# CSE 417T Introduction to Machine Learning

Lecture 7

Instructor: Chien-Ju (CJ) Ho

# Logistics

- HW1: Due Sep 23
  - Reserve time if you have never used Gradescope
  - Check that submission is readable (if you scan your handwriting)
  - Correctly assign pages to each problem (you won't get points otherwise)
- HW2: Will be announce later this week

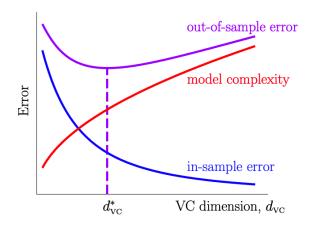
- Exam dates
  - Exam 1: October 27
    - We expect to finish the content for exam1 several lectures before the exam.
  - Exam 2: December 8

# Recap

### VC Generalization Bound

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

- Theoretically characterize 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  $E_{out}(g)$

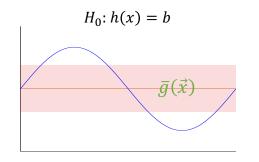


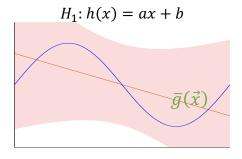
### Bias-Variance Decomposition

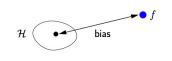
$$\operatorname{Bias}(\vec{x}) \qquad \operatorname{Var}(\vec{x})$$

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

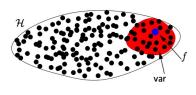
- The performance of your learning, i.e.,  $\mathbb{E}_D[E_{out}(g^{(D)})]$ , depends on
  - How well you can fit your data using your hypothesis set (bias)
  - How stable your learning is for a randomly drawn dataset (variance)







