CSE 417T
Introduction to Machine Learning

Lecture 7

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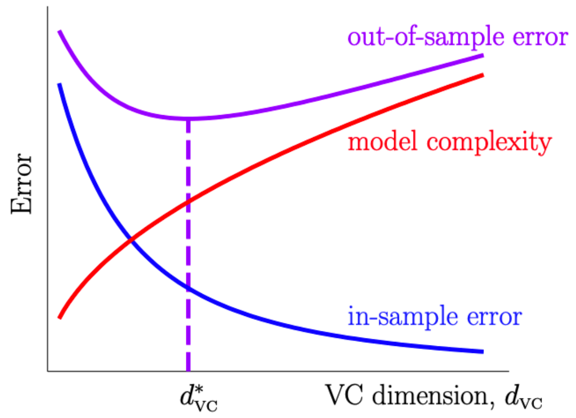
Logistics

- HW1: Due this Friday
  - Reserve time if you have never used Gradescope
  - Check that submission is readable (if you scan your handwriting)
  - Assign pages to each problem
- HW2: Will be announce between this Friday and next Monday
- Exam1: Will announce the date this week
- Contact me: Piazza, not emails

Recap

VC Generalization Bound

- VC Bound: $E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{vc}\frac{\ln N}{N}}\right)$
- Theoretically characterized the feasibility of learning
- The performance of your learning, i.e., $E_{out}(g)$, depends on
  - How well you fit your data ($E_{in}(g)$)
  - How well your $E_{in}(g)$ generalizes to $E_{out}(g)$

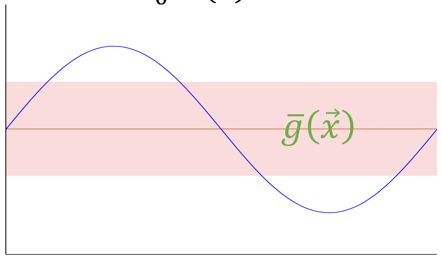


Bias-Variance Decomposition

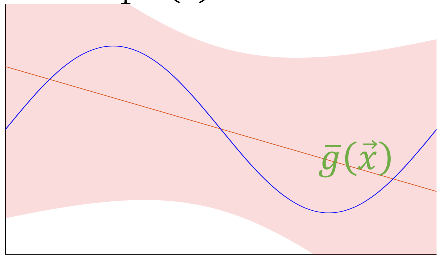
- $$\mathbb{E}_D\left[E_{out}\left(g^{(D)}\right)\right] = \mathbb{E}_{\vec{x}}\left[\overbrace{\left(\bar{g}(\vec{x}) - f(\vec{x})\right)^2}^{\text{Bias}(\vec{x})}\right] + \mathbb{E}_{\vec{x}}\left[\overbrace{\mathbb{E}_D\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)^2\right]}^{\text{Var}(\vec{x})}\right]$$

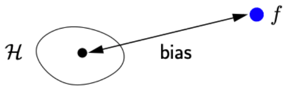
- The performance of your learning, i.e.,$\mathbb{E}_D\left[E_{out}\left(g^{(D)}\right)\right]$, depends on
  - How well you can fit your data using your hypothesis set (bias)
  - How close to the best fit you can get for a given dataset (variance)

