CSE 417T
Introduction to Machine Learning

Lecture 6
Instructor: Chien-Ju (CJ) Ho

Recap

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

- Most of the practical cases involve $M \to \infty$
- Instead of # hypothesis, counting "effective" # hypothesis
- Dichotomy
  - Informally, consider it as "data-dependent" hypothesis
  - Characterized by both 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

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

Why Growth Function?

- Finite-hypothesis Bound

  With prob at least $1-\delta$,

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

- VC Generalization Bound (VC Inequality, 1971)

  With prob at least $1-\delta$

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

If we know the growth function $m_H(N)$ of H, we can obtain the learning guarantee for algorithms operating on H.

Bounding Growth Functions

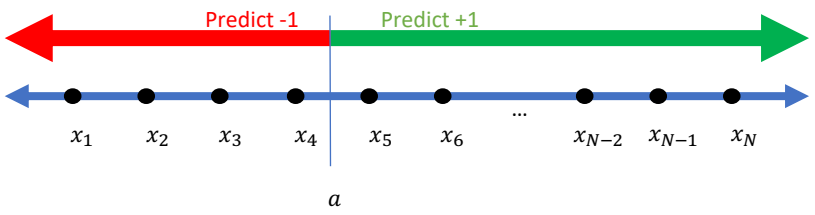
- More definitions….
  - Shatter
    - H **shatters** $(\vec{x}_1, \dots, \vec{x}_N)$ if $|H(\vec{x}_1, \dots, \vec{x}_N)| = 2^N$
    - H can induce all label combinations for $(\vec{x}_1, \dots, \vec{x}_N)$
  - Break point
    - k is a **break point** for H if no data set of size k can be shattered by H
    - k is a break point for $H \leftrightarrow m_H(k) < 2^k$
  - VC Dimension: $d_{vc}(H)$ or d_{vc}
    - The VC dimension of H is the largest N such that $m_H(N) = 2^N$
    - Equivalently, if k^* is the smallest break point for H, $d_{vc}(H) = k^* - 1$

Examples

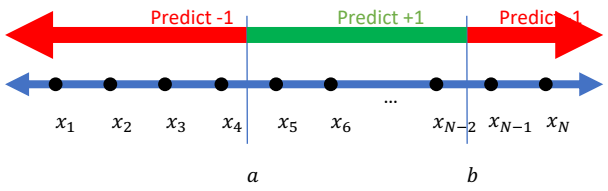
$m_H(N)$

	N=1	N=2	N=3	N=4	N=5	Break Points	VC Dimension
Positive Rays							
Positive Intervals							
Convex Sets							
2D Perceptron							

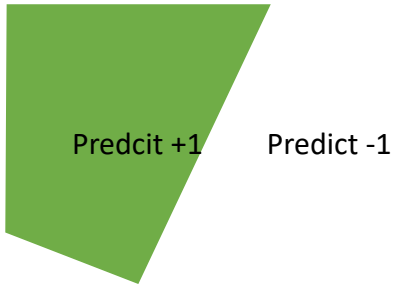
Positive Rays



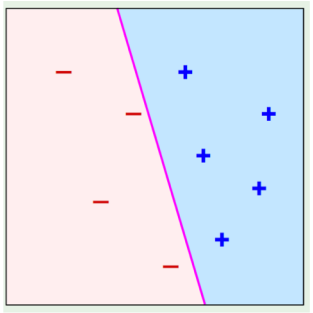
Positive Intervals



Convex Sets



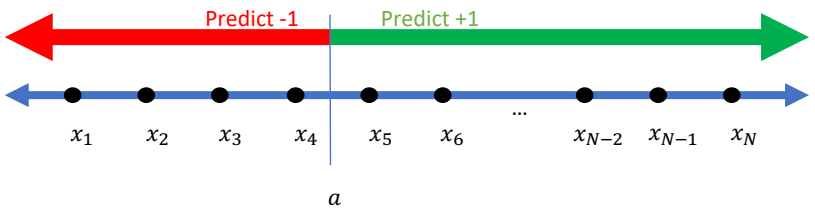
2D Perceptron



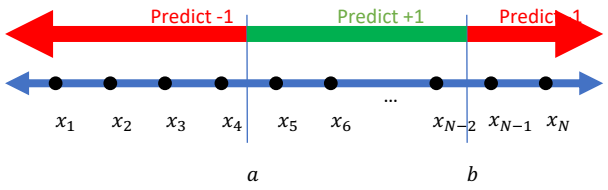
Examples

	$m_H(N)$					
	N=1	N=2	N=3	N=4	N=5	Break Points	VC Dimension
Positive Rays	2	3	4	5	6		
Positive Intervals	2	4	7	11	16		
Convex Sets	2	4	8	16	32		
2D Perceptron	2	4	8	14	?		