Very small model



Very large model

# 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.

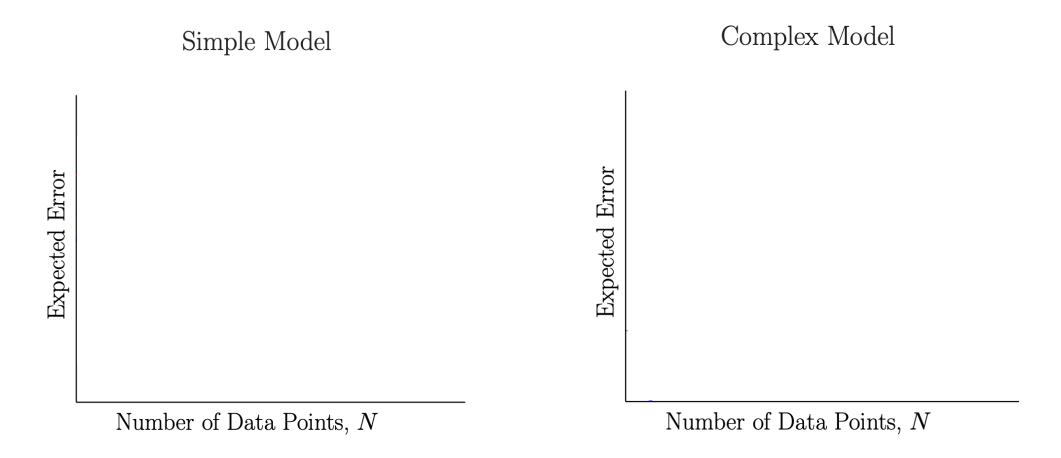
### Two Theories of Generalization

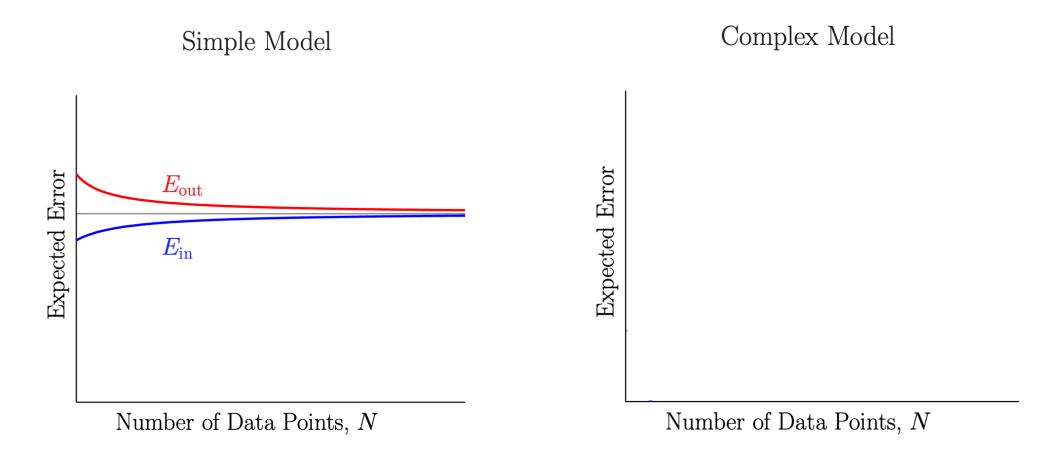
VC Generalization Bound

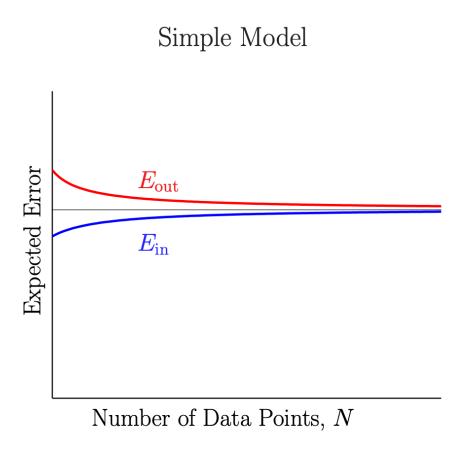
$$E_{out}(g) \le E_{in}(g) + O\left(\sqrt{d_{vc} \frac{\ln N}{N}}\right)$$

