CSE 417T
Introduction to Machine Learning

Lecture 4

Instructor: Chien-Ju (CJ) Ho

Logistics: HW1

- Due: **Feb 14 (Monday), 2022**
  - 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

Logistics: Office Hours

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

Monday	11:30am (Herbert Zhou)	4pm (Dean Yu)	
Tuesday	1pm (Ziqi Xu)	3:30pm (Neal Huang)	
Wednesday	1pm (Eddie Choi)	4:30pm (Weiwei Ma)	
Thursday	10am (Jackie Zhong)	3pm (Fankun Zeng)	
Friday	8am (Shohaib Shaffiey)	1pm (Yunfan Wang)	7pm (Hao Qin)
Sunday	1pm (Jonathan Ma)		

- 60 minutes per session
- Please follow **Piazza** for additional information
- 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 in This Course

Note that by default, $\vec{x}$ is a column vector.

More formally, we should write $\vec{x} = \begin{bmatrix} x_0 \\ \vdots \\ x_d \end{bmatrix}$.

For convenience, I usually write $\vec{x} = (x_0, \ldots, x_d)$.

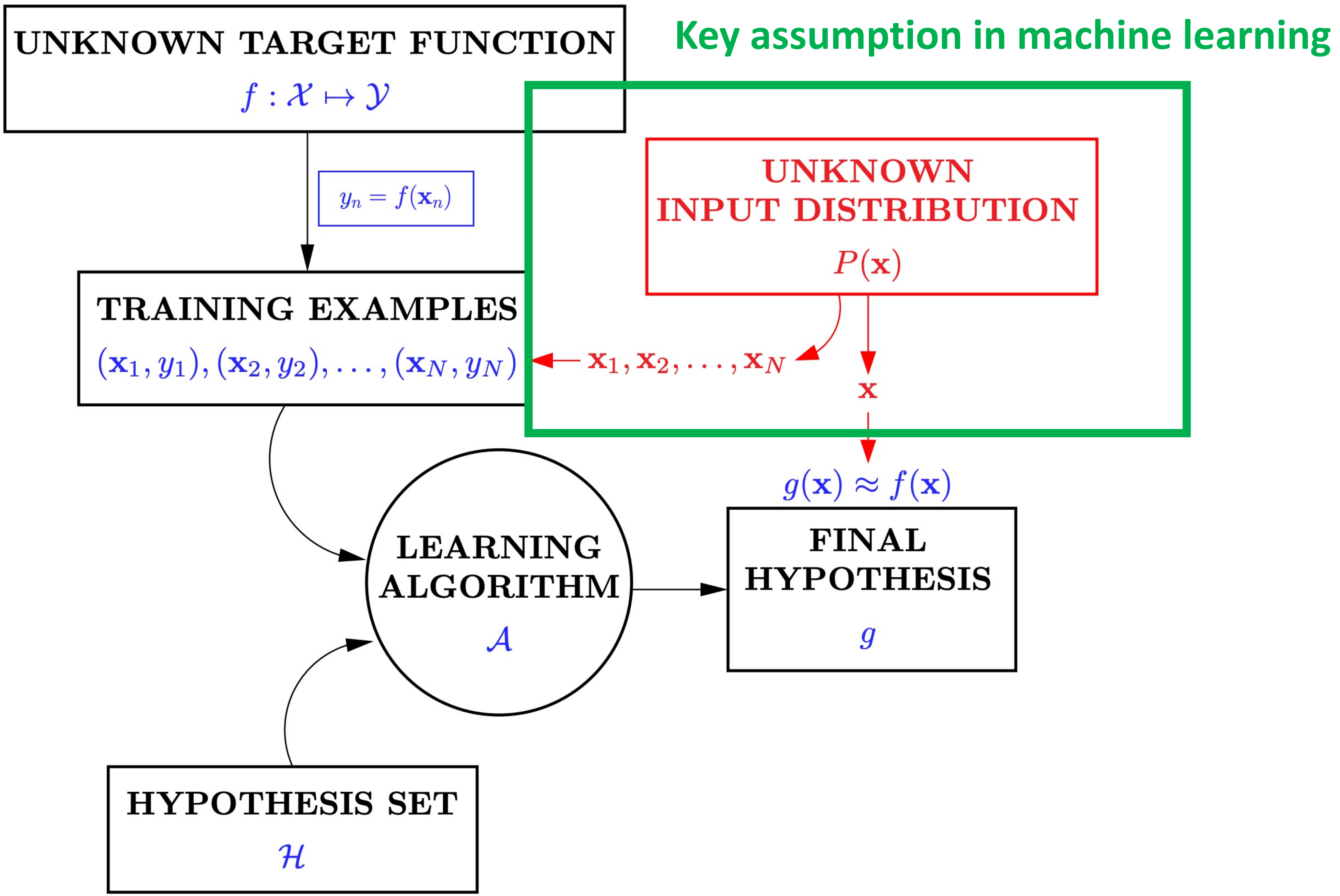
- Data point with augmented x_0: $\vec{x} = (x_0, \ldots, x_d)$
  - We often use d to specify the dimensions of data points
  - We augment $x_0 = 1$ for each data point (Check Lecture 1 for the reasoning)