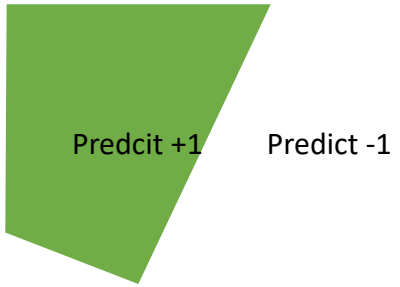
Positive Rays



Positive Intervals



Convex Sets



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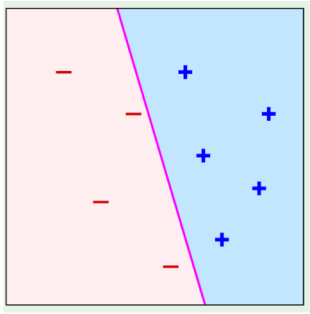
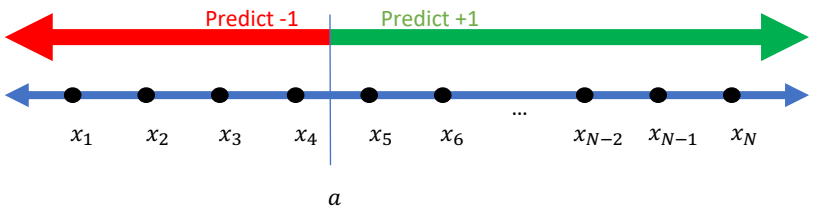


Examples

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

Positive Rays



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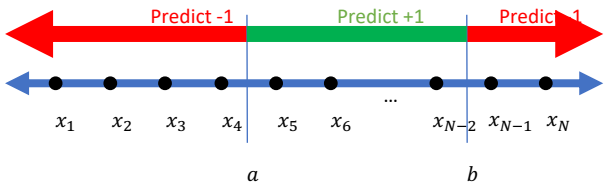
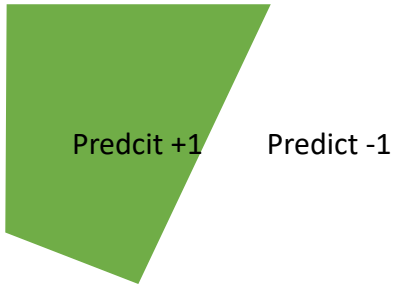


Convex Sets



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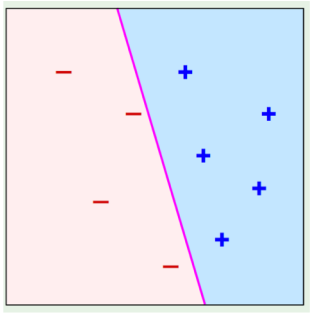
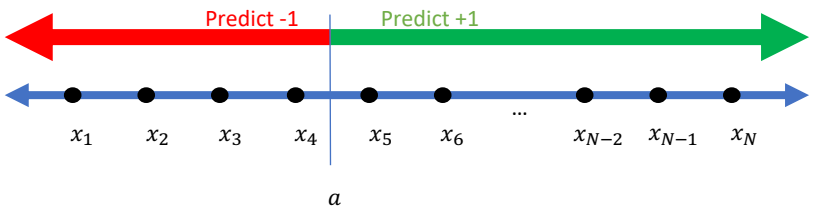


Examples

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

Positive Rays



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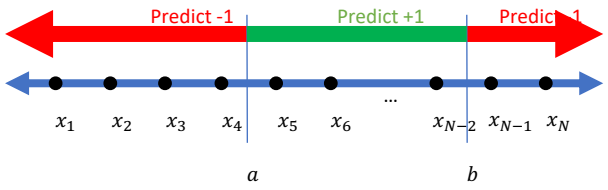