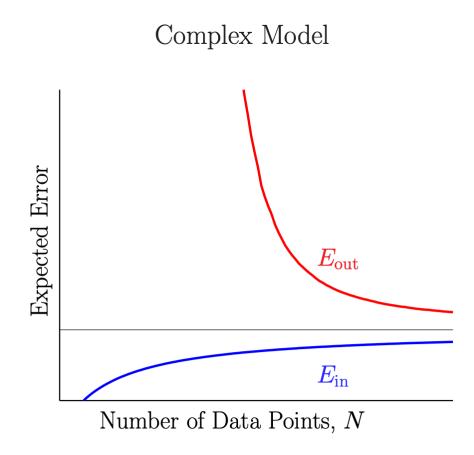
Bias-Variance Tradeoff

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

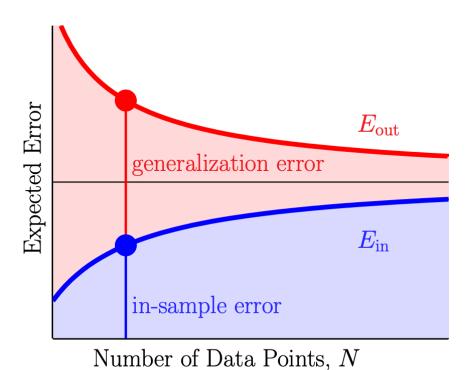






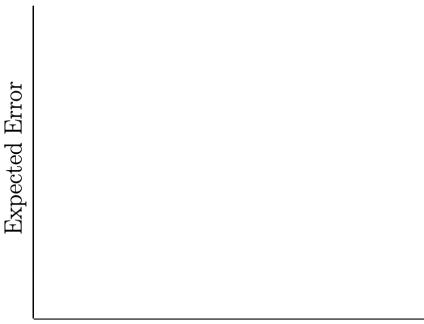


VC Analysis



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

Bias-Variance Analysis

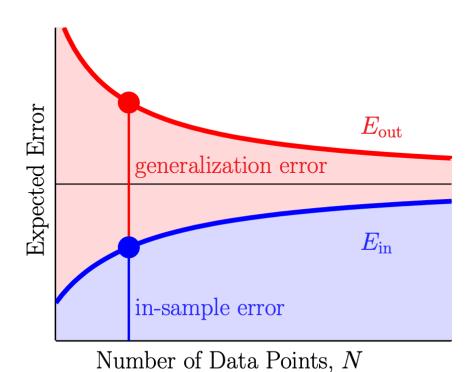


Number of Data Points, N

$$\mathbb{E}_{D}\left[E_{out}(g^{(D)})\right]$$

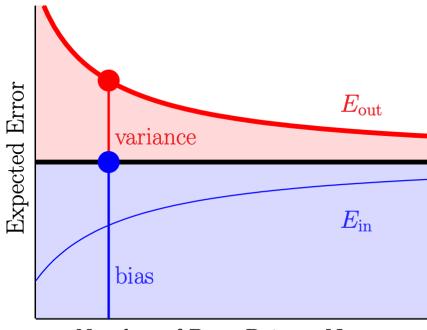
$$= \mathbb{E}_{\vec{x}}\left[\left(\bar{g}(\vec{x}) - f(\vec{x})\right)^{2}\right] + \mathbb{E}_{\vec{x}}\left[\mathbb{E}_{D}\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)^{2}\right]\right]$$