- Dataset: $D = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_N, y_N)\}$
  - 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

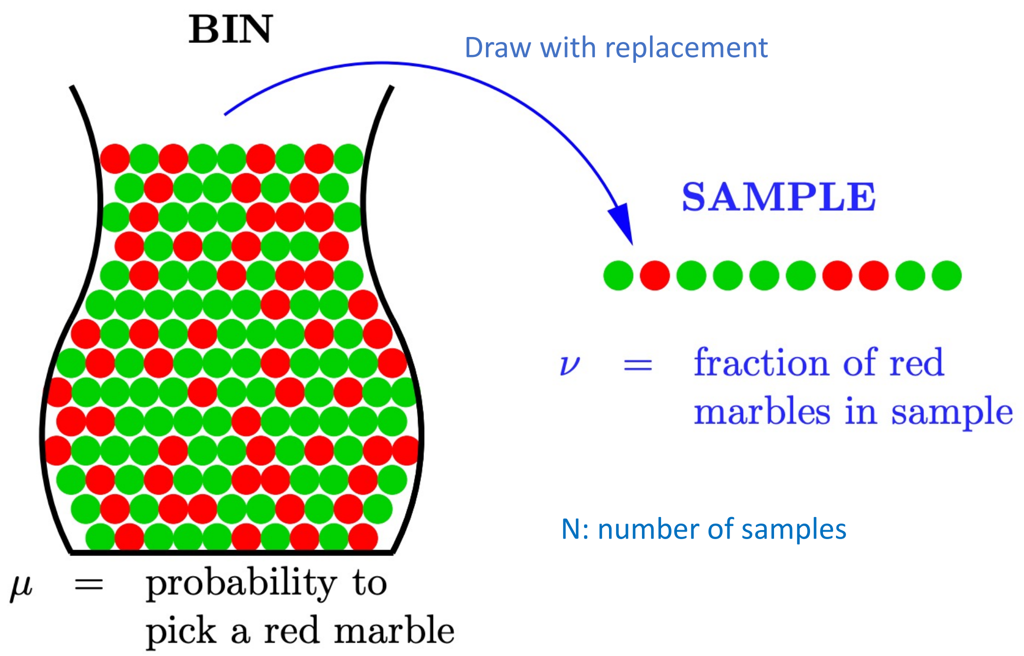
- Indicator variable:
  - $\mathbb{I}[\text{event}] = \begin{cases} 1 & \text{if event is true} \\ 0 & \text{if event is false} \end{cases}$

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



Key assumption in machine learning
UNKNOWN TARGET FUNCTION
$f: \mathcal{X} \mapsto \mathcal{Y}$
$y_n = f(\mathbf{x}_n)$
UNKNOWN INPUT DISTRIBUTION
$P(\mathbf{x})$
TRAINING EXAMPLES
$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)$
$\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$
$\mathbf{x}$
$g(\mathbf{x}) \approx f(\mathbf{x})$
LEARNING ALGORITHM
$\mathcal{A}$
FINAL HYPOTHESIS
g
HYPOTHESIS SET
$\mathcal{H}$

Hoeffding's Inequality



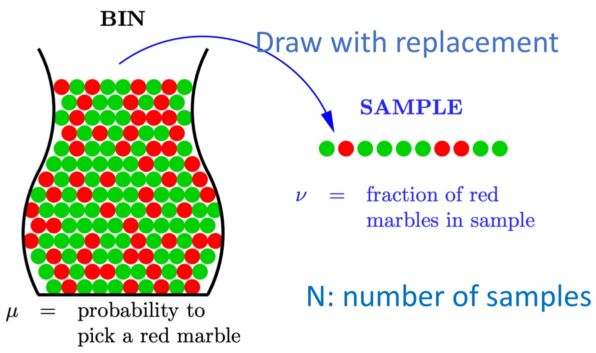
$$\mathbf{Pr}[|\boldsymbol{\mu} - \boldsymbol{\nu}| > \boldsymbol{\epsilon}] \leq \mathbf{2}\boldsymbol{e}^{-\mathbf{2}\boldsymbol{\epsilon}^{\mathbf{2}}\boldsymbol{N}}$$

