CSE 417T Introduction to Machine Learning

Lecture 5

Instructor: Chien-Ju (CJ) Ho

Logistics: Homework 1

- Due: Feb 14 (Monday), 2022
 - http://chienjuho.com/courses/cse417t/hw1.pdf
 - Intended deadline: Feb 10.
 - Recommend to work on it early to spare time for homework 2
 - 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

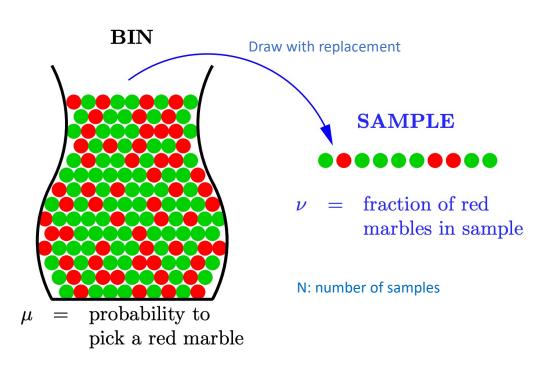
Tentative schedule of TA office hours (starting next Monday)

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

Hoeffding's Inequality



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

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 $D = \{(\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)\}$
 - $E_{in}(h) \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}[h(\vec{x}_n) \neq f(\vec{x}_n)]$ [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]
- Learning bounds
 - Fixed *h* (verification)

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

• Finite hypothesis set: learn $g \in \{h_1, \dots, h_M\}$

$$\Pr[|E_{out}(g) - E_{in}(g)| > \epsilon] \le 2Me^{-2\epsilon^2 N}$$

Dealing with Infinite Hypothesis Set: $M \rightarrow \infty$

- Most of the practical cases involve $M \to \infty$
- Instead of # hypothesis, counting "effective" # hypothesis
- Dichotomies
 - Informally, consider a dichotomy as "data-dependent" hypothesis
 - Characterized by both H and N data points $(\vec{x}_1, ..., \vec{x}_N)$

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

• 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

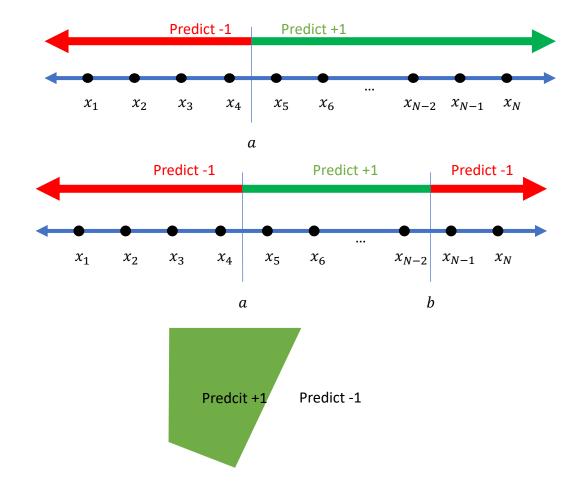
$$m_H(N) = \max_{(\vec{x}_1, ..., \vec{x}_N)} |H(\vec{x}_1, ..., \vec{x}_N)|$$

Examples on Growth Functions

- H = Positive rays
 - $m_H(N) = N + 1$
- H = Positive intervals

•
$$m_H(N) = {N+1 \choose 2} + 1 = \frac{N^2}{2} + \frac{N}{2} + 1$$

- H = Convex sets
 - $m_H(N) = 2^N$



- For all H and for all N
 - $m_H(N) \le 2^N$

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

• VC Generalization Bound (VC Inequality, 1971) With prob at least $1-\delta$

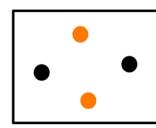
$$E_{out}(g) \le E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4m_H(2N)}{\delta}}$$

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.