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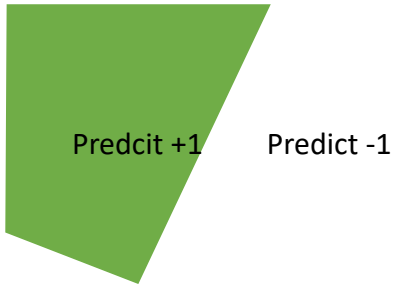

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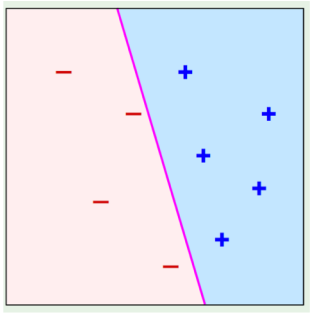

Bounding Growth Functions using Break Points

- Theorem statement:
  - 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

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

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

- Rephrase the above theorem
  - 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 from above. See LFD Problem 2.5]
    - $m_H(N) = O(N^{k-1})$
    - $m_H(N)$ is polynomial in N
  - If d_{vc} is the VC dimension of H, then
    - $m_H(N) \leq \sum_{i=0}^{d_{vc}} \binom{N}{i}$
    - $m_H(N) \leq N^{d_{vc}} + 1$
    - $m_H(N) = O(N^{d_{vc}})$

If d_{vc} is the VC dimension of H, $d_{vc} + 1$ is a break point for H

Vapnik–Chervonenkis (VC) Bound

- VC Generalization Bound

  With prob at least $1 - \delta$

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

- Let d_{vc} be the VC dimension of H, we have $\boldsymbol{m_H(N) \leq N^{d_{vc}} + 1}$. Therefore,

  With prob at least $1 - \delta$

$$E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{8}{N} ln \frac{4((2N)^{d_{vc}}+1)}{\delta}}$$

- If we <u>treat δ as a constant</u>, then we can say, with high probability

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

Brief Lecture Notes Today

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

Let me know if you spot errors.

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If d_{vc} is the VC dimension of H, $d_{vc} + 1$ is a break point for H

Proof Intuitions

- See LFD Section 2.1.2 for the formal proof (safe to skip)
  - [We won't ask questions about this proof in exams/homeworks]

- Key message:

  When there exist break points:

  - strong constraints on the possible dichotomies
  - therefore, we can bound $m_H(N)$

Proof Intuitions

- How many dichotomies can you list on **2 points** when **no 2 points are shattered**

$\vec{x}_1$	$\vec{x}_2$
+1	+1
+1	-1
-1	+1

Proof Intuitions

- How many dichotomies can you list on **4 points** when **no 2 points are shattered**

$\vec{x}_1$	$\vec{x}_2$	$\vec{x}_3$	$\vec{x}_4$
+1	+1	+1	1
+1	+1	+1	+1
+1	+1	-1	+1
+1	-1	+1	+1
-1	+1	+1	+1

Can you add an additional dichotomy?

Proof Intuitions

- How many dichotomies can you list on **4 points** when **no 2 points are shattered**

$\vec{x}_1$	$\vec{x}_2$	$\vec{x}_3$	$\vec{x}_4$
+1	+1	+1	-1
+1	+1	+1	+1
+1	+1	-1	+1
+1	-1	+1	+1
-1	+1	+1	+1

$(\vec{x}_1, \vec{x}_2, \vec{x}_3)$ appear twice, with different $\vec{x}_4$

No 1 points can be shattered

$(\vec{x}_1, \vec{x}_2, \vec{x}_3)$ appear once

No 2 points can be shattered

Proof Intuitions

- How many dichotomies can you list on **4 points** when **no 2 points are shattered**

No 1 points can be shattered

$\vec{x}_1$	$\vec{x}_2$	$\vec{x}_3$	$\vec{x}_4$
+1	+1	+1	-1
+1	+1	+1	+1
+1	+1	-1	+1
+1	-1	+1	+1
-1	+1	+1	+1

No 2 points can be shattered

$\boldsymbol{B(N,k)}$: max # dichotomies on N points when no k points are shattered

A recursive definition:

$$\boldsymbol{B(N,k) \leq B(N-1,k) + B(N-1,k-1)}$$

Prove the bound by **induction**.