VC Analysis



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

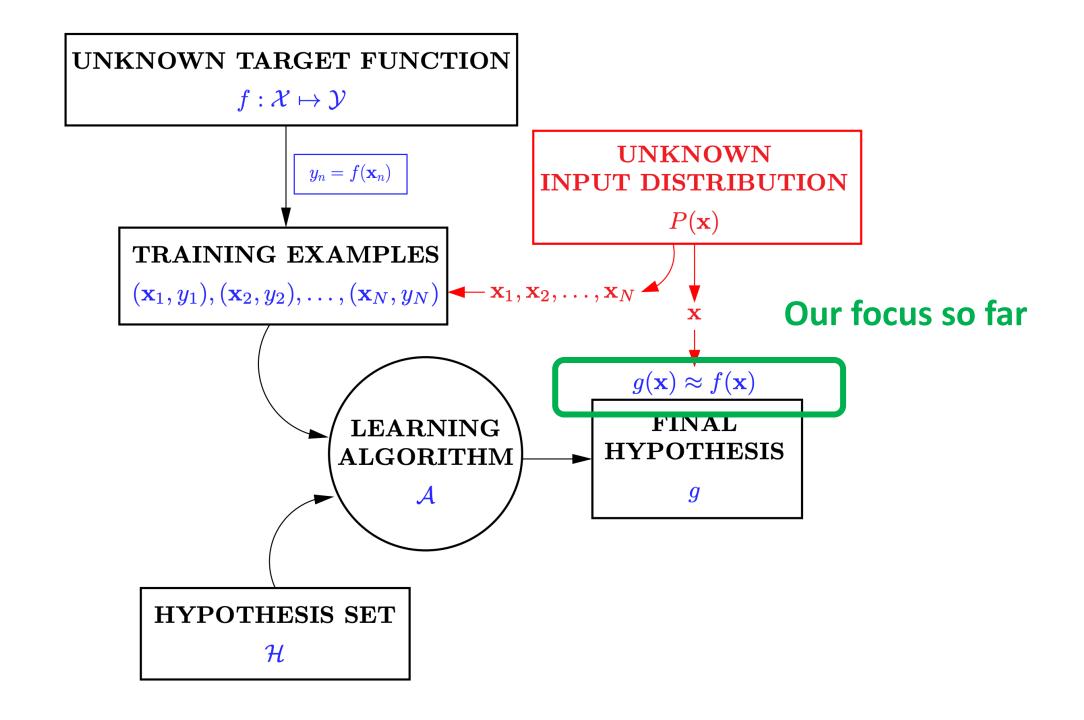
Bias-Variance Analysis

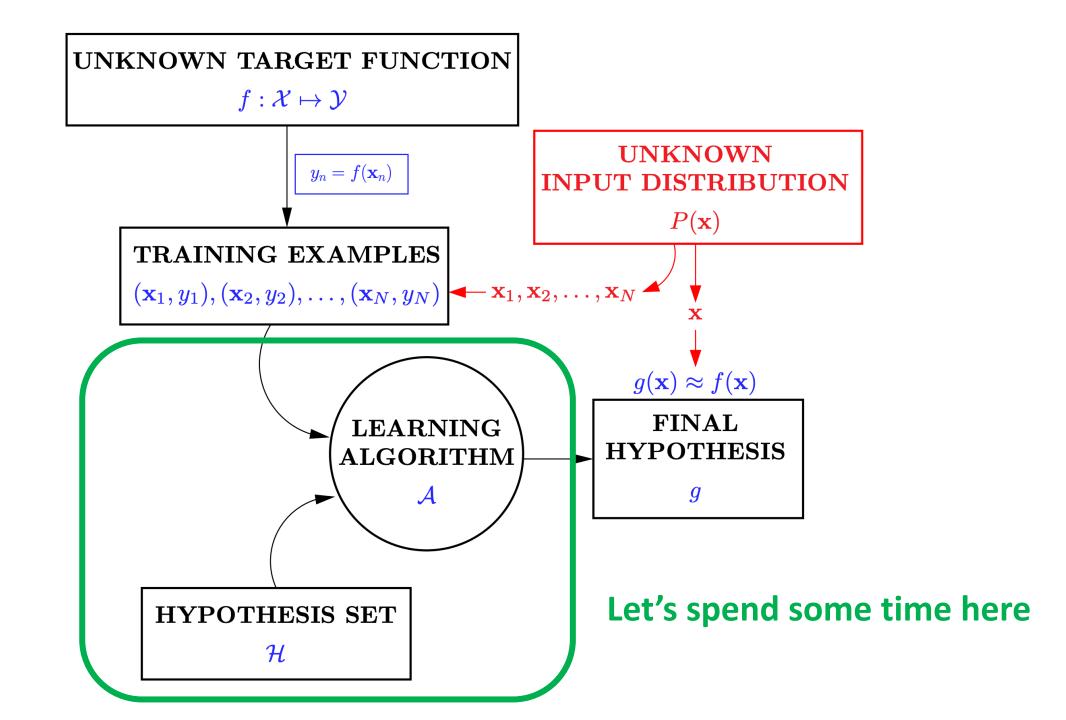


Number of Data Points, N

$$\mathbb{E}_{D}\left[E_{out}(g^{(D)})\right]$$

$$= \mathbb{E}_{\vec{x}}\left[\left(\bar{g}(\vec{x}) - f(\vec{x})\right)^{2}\right] + \mathbb{E}_{\vec{x}}\left[\mathbb{E}_{D}\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)^{2}\right]\right]$$





# 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

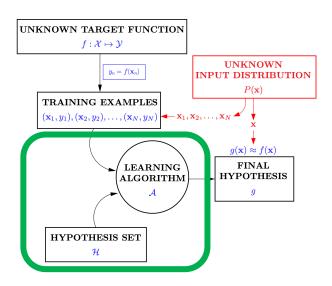
- Linear models:
  - Simple models => Good generalization error

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

- Reminder:
  - We will interchangeably use h and  $\vec{w}$  to represent a hypothesis in linear models

# Learning Algorithm?

• Goal of the algorithm: Find  $g \in H$  that minimizes  $E_{out}(g)$  (We don't know  $E_{out}$ )



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

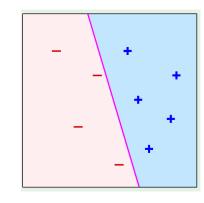
Optimization is a key component in machine learning

# Linear Classification

|                       | 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})\}\$ |