Bounding Growth Function

- What we know so far
 - $H = Positive rays: m_H(N) = N + 1$
 - $H = \text{Positive intervals: } m_H(N) = \binom{N+1}{2} + 1$
 - $H = \text{Convex sets: } m_H(N) = 2^N$
- What about H = 2-D Perceptron?
 - $m_H(3) = 8$
 - $m_H(4) = 14$
 - $m_H(5) = ?$



- Generally hard to write down the growth function exactly
 - Goal: "bound" the growth function using some proxy

Bounding Growth Function

- More definitions....
 - Shatter:
 - *H* shatters $(\vec{x}_1, ..., \vec{x}_N)$ if $|H(\vec{x}_1, ..., \vec{x}_N)| = 2^N$
 - *H* can induce all label combinations for $(\vec{x}_1, ..., \vec{x}_N)$
 - 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:

- $m_H(N) \leq \sum_{i=1}^{k-1} {N \choose i}$, or
- $m_H(N) \leq N^{k-1} + 1$

Practice

Dichotomies

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

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

- 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

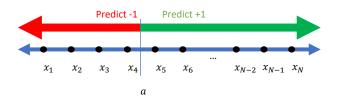
$$m_H(N) = \max_{(\vec{x}_1,...,\vec{x}_N)} |H(\vec{x}_1,...,\vec{x}_N)|$$

• Shatter:

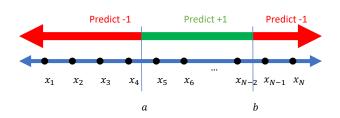
- *H* shatters $(\vec{x}_1, ..., \vec{x}_N)$ if $|H(\vec{x}_1, ..., \vec{x}_N)| = 2^N$
- *H* can induce all label combinations for $(\vec{x}_1, ..., \vec{x}_N)$
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 - k is a break point for H if no data set of size k can be shattered by H

What is the break point for

1. Positive Rays



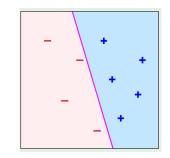
2. Positive Intervals



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 $(\vec{x}_1, ..., \vec{x}_N)$

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

• 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

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

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

 $m_H(N)$

$$m_H(N)$$

$$N=1$$

$$N=2$$

$$N=3$$

$$N=4$$

Break Points

$$N+1$$
 Positive Rays

$$\frac{N^2}{2} + \frac{N}{2} + 1$$
 Posi

Practice

Dichotomies

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

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Growth function

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

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

• Shatter:

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

$m_H(N)$

	N=1	N=2	N=3	N=4	N=5	Break Points
Positive Rays	2	3	4	5	6	k = 2,3,4,
Positive Intervals	2	4	7	11	16	k = 3,4,5,
Convex Sets	2	4	8	16	32	None
2D Perceptron	2	4	8	14	?	k = 4,5,6,

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

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

- 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
 - $m_H(N) \le N^{k-1} + 1$ [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 $1-\delta$

- 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
 - $m_H(N) \le N^{k-1} + 1$ [Can be proven using induction. See LFD Problem 2.5]
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$$E_{out}(g) \le E_{in}(g) + \sqrt{\frac{8}{N}} \ln \frac{4m_H(2N)}{\delta}$$

• In the following discussion, we treat δ as a constant [i.e., with high probability, the following is true]

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

[For example, we can set δ 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:

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



- 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
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 - $m_H(N) = O(N^{k-1})$
 - $m_H(N)$ is polynomial in N
- If there are no break point $(m_H(N) = 2^N)$

$$E_{out}(g) \le E_{in}(g) + \text{Constant}$$
 (This implies that we can't infer E_{out} from E_{in} even when $N \to \infty$)

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

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

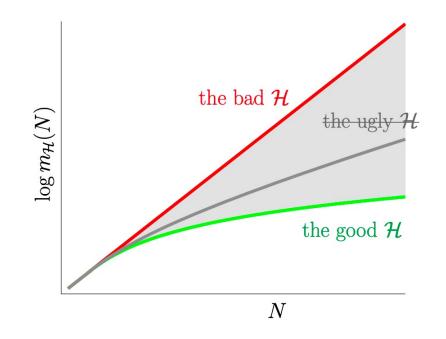
H is Either Good or Bad

- 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
 - $m_H(N) \le N^{k-1} + 1$ [Can be proven using induction. See LFD Problem 2.5]
 - $m_H(N) = O(N^{k-1})$
 - $m_H(N)$ is polynomial in N
- The growth function of *H* is either one of the two
 - Without break points, $m_H(N) = 2^N$
 - With some break point, $m_H(N)$ is polynomial in N (it can be bounded more tightly using the theorem)
 - There is nothing in between!
- Bad hypothesis set

$$E_{out}(g) \le E_{in}(g) + \text{Constant}$$

• Good hypothesis set $m_H(N) = O(N^{k-1})$

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



VC Dimension

- VC Dimension of $H: d_{vc}(H)$ or d_{vc}
 - The VC dimension of H is the largest N such that $m_H(N) = 2^N$.
 - $d_{vc}(H) = \infty$ if $m_H(N) = 2^N$ for all N.
 - Or, let k^* be the smallest break point for H, the VC dimension of H is k^*-1