Bounding Growth Function using Break Points

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

- Rephrase the above theorem
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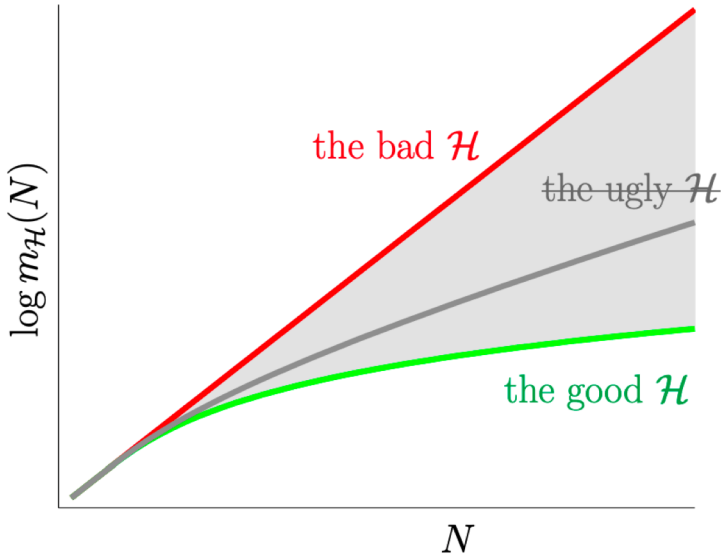
    - $m_H(N) = O(N^{d_{vc}})$

If d_{vc} is the VC dimension of H, $d_{vc} + 1$ is a break point for H

A Hypothesis Set is either “Good” or “Bad”



	N=1	N=2	N=3	N=4	N=5	Break Points	$d_{vc}(H)$	$m_H(N)$
Positive Rays	2	3	4	5	6	$k = 2,3,4, \ldots$	1	$\leq N + 1$
Positive Intervals	2	4	7	11	16	$k = 3,4,5, \ldots$	2	$\leq N^2 + 1$
Convex Sets	2	4	8	16	32	None	∞	2^N
2D Perceptron	2	4	8	14	?	$k = 4,5,6, \ldots$	3	$\leq N^3 + 1$
Some H	2	4	8	16	<32	$k = 5,6,7, \ldots$	4	$\leq N^4 + 1$

VC Bound with VC Dimension

- VC Generalization Bound

  With prob at least $1 - \delta$

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

- Let d_{vc} be the VC dimension of H, we have $m_H(N) \leq N^{d_{vc}} + 1$. Therefore,

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- If we <u>treat δ as a constant</u>, then we can say, with high probability

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Discussion on the VC Theory

Build on the i.i.d. data assumption

The bound derivation is loose

All models are wrong
but some are useful

George E.P. Box

Discussion on the VC Theory

Build on the i.i.d. data assumption

The bound derivation is loose

It characterizes the practice reasonably well and provides good insights

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

- How to determine the sample complexity?
  - Set $\sqrt{\frac{8}{N} ln \frac{4((2N)^{d_{VC}}+1)}{\delta}} \leq \epsilon$
  - We get $N \geq \frac{8}{\epsilon^2} ln\left(\frac{4\left(1+(2N)^{d_{VC}}\right)}{\delta}\right)$

- $N \propto 1/\epsilon^2$
- $N = O(d_{vc} \ln N)$
  - In practice, roughly, $N \propto d_{vc}$