H_0: $h(x) = b$

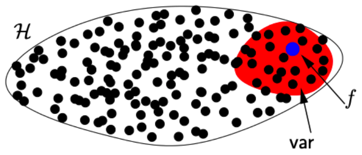


H_1: $h(x) = ax + b$



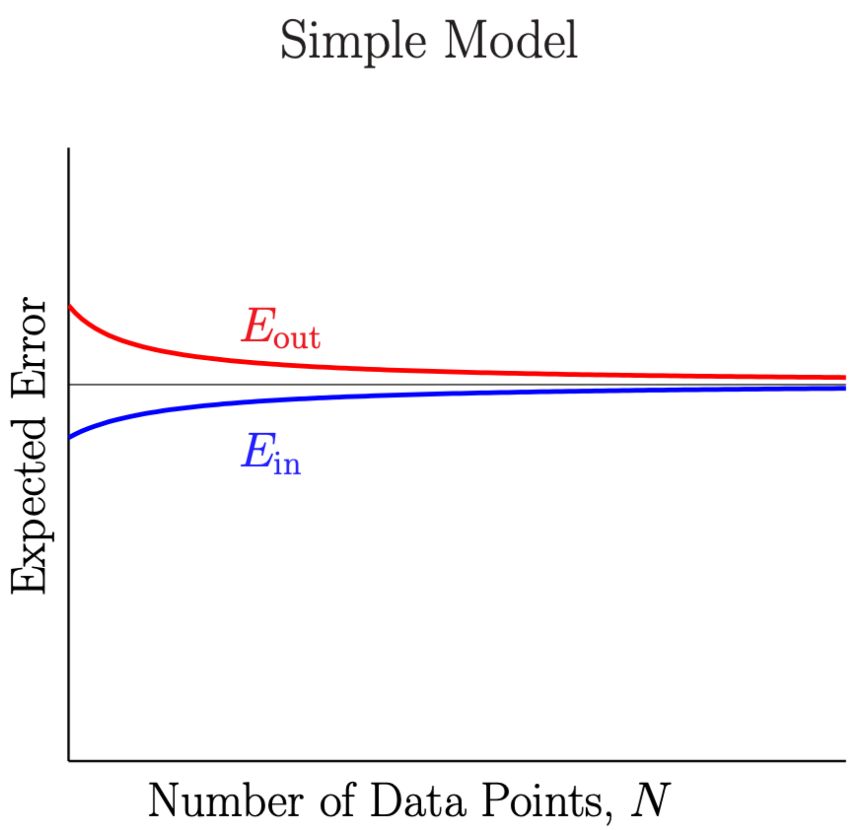


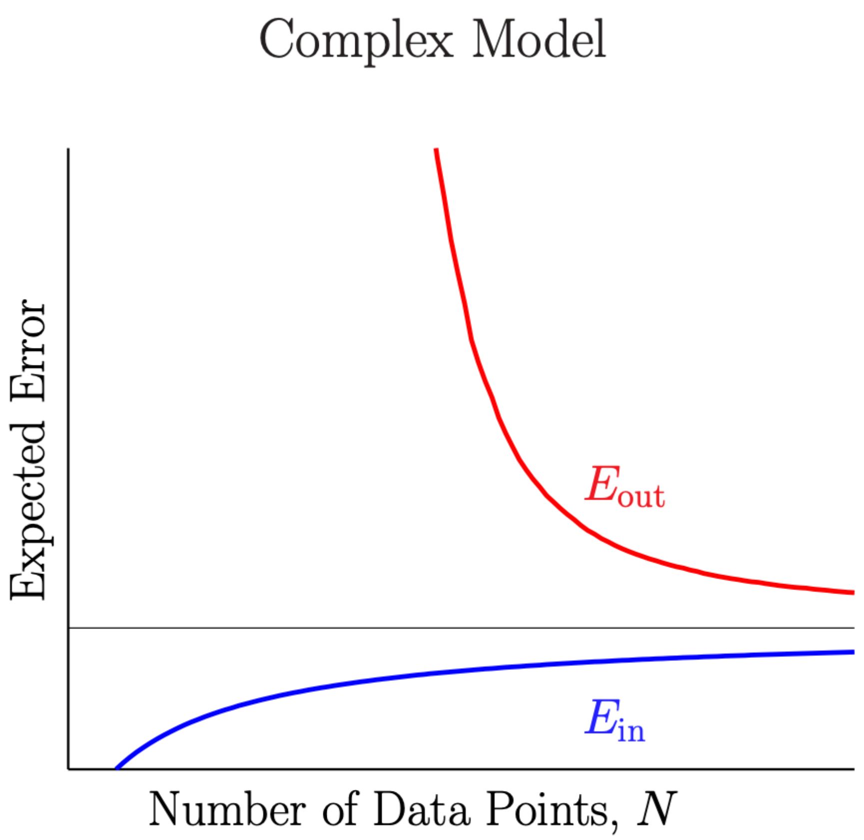
Very small model



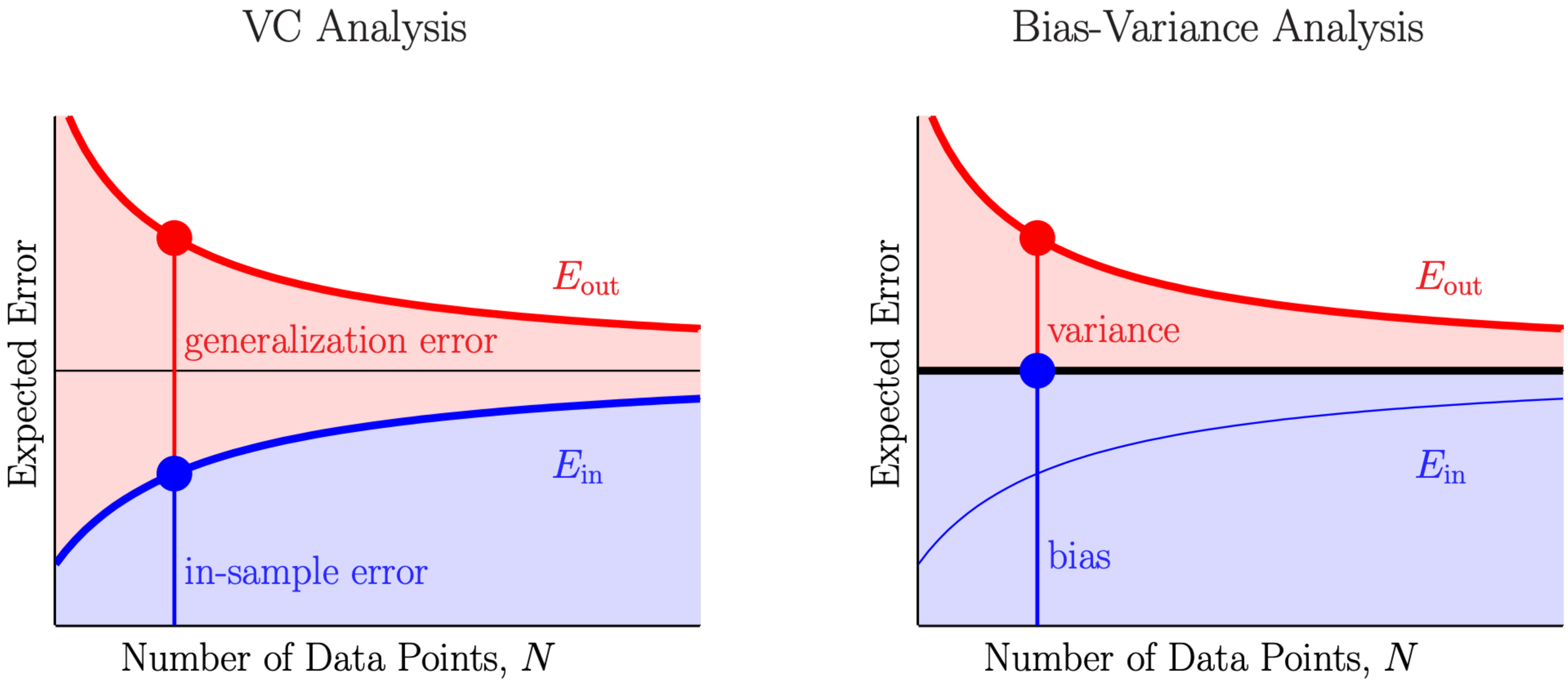
Very large model

Learning Curves





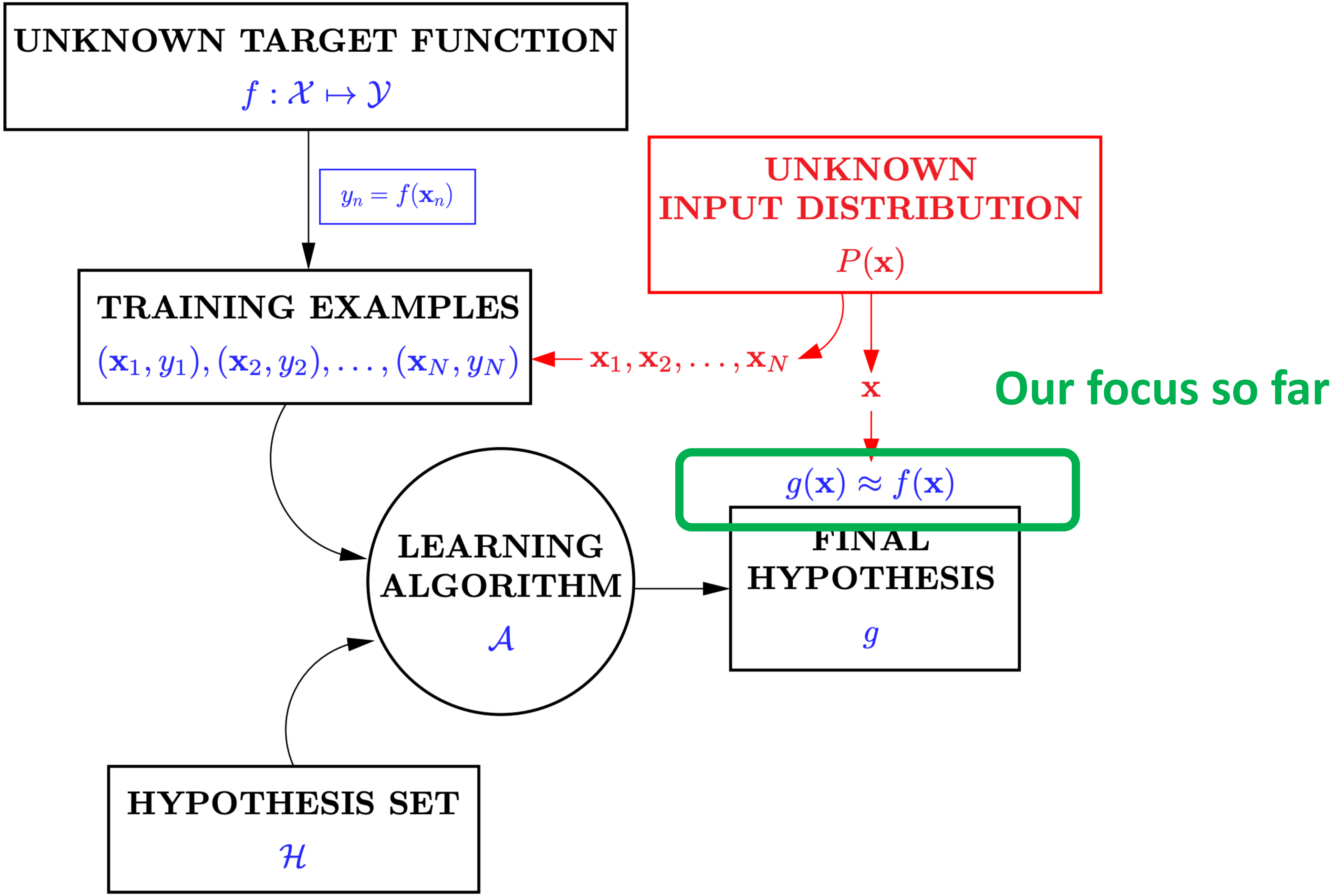
Learning Curves



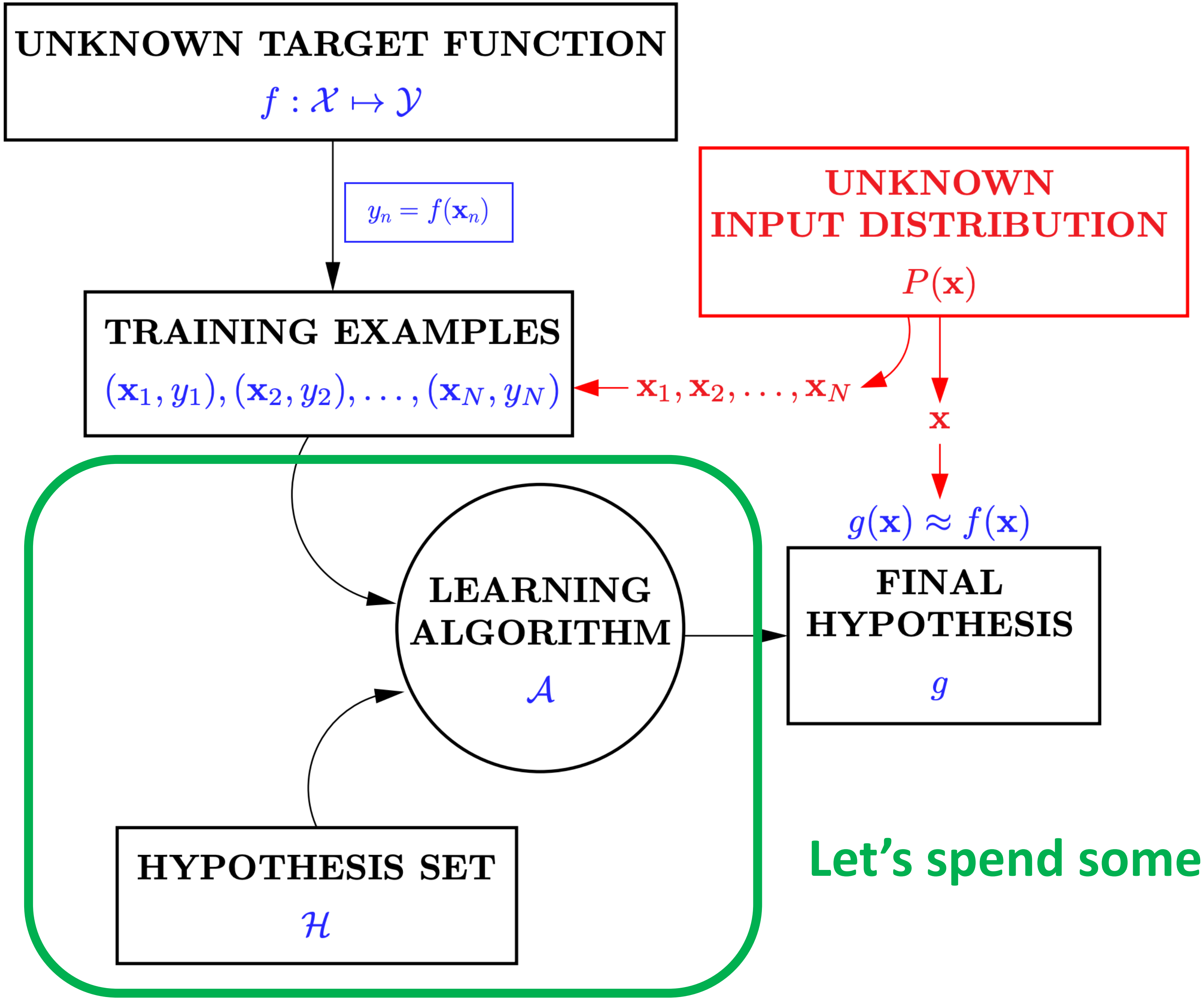
Today’s Lecture

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

Let me know if you spot errors.