	$m_H(N)$						
	N=1	N=2	N=3	N=4	N=5	Break Points	VC Dimension
Positive Rays	2	3	4	5	6	k = 2,3,4,	
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Positive Intervals	2	4	7	11	16	k = 3,4,5,	2
Convex Sets	2	4	8	16	32	None	∞
2D Perceptron	2	4	8	14	?	k = 4,5,6,	3

VC Dimension

• If there are no break point $(m_H(N)=2^N)$ $E_{out}(g) \leq E_{in}(g) + \text{Constant}$ • If k is a break point for H, i.e., $m_H(N) = O(N^{k-1})$ $E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{(k-1)\frac{\ln N}{N}}\right)$

- VC Dimension of $H: d_{vc}(H)$ or d_{vc}
 - The VC dimension of H is the largest N such that $m_H(N) = 2^N$.
 - $d_{vc}(H) = \infty$ if $m_H(N) = 2^N$ for all N.
 - Or, let k^* be the smallest break point for H, the VC dimension of H is k^*-1

Plug the definition into VC Generalization Bound

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

All models are wrong but some are useful



George E.P. Box

VC Bound

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

- Built on top of the i.i.d. data assumption
- The bound is "loose"
 - Depends only on H and N
 - The analysis is loose in many places
- However, it qualitatively characterizes the practice reasonably well
 - (the bound is roughly equally loose for every H)

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

- Goal of learning: Minimize $E_{out}(g)$
- How to achieve that
 - Minimize $E_{in}(g)$
 - Choose a hypothesis set with large d_{VC} (complex hypothesis likely fit data better)
 - Minimize generalization error
 - Choose a hypothesis with small d_{VC}
 - Have a lot of data points to train on (N is large)
- Think about the high-level tradeoff of choosing d_{VC} and its dependency on N

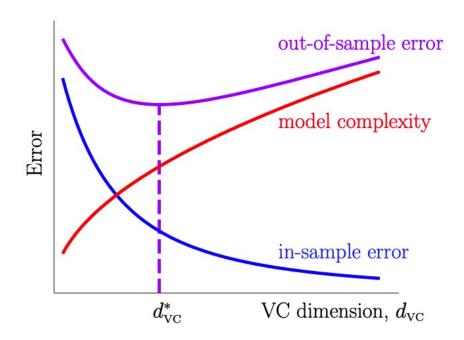
- It establishes the feasibility of learning for infinite hypothesis set
- It provides nice intuitions on what's happening underneath ML
 - A single parameter to characterize complexity of H

$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{\frac{\ln N}{N}}\right) \qquad \stackrel{\text{Let}}{\sqsubseteq}$$

$$\text{VC dimension, } d_{\text{VC}}$$

- It establishes the feasibility of learning for infinite hypothesis set.
- It provides nice intuitions on what's happening underneath ML.
 - A single parameter to characterize complexity of H

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



Sample Complexity

- Sample complexity:
 - Analogy to time/space complexity
 - How many data points do we need to achieve generalization error less than ϵ with prob $1-\delta$?
- Recall the (full) VC Bound:

With prob at least
$$1 - \delta$$
, $E_{out}(g) \le E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4((2N)^{d_{vc}+1)}}{\delta}}$

How to determine the sample complexity?