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



- 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 ν]
  - $E_{out}(h) \stackrel{\text{def}}{=} \Pr_{\vec{x}\sim P(\vec{x})}[h(\vec{x}) \neq f(\vec{x})]$ [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 $H = \{h_1, \ldots, h_M\}$
- Apply some learning algorithm on D, output a $g \in H$

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

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

Intuitions:

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

   g is selected within $\{h_1, \ldots, h_M\}$
   => bad event of g is within the union of the bad events of $h_1, \ldots, h_M$

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

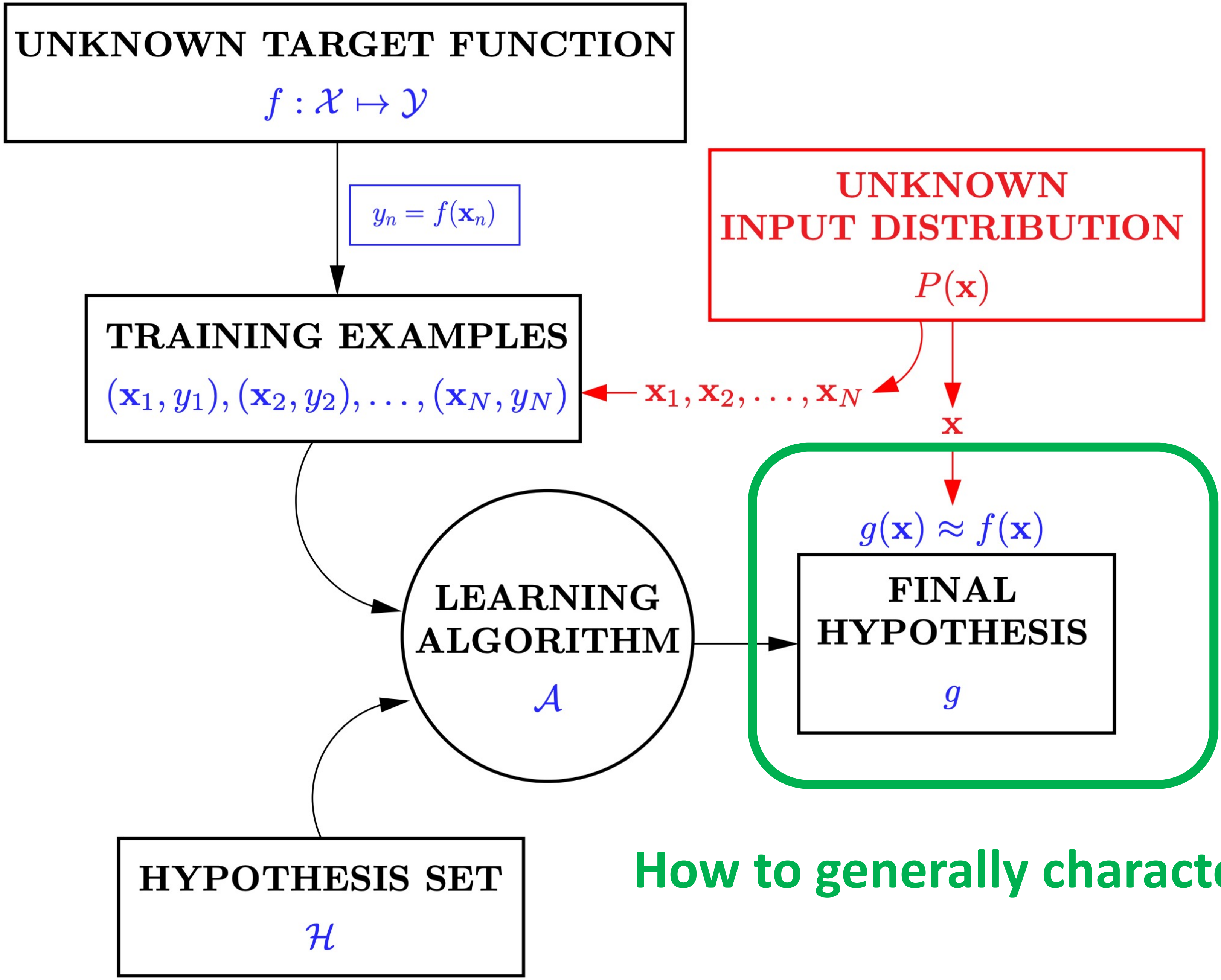
   each of the $\Pr[B(h_m)]$ follows Hoeffding's inequality