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



Let's spend some time here

Linear Models

Linear Models

This is why it's called linear models

- H contains hypothesis $h(\vec{x})$ as **some function of $\vec{w}^T\vec{x}$**

	Domain	Model
Linear Classification	$y \in \{-1, +1\}$	$H = \{h(\vec{x}) = sign(\vec{w}^T\vec{x})\}$
Linear Regression	$y \in \mathbb{R}$	$H = \{h(\vec{x}) = \vec{w}^T\vec{x}\}$
Logistic Regression	$y \in [0,1]$	$H = \{h(\vec{x}) = \theta(\vec{w}^T\vec{x})\}$

Credit Card Example

Approve or not

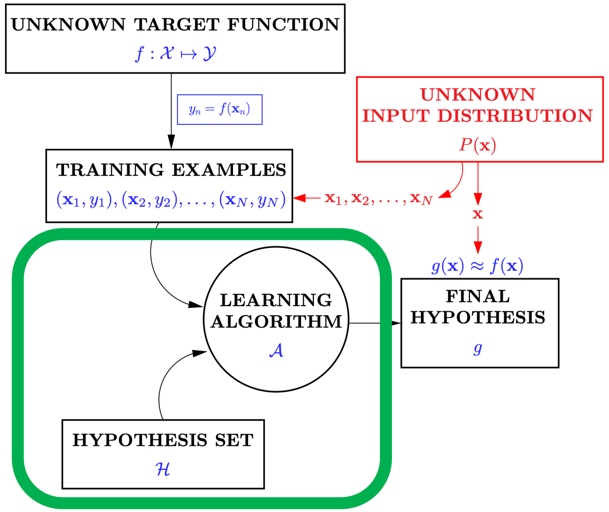
Credit line

Prob. of default

$$\theta(s) = \frac{e^s}{1 + e^s}$$

- Linear models:
  - Simple models => Good generalization error
- Reminder:
  - We will **interchangeably use h and $\vec{w}$** to represent a hypothesis in linear models

Learning Algorithm?



- Goal of the learning algorithm:
  - Find $g \in H$ such that $g \approx f$
  - Define error measures to quantify $g \approx f$
  - Find $g \in H$ that minimizes $E_{out}(g)$ (but we don't know E_{out})

- Recall on the error measure
  - Often focus on point-wise error $e\big(h(\vec{x})\big), f(\vec{x}))$
    - Binary error for classification
    - Squared error for regression
  - In-sample and out-of-sample errors
    - $E_{in}(h) = \frac{1}{N}\sum_{n=1}^{N} e(h(\vec{x}_n), f(\vec{x}_n))$
    - $E_{out}(h) = \mathbb{E}_{\vec{x}}[e(h(\vec{x}), f(\vec{x})]$

Learning Algorithm?

