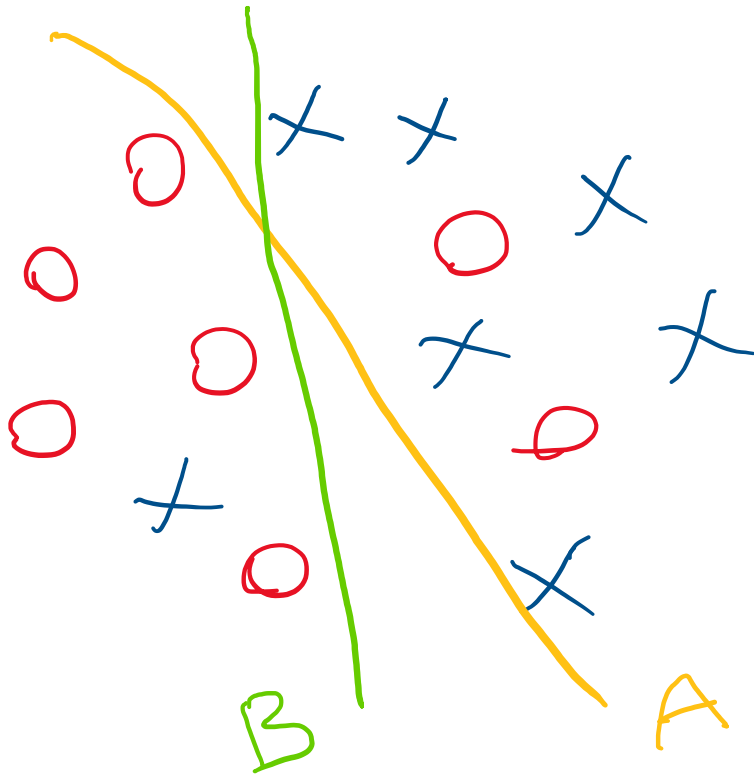
The two linear separators on the left make the same predictions for most points.

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?




For this dataset,  
any difference between **A** and **B**?

For this dataset, probably no difference.

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'kädəmē/*  
*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 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  $\vec{x}_1, \dots, \vec{x}_N$

- Growth function

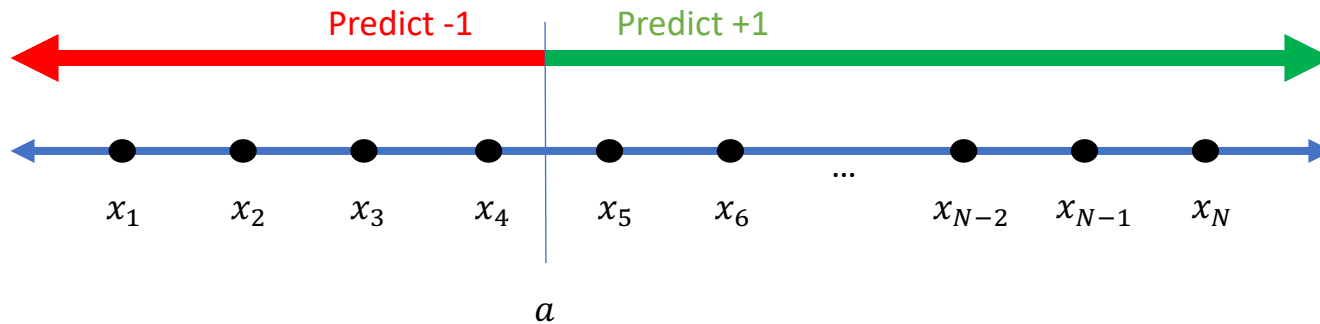
- Largest number of dichotomies  $H$  can induce across all possible data sets of size  $N$