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 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

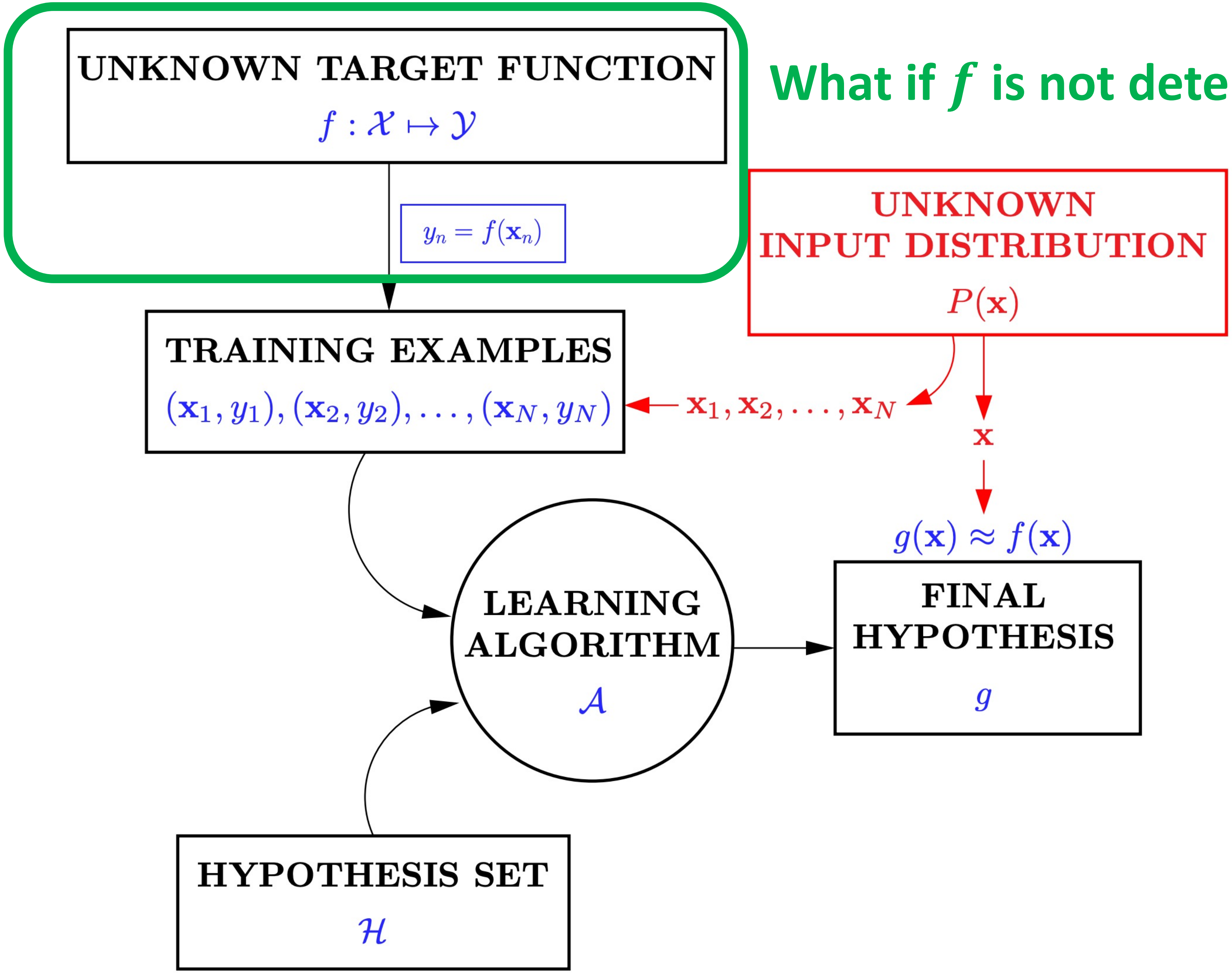
How to choose the error function?

- 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

What if f is not deterministic?