# Linear Classification (Perceptron)

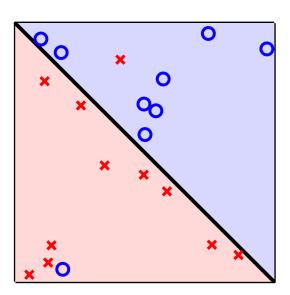
- Formulation
  - Hypothesis set  $H = \{h(\vec{x}) = sign(\vec{w}^T\vec{x})\}$
  - Error measure: binary error  $e(h(\vec{x}), y) = \mathbb{I}[h(\vec{x}) \neq y]$



- Property
  - Simple model (Fact: the VC dimension of d-dim perceptron is d+1)
  - Good generalization error
- When data is linearly separable
  - Run PLA
    - $\Rightarrow$  find g with  $E_{in}(g) = 0$
    - $\Rightarrow E_{out}(g)$  is close to  $E_{in}(g) = 0$

# Non-Separable Data

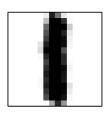
- Generally a hard problem
  - Minimizing  $E_{in}$  is NP-hard
  - Reason: binary error is discrete and hard to optimize

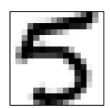


- Alternative approaches
  - Pocket algorithm
    - Run PLA for a finite pre-determined T rounds
    - Keep track of the best weights  $\vec{w}^*$  ( $\vec{w}(t)$  that minimizes  $E_{in}$ )
  - Engineering the features to make data closer to be separable
    - Feature engineering (requiring domain knowledge, e.g., see LFD Example 3.1)
  - Non-linear transformation (will discuss this in later lectures)
  - Changing the problem formulation
    - Treat it as a logistic regression problem (what's the probability for the label to be +1)
    - Another example: Support vector machines in 2<sup>nd</sup> half of the semester

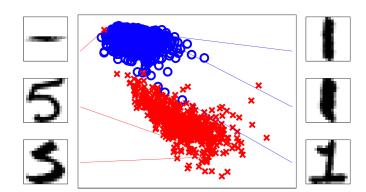
# Example on Feature Engineering

• Task: Classify handwritten digits of 1 and 5





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

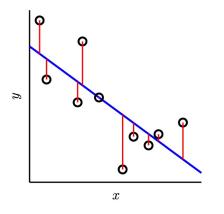


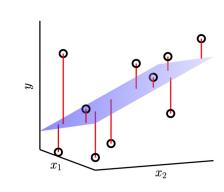
# Linear Regression

|                       | 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})\}\$ |

# 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  $D = \{(\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)\}$ 
  - $E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^{N} (\vec{w}^T \vec{x}_n y_n)^2$
- Goal: find  $\overrightarrow{w}_{lin} = argmin_{\overrightarrow{w}} E_{in}(\overrightarrow{w})$

# Matrix Representation

• 
$$D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$$

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

**Predictions** made by hypothesis  $\vec{w}$ 

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

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

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

# Rewriting the In-Sample Error In Matrix Form

$$E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^{N} (\vec{w}^T \vec{x}_n - y_n)^2 \qquad \begin{bmatrix} x = \begin{bmatrix} \vec{x}_1^T \\ \vec{x}_N^T \end{bmatrix}; \ \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \end{bmatrix} \begin{pmatrix} x \vec{w} = \begin{bmatrix} \vec{x}_1^T \vec{w} \\ \vdots \\ \vec{x}_N^T \vec{w} \end{bmatrix} \\ = \frac{1}{N} \sum_{n=1}^{N} (\vec{x}_n^T \vec{w} - y_n)^2 \qquad \begin{bmatrix} \|\vec{z}\| = \sqrt{\vec{z}^T \vec{z}} = \sqrt{\sum_{i=1}^d z_i^2} \\ \|\vec{z}\|^2 = \vec{z}^T \vec{z} = \sum_{i=1}^d z_i^2 \end{bmatrix} \\ = \frac{1}{N} \|X \vec{w} - \vec{y}\|^2 \qquad \qquad E_{in}(\vec{w}) = \frac{1}{N} ((X \vec{w})^T - \vec{y}^T) (X \vec{w} - \vec{y}) \\ = \frac{1}{N} (X \vec{w} - \vec{y})^T (X \vec{w} - \vec{y}) \qquad \qquad -\frac{1}{N} (\vec{w}^T Y^T Y \vec{w} - 2\vec{w}^T Y^T \vec{y} + \vec{y}^T \vec{y})$$