• Set
$$\sqrt{\frac{8}{N}} \ln \frac{4((2N)^{d_{vc}+1)}}{\delta} \le \epsilon$$

• We get
$$N \ge \frac{8}{\epsilon^2} ln \left(\frac{4(1 + (2N)^d VC)}{\delta} \right)$$

•
$$N \propto 1/\epsilon^2$$

•
$$N = O(d_{vc} \ln N)$$

• In practice, roughly, $N \propto d_{vc}$

Test Set

- Goal of learning: Minimize $E_{out}(g)$
- Can we estimate E_{out} directly?
 - Reserve a test set (D_{test}) before learning
 - Ensure D_{test} is not used at all in any way for learning
 - For D_{test} , g is a "fixed" hypothesis and standard Hoeffding's inequality is valid
 - Let $E_{test}(g)$ be the error in the test set

$$P\{|E_{test}(g) - E_{out}(g)| > \epsilon\} \le 2e^{-2\epsilon^2 N_{test}}$$
 where $N_{test} = |D_{test}|$

Test Set

- Test set is great: we can obtain an unbiased estimate of E_{out}
- At what cost?
 - We have a finite amount of data
 - Data points in test set cannot be involved in learning at all
 - More points in test set
 - Better estimate of *E*_{out}
 - Less data points in training set -> often leads to worse learned hypothesis

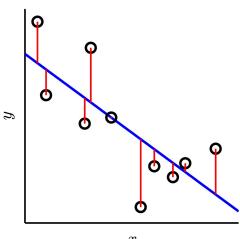
- Practical rule of thumb (i.e., a common heuristic, not really a gold rule)
 - 80% for training, 20% for testing

Bias-Variance Decomposition

Another theory of generalization

Real-Value Target and Squared Error

- So far, we focus on binary target function and binary error
 - Binary target function $f(\vec{x}) \in \{-1,1\}$
 - Binary error $e(h(\vec{x}), f(\vec{x})) = \mathbb{I}[h(\vec{x}) \neq f(\vec{x})]$
- Real-value functions ["regression"] and squared error?
 - Real-value target function $f(\vec{x}) \in \mathbb{R}$
 - Square error $e(h(\vec{x}), f(\vec{x})) = (h(\vec{x}) f(\vec{x}))^2$



Real-Value Target and Square Error

- Real-value functions [called "regression"] and squared error?
 - Real-value target function $f(\vec{x}) \in \mathbb{R}$
 - Square error $e(h(\vec{x}), f(\vec{x})) = (h(\vec{x}) f(\vec{x}))^2$
- Errors:
 - In-sample error: $E_{in}(g) = \frac{1}{N} \sum_{n=1}^{N} e(h(\vec{x}_n), f(\vec{x}_n)) = \frac{1}{N} \sum_{n=1}^{N} (h(\vec{x}_n) f(\vec{x}_n))^2$
 - Out-of-sample error: $E_{out}(g) = \mathbb{E}_{\vec{x}}[e(h(\vec{x}), f(\vec{x}))] = \mathbb{E}_{\vec{x}}[(g(\vec{x}) f(\vec{x}))^2]$
- Theory of generalization: What can we say about $E_{out}(g)$?

- Note that g is learned by some algorithm on the dataset D
 - We'll make the dependency on D explicit and write it as $g^{(D)}$ here.
 - [In VC theory, we consider the worst-case D through the definition of growth function $m_H(N)$]

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

• $\mathbb{E}_D[E_{out}(g^{(D)})]$

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

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

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

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

• Note that
$$\mathbb{E}_D\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)\left(\bar{g}(\vec{x}) - f(\vec{x})\right)\right] = \left(\bar{g}(\vec{x}) - f(\vec{x})\right)\mathbb{E}_D\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)\right] = 0$$

Define "expected" hypothesis $\bar{g}(\vec{x}) = \mathbb{E}_D \big[g^{(D)}(\vec{x}) \big]$

$\bar{g}(\vec{x}) = \mathbb{E}_D \big[g^{(D)}(\vec{x}) \big]$

Finishing Up

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

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

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

- = $\mathbb{E}_{\vec{x}}$ [Variance of $g^{(D)}(\vec{x})$ + Bias of $\bar{g}(\vec{x})$]
- = Variance + Bias

Bias-Variance Decomposition

X: a random variable μ : the mean of X

Variance of X: $Var(X) = \mathbb{E}[(X - \mu)^2]$

Discussion

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

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

- This is a conceptual decomposition
 - Both \bar{g} and f are unknown
 - We can't really calculate bias and variance in practice
- However, it provides a conceptual guideline in decreasing E_{out}