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



# 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 a “data-dependent” hypothesis
- Characterized by both hypothesis set  $H$  and  $N$  data points  $(\vec{x}_1, \dots, \vec{x}_N)$ 
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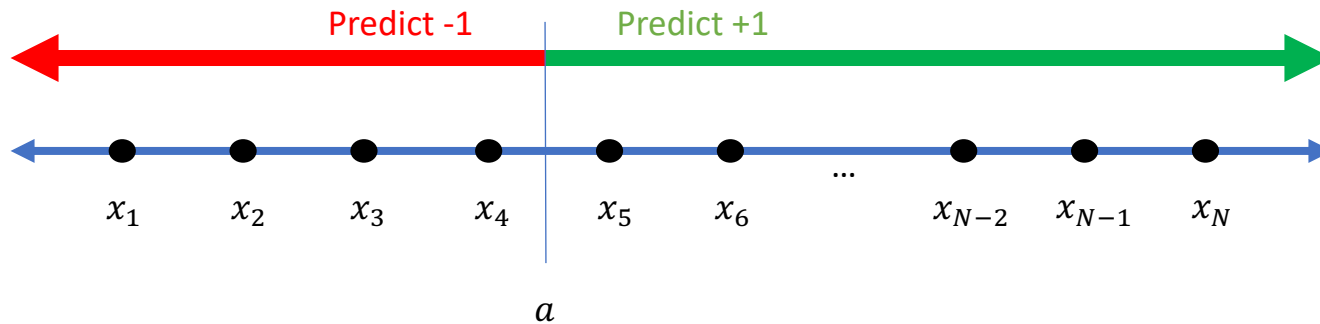
## • Growth function

- 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 a “data-dependent” hypothesis
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## • Growth function

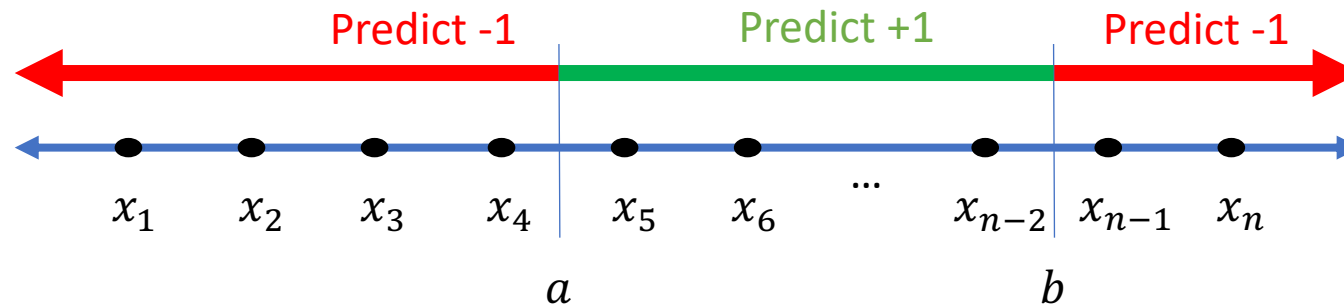
- Largest number of dichotomies  $H$  can induce across all possible data sets of size  $N$