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

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

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

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

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

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

- 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  $\nabla_{\overrightarrow{w}} E_{in}(\overrightarrow{w}) = 0$ 
  - Think about what you'll do for one-dimensional case

#### Derivations

• 
$$E_{in}(\overrightarrow{w}) = \frac{1}{N}(\overrightarrow{w}^T X^T X \overrightarrow{w} - 2\overrightarrow{w}^T X^T \overrightarrow{y} + \overrightarrow{y}^T \overrightarrow{y})$$

• 
$$\nabla_{\overrightarrow{w}} E_{in}(\overrightarrow{w}) = \frac{1}{N} (2X^T X \overrightarrow{w} - 2X^T \overrightarrow{y})$$

• 
$$\nabla_{\overrightarrow{w}} E_{in}(\overrightarrow{w}_{lin}) = 0 \implies X^T X \overrightarrow{w}_{lin} = X^T \overrightarrow{y}$$

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

• 
$$X^T X \overrightarrow{w}_{lin} = X^T \overrightarrow{y}$$

- Two cases:
  - If  $X^TX$  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  $X^TX$  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  $X^TX$  is invertible,  $X^{\dagger} = (X^TX)^{-1}X^T$
    - When  $X^TX$  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:  $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), ..., (\vec{x}_N, y_N)\}$
- 1. Construct X and  $\vec{y}$
- 2. Compute the pseudo-inverse of  $X: X^{\dagger}$   $(X^{\dagger} = (X^T X)^{-1} X^T \text{ when } (X^T X) \text{ is invertible})$
- 3. Compute  $\vec{w}_{lin} = X^{\dagger} \vec{y}$
- Output:  $\overrightarrow{w}_{lin}$

### **Short Discussion**

#### Linear Regression "Algorithm"

- Input:  $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), ..., (\vec{x}_N, y_N)\}$
- 1. Construct X and  $\vec{y}$
- 2. Compute the pseudo-inverse of  $X: X^{\dagger}$   $(X^{\dagger} = (X^TX)^{-1}X^T \text{ when } (X^TX) \text{ is invertible})$
- 3. Compute  $\vec{w}_{lin} = X^{\dagger} \vec{y}$
- Output:  $\overrightarrow{w}_{lin}$

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

### **Short Discussion**

#### Linear Regression "Algorithm"

- Input:  $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), ..., (\vec{x}_N, y_N)\}$
- 1. Construct X and  $\vec{y}$
- 2. Compute the pseudo-inverse of  $X: X^{\dagger}$   $(X^{\dagger} = (X^TX)^{-1}X^T \text{ when } (X^TX) \text{ is invertible})$
- 3. Compute  $\vec{w}_{lin} = X^{\dagger} \vec{y}$
- Output:  $\vec{w}_{lin}$

Special case of zero—dimensional space

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

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

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

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:  $g(\vec{x}) = \text{sign}(\vec{w}_{lin}^T \vec{x})$
  - Alternatively, use  $\vec{w}_{lin}$  as the initialization for Pocket Algorithm

# Logistic Regression

|                       | 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})\}\$ |

# Logistic Regression: Predicting a Probability

Will this patient have a heart attack within the next year?

| age         | 62 years        |
|-------------|-----------------|
| gender      | male            |
| blood sugar | 120 mg/dL40,000 |
| HDL         | 50              |
| LDL         | 120             |
| Mass        | 190 lbs         |
| Height      | 5' 10"          |
|             | • • •           |

Classification: Yes/No

Logistic regression: Probability of Yes

- A hypothesis  $h(\vec{x})$  outputs a value in [0,1]
  - Interpreting it as the probability of yes