- Goal of the algorithm: Find $g \in H$ that minimizes $E_{out}(g)$

- Common algorithms:
  - $g = argmin_{h \in H} E_{in}(h)$
    - Works well when the model is simple (generalization error is small)
    - Will focus on this in the discussion of linear models

  - $g = argmin_{h \in H} \{E_{in}(h) + \Omega(h)\}$
    - $\Omega(h)$: penalty for complex h
    - Will discuss this when we get to LFD Section 4

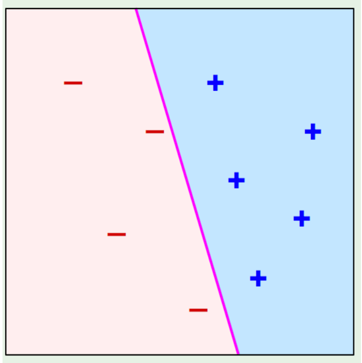
VC Bound: $E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{vc} \frac{\ln N}{N}}\right)$

- Optimization is a key component in machine learning

Linear Classification

Linear Classification

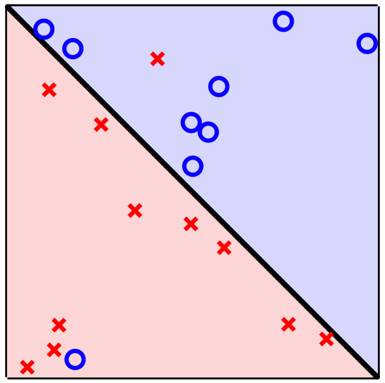
- Formulation
  - Hypothesis set $H = \{h(\vec{x}) = sign(\vec{w}^T \vec{x})\}$
  - Error measure: binary error $e(h(\vec{x}), y) = \mathbb{I}[h(\vec{x}) \neq y]$



- Property
  - Simple model (Fact: the VC dimension of d-dim perceptron is d+1)
  - Good generalization error

- When data is linearly separable
  - Run PLA
    => find g with $E_{in}(g) = 0$
    => $E_{out}(g)$ is close to $E_{in}(g) = 0$

Non-Separable Data

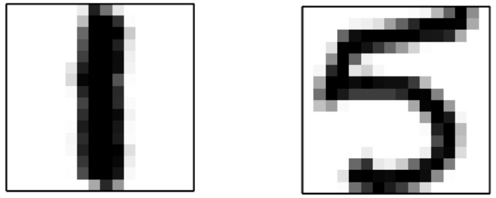


- Generally a hard problem
  - Minimizing E_{in} is a NP-hard problem
  - Reason: binary error is discrete and hard to optimize

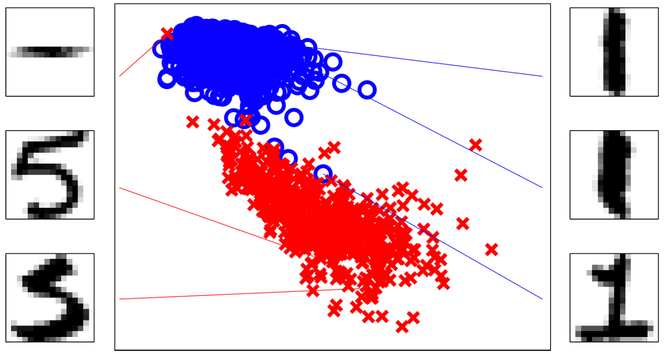
- Alternative approaches
  - Pocket algorithm
    - Run PLA for a finite pre-determined T rounds
    - Keep track of the best weights $\vec{w}^*$ ($\vec{w}(t)$ that minimizes E_{in})
  - Engineering the features to make data closer to be separable
    - Feature engineering (requiring domain knowledge, e.g., see LFD Example 3.1)
  - Non-linear transformation (will discuss this in later lectures)
  - Changing the problem formulation (will discuss this in later lectures)
    - Example: Support vector machines in 2^{nd} half of the semester