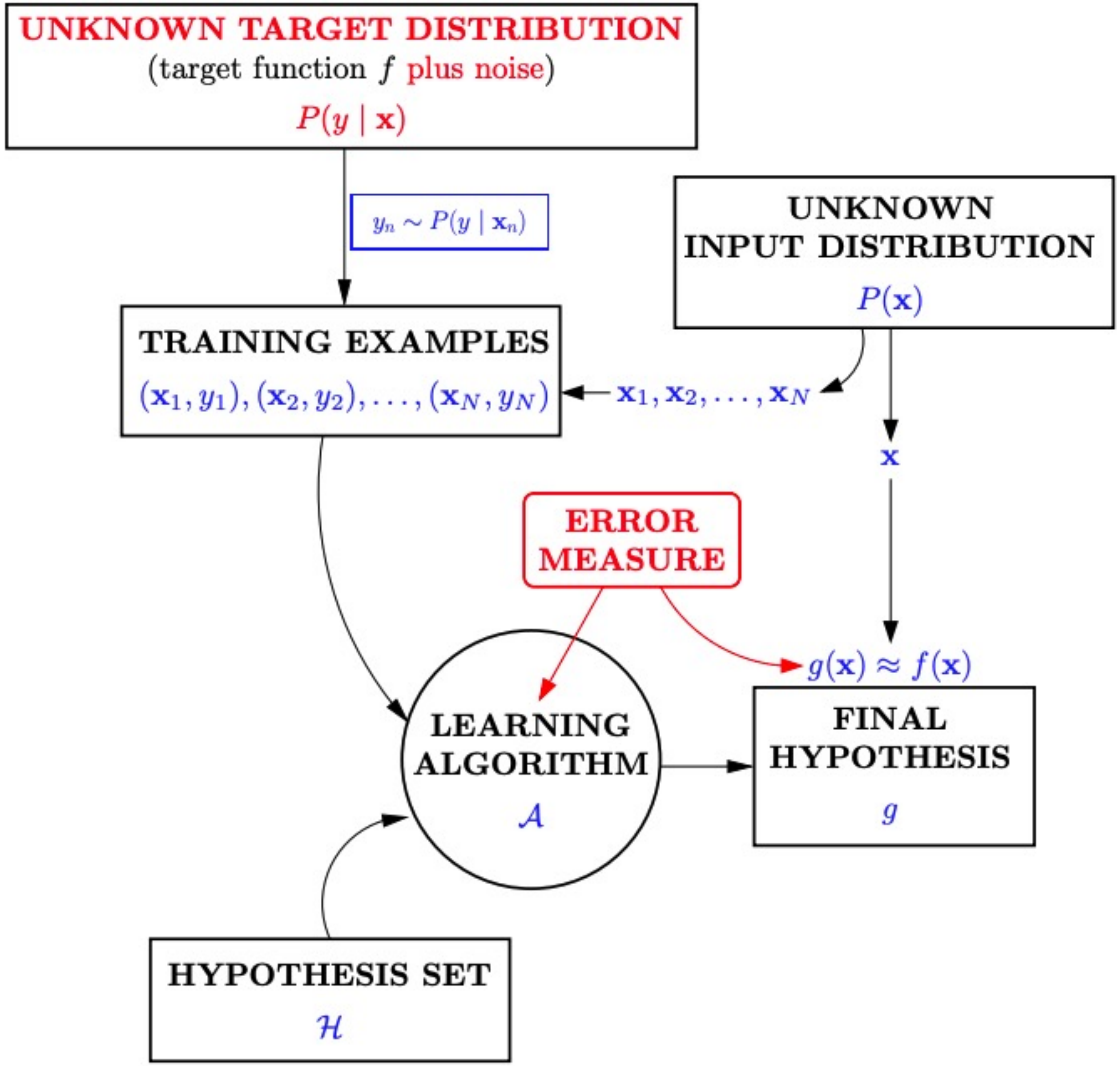
Noisy Target

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

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

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

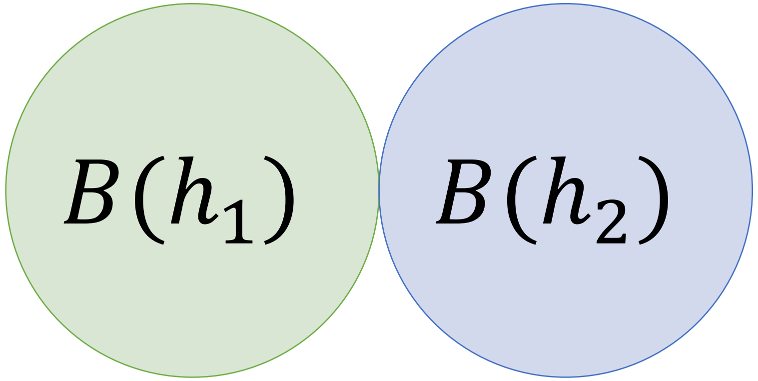
What if M is infinite?