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

# What is $m_H(N)$ ?

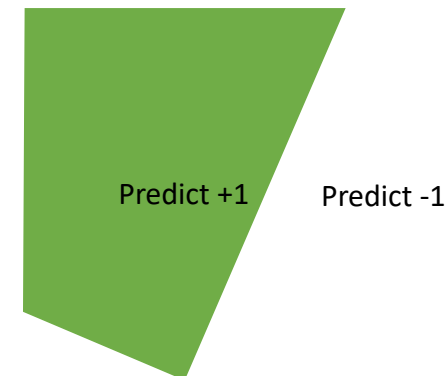
- $H$  = Positive Intervals

- 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

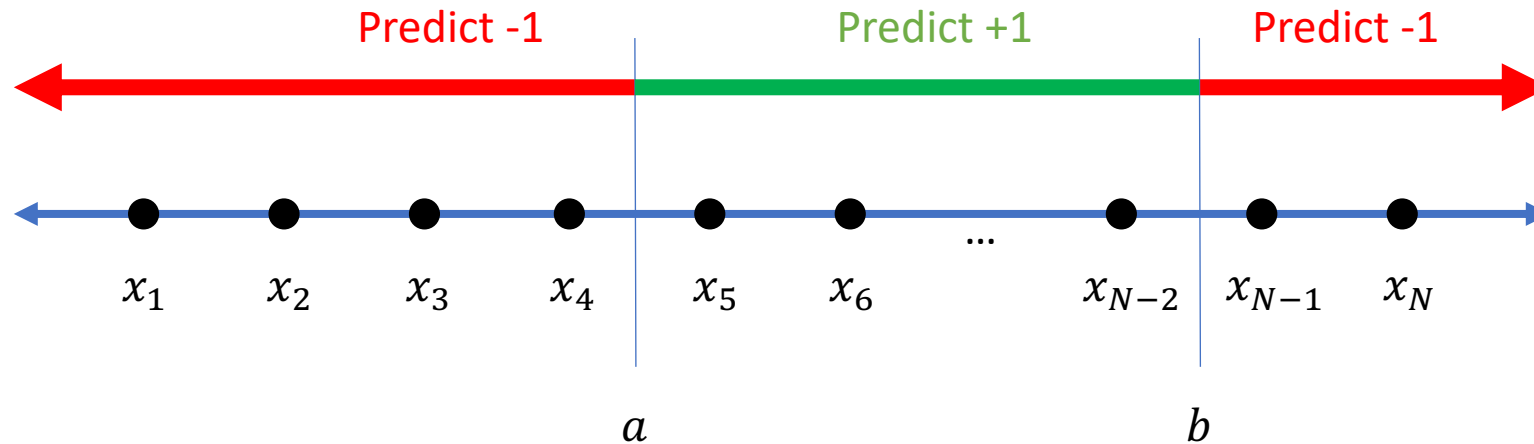
- Informally, consider a dichotomy as a “data-dependent” hypothesis
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- Growth function

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

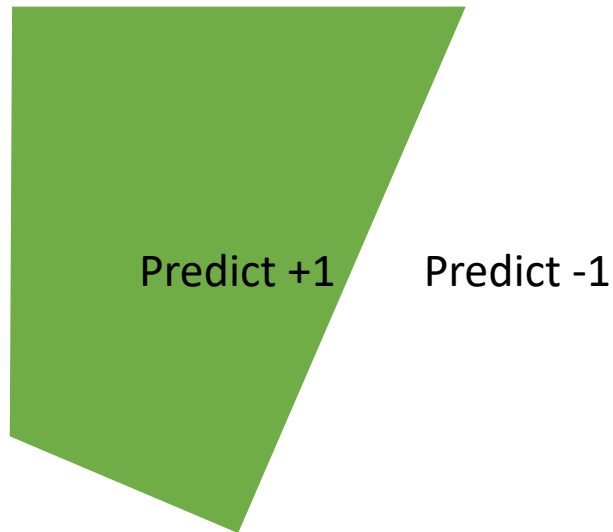
$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

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

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

- Dichotomies

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

- 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  $m_H(3)$
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- 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 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
- $m_H(N) \leq N^{k-1} + 1$

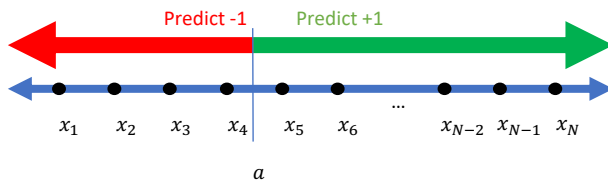
# Practice

$x_5$

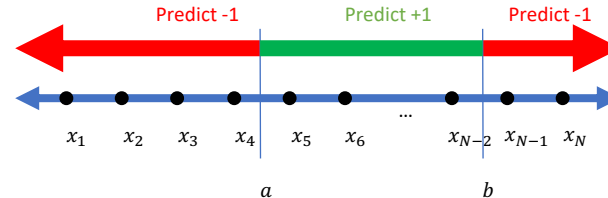
- Shatter:
  - $H$  **shatters**  $(\vec{x}_1, \dots, \vec{x}_N)$  if  $|H(\vec{x}_1, \dots, \vec{x}_N)| = 2^N$
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- Break point
  - $k$  is a **break point** for  $H$  if no data set of size  $k$  can be shattered by  $H$

- What are the break points for

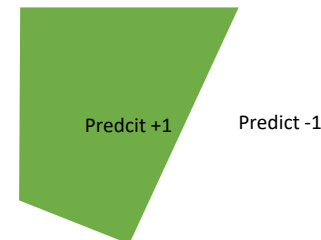
## 1. Positive Rays



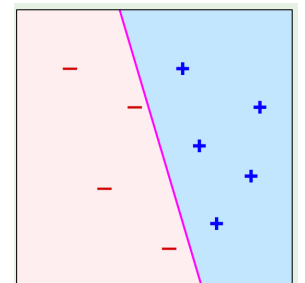
## 2. Positive Intervals



## 3. Convex Sets



## 4. 2-D Perceptron



# Practice

- Dichotomies
  - 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  $\vec{x}_1, \dots, \vec{x}_N$
- Growth function
  - Largest number of dichotomies  $H$  can induce across all possible data sets of size  $N$ 