Example on Feature Engineering

- Task: Classify handwritten digits of 1 and 5



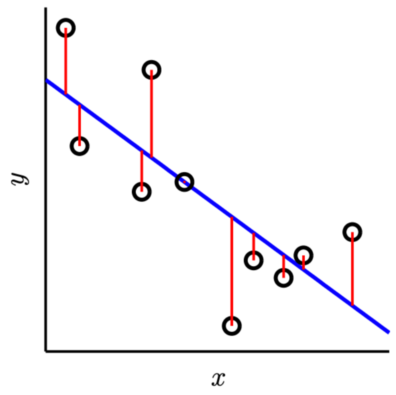
- Linearly separable?
  - What are the features $\vec{x}$?
    - Each pixel as a feature (deep learning approach. requires data)
    - $\vec{x} = (\text{intensity}, \text{symmtry})$

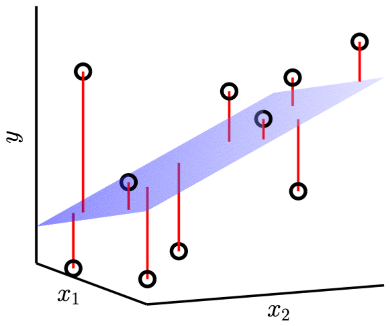


Feature engineer is a practical issue in applied ML but not the focus of this course (requires domain knowledge).

Linear Regression

Linear Regression





- Formulation
  - Hypothesis set $H = \{h(\vec{x}) = \vec{w}^T\vec{x}\}$
  - Squared error $e(h(\vec{x}), y) = (h(\vec{x}) - y)^2$

- Given dataset $D = \{(\vec{x}_1, y_1), \ldots, (\vec{x}_N, y_N)\}$
  - $E_{in}(\vec{w}) = \frac{1}{N}\sum_{n=1}^{N}(\vec{w}^T\vec{x}_n - y_n)^2$

- Goal: find $\vec{w}_{lin} = argmin_{\vec{w}}\, E_{in}(\vec{w})$

Matrix Representation

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

- $X = \begin{bmatrix} \vec{x}_1^T \\ \vdots \\ \vec{x}_N^T \end{bmatrix} = \begin{bmatrix} x_{1,0} & x_{1,1} & \cdots & x_{1,d} \\ x_{2,0} & x_{2,1} & \cdots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{2,0} & x_{N,1} & \cdots & x_{N,d} \end{bmatrix}$

$x_{n,i}$: the i-th element of vector $\vec{x}_n$

- $\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$

Rewriting the In-Sample Error In Matrix Form

$$E_{in}(\vec{w}) = \frac{1}{N}\sum_{n=1}^{N}(\vec{w}^T\vec{x}_n - y_n)^2$$

$$= \frac{1}{N}\sum_{n=1}^{N}(\vec{x}_n^T\vec{w} - y_n)^2$$

$$= \frac{1}{N}\|X\vec{w} - \vec{y}\|^2$$

$$= \frac{1}{N}(X\vec{w} - \vec{y})^{\mathrm{T}}(X\vec{w} - \vec{y})$$

$$X = \begin{bmatrix} \vec{x}_1^T \\ \vdots \\ \vec{x}_N^T \end{bmatrix}; \quad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

$$X\vec{w} = \begin{bmatrix} \vec{x}_1^T\vec{w} \\ \vdots \\ \vec{x}_N^T\vec{w} \end{bmatrix}$$

$$X\vec{w} - \vec{y} = \begin{bmatrix} \vec{x}_1^T\vec{w} - y_1 \\ \vdots \\ \vec{x}_N^T\vec{w} - y_N \end{bmatrix}$$

$$\|\vec{z}\| = \sqrt{\vec{z}^T\vec{z}} = \sqrt{\Sigma_{i=1}^{d} z_i^2}$$

$$\|\vec{z}\|^2 = \vec{z}^T\vec{z} = \Sigma_{i=1}^{d} z_i^2$$

$$\longrightarrow$$

$$E_{in}(\vec{w}) = \frac{1}{N}\left((X\vec{w})^T - \vec{y}^{\mathrm{T}}\right)(X\vec{w} - \vec{y})$$

$$= \frac{1}{N}(\vec{w}^T X^T X\vec{w} - 2\vec{w}^T X^T\vec{y} + \vec{y}^T\vec{y})$$

How to find $\vec{w}_{lin} = argmin_{\vec{w}}\, E_{in}(\vec{w})$?