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

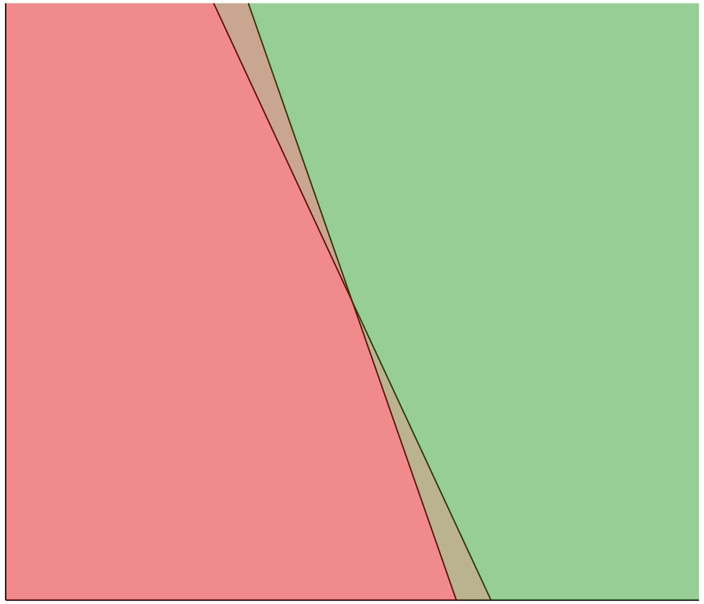
$\leq \Pr[B(h_1)] + \Pr[B(h_2)]$ (Union Bound)



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

Do Bad Events Overlap?

- Oftentimes, they overlap a lot!



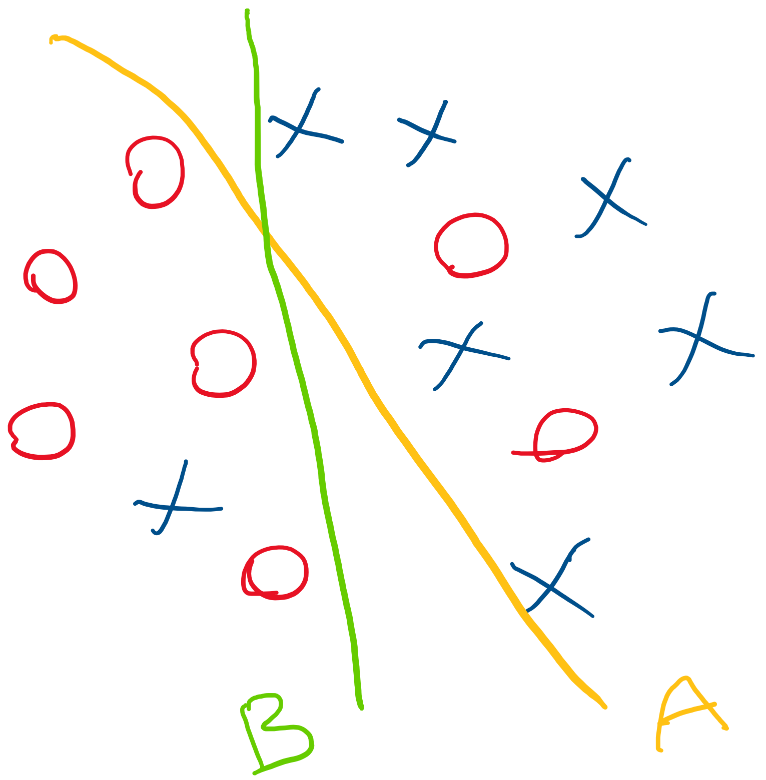
The two linear separators on the left make the same predictions for most points.

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

”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 $h: X \rightarrow \{-1, +1\}$
- 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