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

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	$m_H(N)$					
$m_H(N)$	N=1	N=2	N=3	N=4	N=5	Break Points
$N + 1$						Positive Rays
$\frac{N^2}{2} + \frac{N}{2} + 1$						Positive Intervals
$2^N$						Convex Sets
						2D Perceptron

# Practice

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

$$H(\vec{x}_1, \dots, \vec{x}_N) = \{(h(\vec{x}_1), \dots, h(\vec{x}_N)) | h \in H\}$$
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- Shatter:
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		$m_H(N)$					
$m_H(N)$		N=1	N=2	N=3	N=4	N=5	Break Points
$N + 1$	Positive Rays	2	3	4	5	6	$k = 2,3,4, \dots$
$\frac{N^2}{2} + \frac{N}{2} + 1$	Positive Intervals						
$2^N$	Convex Sets						
	2D Perceptron						

# Practice

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

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

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

- 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  $H$

		$m_H(N)$					
$m_H(N)$		N=1	N=2	N=3	N=4	N=5	Break Points
$N + 1$	Positive Rays	2	3	4	5	6	$k = 2,3,4, \dots$
$\frac{N^2}{2} + \frac{N}{2} + 1$	Positive Intervals	2	4	7	11	16	$k = 3,4,5, \dots$
$2^N$	Convex Sets	2	4	8	16	32	None
	2D Perceptron	2	4	8	14	?	$k = 4,5,6, \dots$

# Why Break Points?

- Theorem statement (Again, take it as a fact for now)
  - If there is no break point for  $H$ , then  $m_H(N) = 2^N$  for all  $N$ .
  - If  $k$  is a break point for  $H$ , i.e., if  $m_H(k) < 2^k$  for some value  $k$ , then

$$m_H(N) \leq \sum_{i=0}^{k-1} \binom{N}{i}$$

- Rephrase the above theorem
  - If there is no break point for  $H$ , then  $m_H(N) = 2^N$  for all  $N$ .
  - If  $k$  is a break point for  $H$ , the following statements are true
    - $m_H(N) \leq N^{k-1} + 1$  [Can be proven using induction. See LFD Problem 2.5]
    - $m_H(N) = O(N^{k-1})$
    - $m_H(N)$  is polynomial in  $N$
- We can “bound” the growth function without knowing it exactly.
  - Find break point!

# Why Break Points?

- VC Generalization Bound

With prob  $1 - \delta$

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

- In the following discussion, we treat  $\delta$  as a constant [i.e., with high probability, the following is true]

$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{\frac{1}{N} \ln m_H(N)}\right)$$

- Rephrase the above theorem

- If there is no break point for  $H$ , then  $m_H(N) = 2^N$  for all  $N$ .
- If  $k$  is a break point for  $H$ , the following statements are true
  - $m_H(N) \leq N^{k-1} + 1$  [Can be proven using induction. See LFD Problem 2.5]
  - $m_H(N) = O(N^{k-1})$
  - $m_H(N)$  is polynomial in  $N$

[For example, we can set  $\delta$  to be a small constant, say 0.01. Then every time we wrote the above inequality, we mean that it is true with probability at least 99%.]

# Applying Break Points in VC Bound

- VC Bound:

$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{\frac{1}{N} \ln m_H(N)}\right)$$



- Rephrase the above theorem

- If there is no break point for  $H$ , then  $m_H(N) = 2^N$  for all  $N$ .
- If  $k$  is a break point for  $H$ , the following statements are true
  - $m_H(N) \leq N^{k-1} + 1$  [Can be proven using induction. See LFD Problem 2.5]
  - $m_H(N) = O(N^{k-1})$
  - $m_H(N)$  is polynomial in  $N$

- If there are no break point ( $m_H(N) = 2^N$ )

$$E_{out}(g) \leq E_{in}(g) + O(1)$$

(This implies that we can't infer  $E_{out}$  from  $E_{in}$  even when  $N \rightarrow \infty$ )

- If  $k$  is a break point for  $H$ , i.e.,  $m_H(N) = O(N^{k-1})$

$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{(k-1) \frac{\ln N}{N}}\right)$$