# Logistic Regression: Predicting a Probability

- Hypothesis set  $H = \{h(\vec{x}) = \theta(\vec{w}^T\vec{x})\}$ 
  - Want  $\theta$  to map from  $(-\infty, \infty)$  to [0,1]

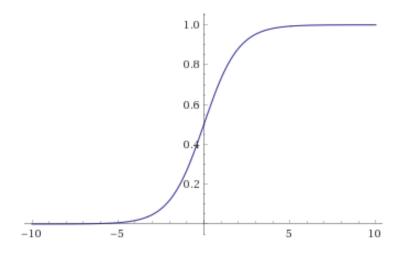
• 
$$\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}$$

A sigmoid function ("S"-shaped function)

• 
$$\theta(s) = \begin{cases} 1 & \text{when } s \to \infty \\ 0.5 & \text{when } s = 0 \\ 0 & \text{when } s \to -\infty \end{cases}$$

Useful property

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



### What Kind of Dataset do We Get?

• Dataset  $D = \{(\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)\}$ 

| age         | 62 years        |
|-------------|-----------------|
| gender      | male            |
| blood sugar | 120 mg/dL40,000 |
| HDL         | 50              |
| LDL         | 120             |
| Mass        | 190 lbs         |
| Height      | 5' 10"          |
|             | • • •           |

- What are the values of  $y_n$ ?
  - Ideally, we want to have  $y_n$  to be the probability value
  - In practice, we cannot measure a probability
  - We can only see the occurrence of an event and infer the probability
  - (We often only observe whether the person had heart attack, we don't observe the "probability")
- Need to address the case when  $y_n \in \{-1, +1\}$  in the given dataset D

# Error Measure: Quantifying $g \approx f$

• Target function  $f(\vec{x}) = \Pr(y = +1|\vec{x})$ 

Side note:

You probably can guess why the property  $1 - \theta(s) = \theta(-s)$  might be helpful

- Another way to write it:  $\Pr(y|\vec{x}) = \begin{cases} f(\vec{x}) & \text{for } y = +1 \\ 1 f(\vec{x}) & \text{for } y = -1 \end{cases}$
- How do we define the error measure to quantify  $g \approx f$ 
  - Ideally, we want it to be meaningful
    - Binary error for classification: tell us the number of mistakes we make
    - Squared error for regression: the error minimizer is the "mean (average)"
  - We also want it to be easy to optimize

# Cross Entropy Error

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

- It looks complicated, but
  - It has nice interpretations (min error => max likelihood)
  - It is easy to optimize (continuous, differentiable, convex)

# Minimizing Cross Entropy Error



Maximizing Likelihood

#### Maximum Likelihood Estimation

- Likelihood Pr(D|h)
  - The probability of seeing dataset D if D is generated according to h
  - $Pr(D|h) = Pr((\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)|h)$
  - Maximum likelihood estimation (MLE)
    - $g = argmax_{h \in H} Pr(D|h)$
- Sidenote: Two different concepts in ML
  - Likelihood: Pr(D|h) [Focus of this course]
  - Posterior: Pr(h|D) [Focus of Bayesian machine learning: More in 515T]
  - Connection:  $Pr(h|D) = \frac{Pr(h)Pr(D|h)}{Pr(D)}$ 
    - Prior Pr(h): the additional assumption Bayesian ML makes

#### Write Down the Likelihood

- How are  $D = \{(\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)\}$  generated?
  - $(\vec{x}_1, ..., \vec{x}_N)$  are i.i.d. drawn from a distribution
  - $(y_1, ..., y_N)$  are labeled according to target function  $f(\vec{x})$
- UNKNOWN TARGET DISTRIBUTION (target function f plus noise)  $P(y \mid \mathbf{x})$ UNKNOWN INPUT DISTRIBUTION  $P(\mathbf{x})$ TRAINING EXAMPLES ( $\mathbf{x}_1, y_1$ ), ( $\mathbf{x}_2, y_2$ ),..., ( $\mathbf{x}_N, y_N$ )  $\mathbf{ERROR}$ MEASURE  $\mathbf{MEASURE}$   $\mathbf{MEASURE}$   $\mathbf{HYPOTHESIS}$   $\mathbf{J}$ HYPOTHESIS SET  $\mathcal{H}$