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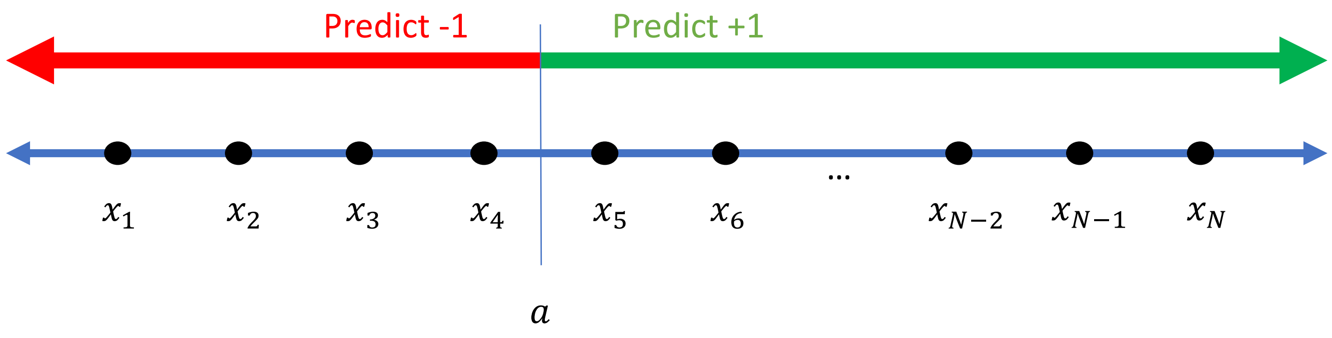
$$m_H(N) = \max_{(\vec{x}_1,\dots,\vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

- 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 $m_H(N)$?

Example: H = Positive Rays

- Dichotomies
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  - 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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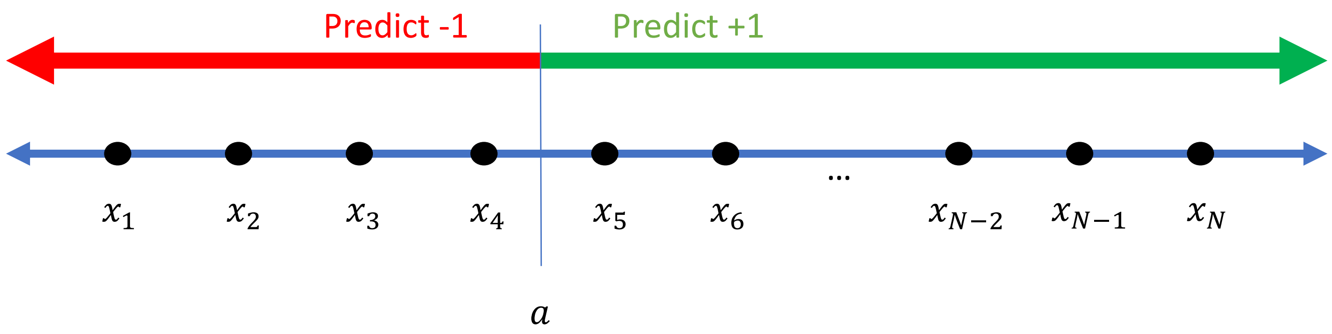

- What is $H(\vec{x}_1, \dots, \vec{x}_N)$?

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

- What is $m_H(N)$?

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

What is $m_H(N)$?

- Dichotomies
  - Informally, consider a dichotomy as “data-dependent” hypothesis
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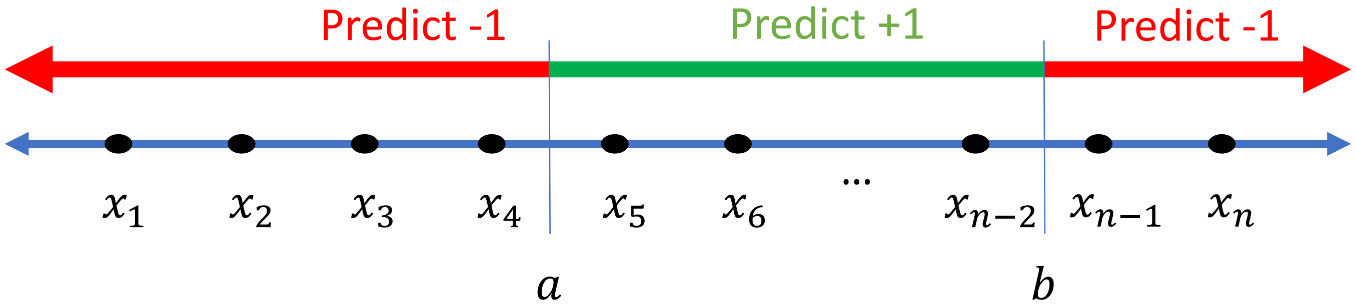
$$H(\vec{x}_1, \dots \vec{x}_N) = \{h(\vec{x}_1), \dots, h(\vec{x}_N) | h \in H\}$$