- Given $E_{in}(\vec{w}) = \frac{1}{N}(\vec{w}^T X^T X \vec{w} - 2\vec{w}^T X^T \vec{y} + \vec{y}^T \vec{y})$
- Solve for $\nabla_{\vec{w}} E_{in}(\vec{w}) = 0$
  - Think about what you'll do for one-dimensional case

$$\nabla f(\vec{w}) = \nabla_{\vec{w}} f(\vec{w}) = \begin{bmatrix} \frac{\partial}{\partial w_0} f(\vec{w}) \\ \frac{\partial}{\partial w_1} f(\vec{w}) \\ \vdots \\ \frac{\partial}{\partial w_d} f(\vec{w}) \end{bmatrix}$$

- Derivations
  - $E_{in}(\vec{w}) = \frac{1}{N}(\vec{w}^T X^T X \vec{w} - 2\vec{w}^T X^T \vec{y} + \vec{y}^T \vec{y})$
  - $\nabla_{\vec{w}} E_{in}(\vec{w}) = \frac{1}{N}(2X^T X \vec{w} - 2X^T \vec{y})$
  - $\nabla_{\vec{w}} E_{in}(\vec{w}_{lin}) = 0$ ==> $X^T X \vec{w}_{lin} = 2X^T \vec{y}$

- $X^T X \vec{w}_{lin} = 2X^T \vec{y}$

- Two cases:
  - If $X^T X$ is invertible (When $N \gg d$, most of the time, it is invertible)
    - $\vec{w}_{lin} = (X^T X)^{-1} X^T \vec{y}$
  - If $X^T X$ is not invertible
    - Requires special handling (See LFD Problem 3.15 for an example)

- In practice
  - Define $X^\dagger$ as the pseudo-inverse of X
    - When $X^T X$ is invertible, $X^\dagger = (X^T X)^{-1} X^T$
    - When $X^T X$ is not invertible, "handle" it appropriately (usually done in the library for you)

- Linear regression algorithm (a single step algorithm):
  - $\vec{w}_{lin} = X^\dagger \vec{y}$

Linear Regression "Algorithm"

- Input: $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \dots, (\vec{x}_N, y_N)\}$

1. Construct X and $\vec{y}$
2. Compute the pseudo-inverse of X: $X^\dagger$
   ($X^\dagger = (X^T X)^{-1} X^T$ when $(X^T X)$ is invertible)
3. Compute $\vec{w}_{lin} = \mathrm{X}^\dagger \vec{y}$

- Output: $\vec{w}_{lin}$

Break and Practice

Linear Regression "Algorithm"

- Input: $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \dots, (\vec{x}_N, y_N)\}$

1. Construct X and $\vec{y}$
2. Compute the pseudo-inverse of X: $X^\dagger$
   ($X^\dagger = (X^T X)^{-1} X^T$ when $(X^T X)$ is invertible)
3. Compute $\vec{w}_{lin} = \mathrm{X}^\dagger \vec{y}$

- Output: $\vec{w}_{lin}$

- What happens in 0-dimensional model
  - $\vec{x} = (x_0)$
  - Given $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \dots, (\vec{x}_N, y_N)\}$
  - What's $\vec{w}_{lin}$

Discussion

Linear Regression "Algorithm"

- Input: $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_N, y_N)\}$

1. Construct X and $\vec{y}$
2. Compute the pseudo-inverse of X: $X^\dagger$
   ($X^\dagger = (X^TX)^{-1}X^T$ when (X^TX) is invertible)
3. Compute $\vec{w}_{lin} = \mathrm{X}^\dagger \vec{y}$

- Output: $\vec{w}_{lin}$

- Special case of zero–dimensional space

$$X = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \Rightarrow X^TX = N \Rightarrow (X^TX)^{-1} = 1/\mathrm{N}$$

$$\vec{w}_{lin} = (X^TX)^{-1}X^T\vec{y}$$

$$= \begin{bmatrix} \frac{1}{N} \cdots \frac{1}{N} \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} = \frac{1}{N} \sum_{n=1}^{N} y_n$$

Squared error => mean

Discussion

- Linear regression generalizes very well
  - Under mild conditions (See LFD Exercise 3.4 for an example)

$$E_{out}(g) = E_{in}(g) + O\left(\frac{d}{N}\right)$$

- Use regression for classification
  - Note that $\{-1, +1\} \subset \mathbb{R}$
  - Use linear regression to find $\vec{w}_{lin} = (X^T X)^{-1} X^T \vec{y}$ for data with $y \in \{-1, +1\}$
  - Use $\vec{w}_{lin}$ for classification: $g(\vec{x}) = \text{sign}\left(\vec{w}_{lin}^T \vec{x}\right)$

  - Alternatively, use $\vec{w}_{lin}$ as the initialization for Pocket Algorithm

Logistic Regression