- Likelihood Pr(D|h)
  - The probability of seeing dataset D if D is generated according to h

• 
$$\Pr(D|h) = \Pr((\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)|h)$$
  
 $= \Pr(\vec{x}_1, ..., \vec{x}_N) \Pr((y_1, ..., y_N)|(\vec{x}_1, ..., \vec{x}_N), h)$   
 $= \prod_{n=1}^{N} \Pr(\vec{x}_n) \prod_{n=1}^{N} \Pr(y_n|\vec{x}_n, h)$  (Assumption of independent data)

### Maximum Likelihood

Choosing the hypothesis that maximizes the likelihood

```
• g = argmax_{h \in H} \Pr(D|h)

= argmax_{h \in H} \prod_{n=1}^{N} \Pr(\vec{x}_n) \prod_{n=1}^{N} \Pr(y_n|\vec{x}_n, h)

= argmax_{h \in H} \prod_{n=1}^{N} \Pr(y_n|\vec{x}_n, h)
```

 $\prod_{n=1}^{N} \Pr(\vec{x}_n)$  doesn't depend on h

• We interpret  $h(\vec{x})$  as the probability of y=+1

• 
$$\Pr(y|\vec{x},h) = \begin{cases} h(\vec{x}) = \theta(\vec{w}^T \vec{x}) & \text{for } y = +1\\ 1 - h(\vec{x}) = 1 - \theta(\vec{w}^T \vec{x}) & \text{for } y = -1 \end{cases}$$

- Since  $1 \theta(s) = \theta(-s)$ 
  - $Pr(y|\vec{x}, h) = \theta(y \vec{w}^T \vec{x})$

### Maximum Likelihood

Choosing the hypothesis that maximizes the likelihood

```
• g = argmax_{h \in H} \Pr(D|h)
= argmax_{h \in H} \prod_{n=1}^{N} \Pr(y_n | \vec{x}_n, h)
```

• 
$$\overrightarrow{w}^* = argmax_{\overrightarrow{w}} \prod_{n=1}^{N} \theta(y_n \overrightarrow{w}^T \overrightarrow{x}_n)$$
  

$$= argmax_{\overrightarrow{w}} \ln(\prod_{n=1}^{N} \theta(y_n \overrightarrow{w}^T \overrightarrow{x}_n))$$
  

$$= argmax_{\overrightarrow{w}} \sum_{n=1}^{N} \ln(\theta(y_n \overrightarrow{w}^T \overrightarrow{x}_n))$$
  

$$= argmin_{\overrightarrow{w}} - \sum_{n=1}^{N} \ln(\theta(y_n \overrightarrow{w}^T \overrightarrow{x}_n))$$
  

$$= argmin_{\overrightarrow{w}} \sum_{n=1}^{N} \ln \frac{1}{\theta(y_n \overrightarrow{w}^T \overrightarrow{x}_n)}$$
  

$$= argmin_{\overrightarrow{w}} \sum_{n=1}^{N} \ln(1 + e^{-y_n \overrightarrow{w}^T \overrightarrow{x}_n})$$
  

$$= argmin_{\overrightarrow{w}} \sum_{n=1}^{N} \ln(1 + e^{-y_n \overrightarrow{w}^T \overrightarrow{x}_n})$$

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

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

# Cross Entropy Error

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

- Minimizing  $E_{in}(\vec{w})$  is the same as maximizing likelihood
- Next question: How to solve  $\vec{w}^* = argmin_{\vec{w}} E_{in}(\vec{w})$ 
  - Answer: Solve for  $\nabla_{\overrightarrow{w}} E_{in}(\overrightarrow{w}) = 0$
  - No single-step solution like we have in linear regression