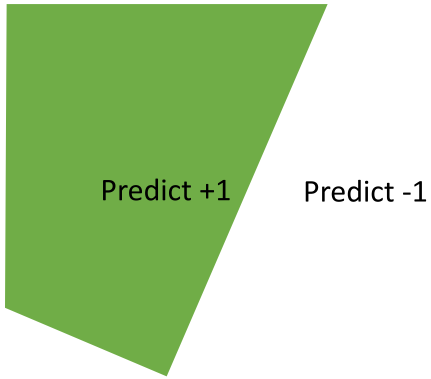
  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \dots, \vec{x}_N$
- Growth function
  - Largest number of dichotomies H can induce across all possible data sets of size N

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

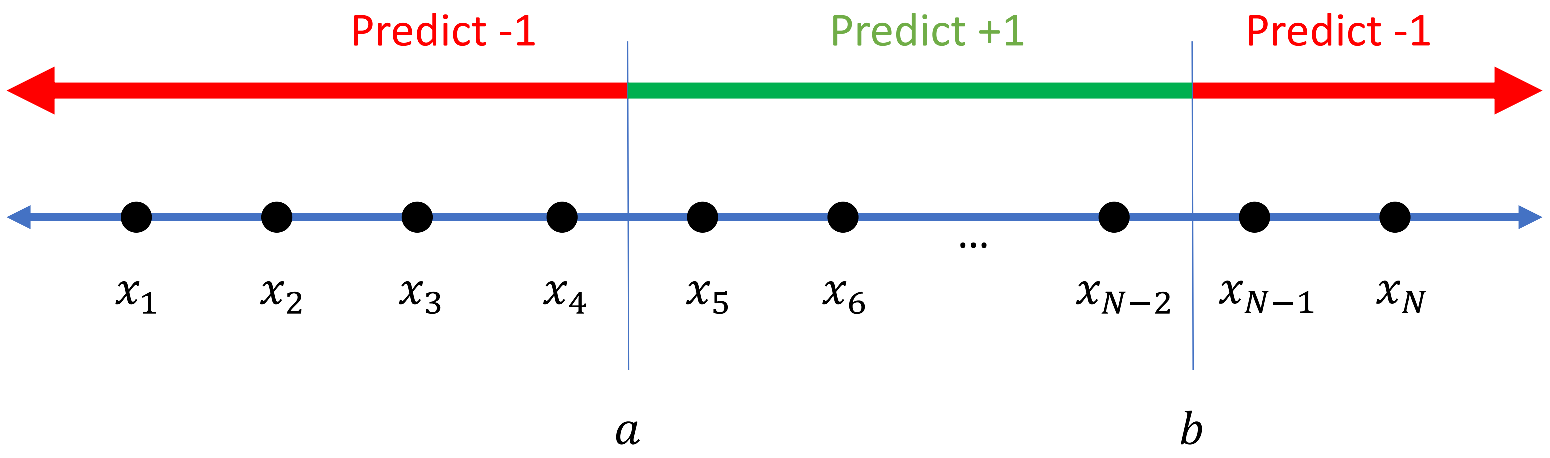
- H = Positive Intervals
  - Data points are in one-dimensional space
  - Choose two thresholds. Predict +1 within the interval, -1 outside



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

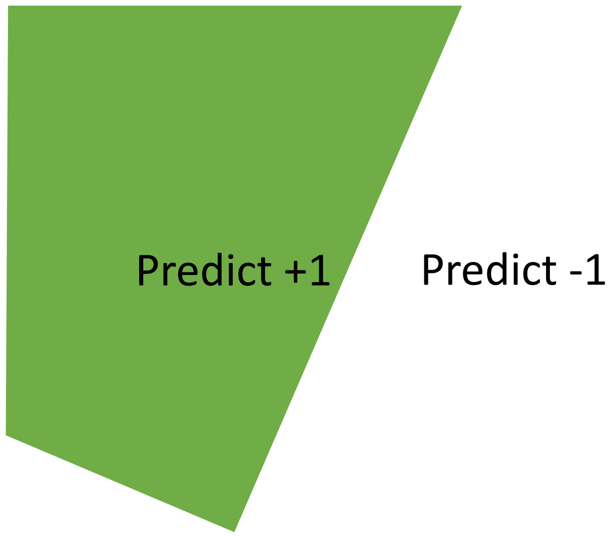


Example: H = Positive Intervals



- 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?

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

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

  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \ldots, \vec{x}_N$
- Growth function
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    $$m_H(N) = \max_{(\vec{x}_1, \ldots, \vec{x}_N)} |H(\vec{x}_1, \ldots, \vec{x}_N)|$$

- 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 $1 - \delta$

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

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

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Growth Functions for Other H

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

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

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