Approximation-Generalization Tradeoff

What we want to minimize

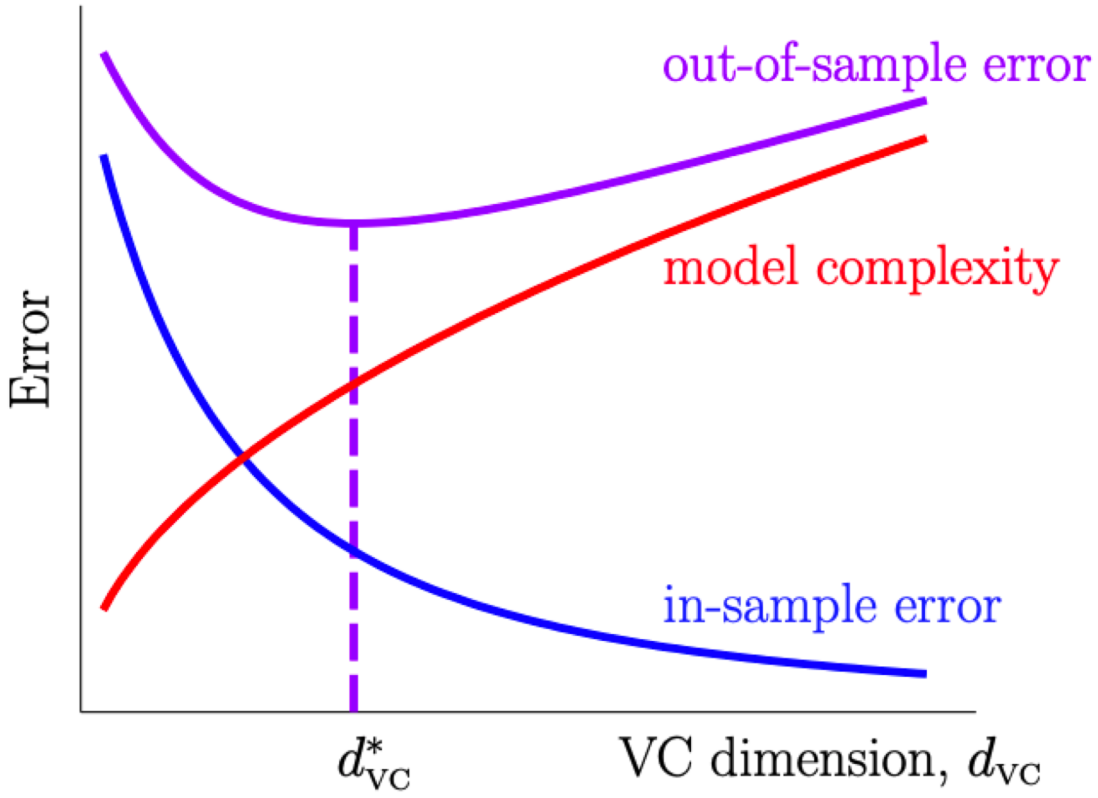
How well g generalizes

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

How well g approximates f in training data

Approximation-Generalization Tradeoff

- VC Dimension: A single parameter to characterize complexity of H



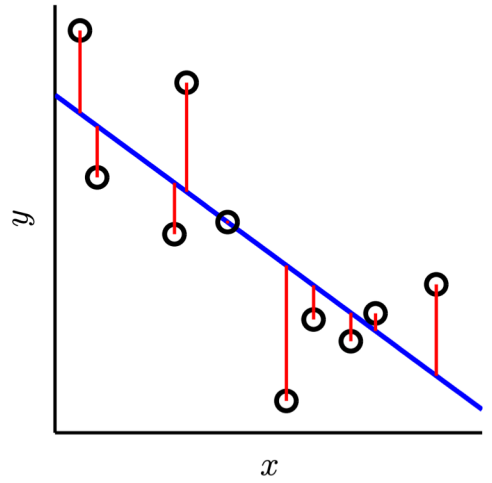
Bias-Variance Decomposition

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 $e\big(h(\vec{x}), f(\vec{x})\big) = \mathbb{I}[h(\vec{x}_n) \neq f(\vec{x}_n)]$

- Real-value functions [”**regression**”] and squared error?
  - Real-value target function $f(\vec{x}) \in \mathbb{R}$
  - Square error $e\big(h(\vec{x}), f(\vec{x})\big) = \big(h(\vec{x}_n) - f(\vec{x}_n)\big)^2$



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 $e\big(h(\vec{x}), f(\vec{x})\big) = \big(h(\vec{x}_n) - f(\vec{x}_n)\big)^2$

- Errors:
  - In-sample error: $E_{in}(g) = \frac{1}{N}\sum_{n=1}^{N} e(h(\vec{x}_n), f(\vec{x}_n)) = \frac{1}{N}\sum_{n=1}^{N}\big(h(\vec{x}_n) - f(\vec{x}_n)\big)^2$
  - Out-of-sample error: $E_{out}(g) = \mathbb{E}_{\vec{x}}[e\big(h(\vec{x}_n), f(\vec{x}_n)\big)] = \mathbb{E}_{\vec{x}}[\big(g(\vec{x}) - f(\vec{x})\big)^2]$

- 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 $\boldsymbol{g^{(D)}}$ here.
  - [In VC Theory, we consider the worst-case D through the definition of growth function $m_H(N)$]

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

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

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

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

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

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

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

Finishing Up

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

X: a random variable
μ: the mean of X

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

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

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

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

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

$$= \text{Variance} + \text{Bias}$$

- Bias-Variance Decomposition

Discussion

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

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

- 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 an conceptual guideline in decreasing E_{out}

Example of Bias-Variance Decomposition

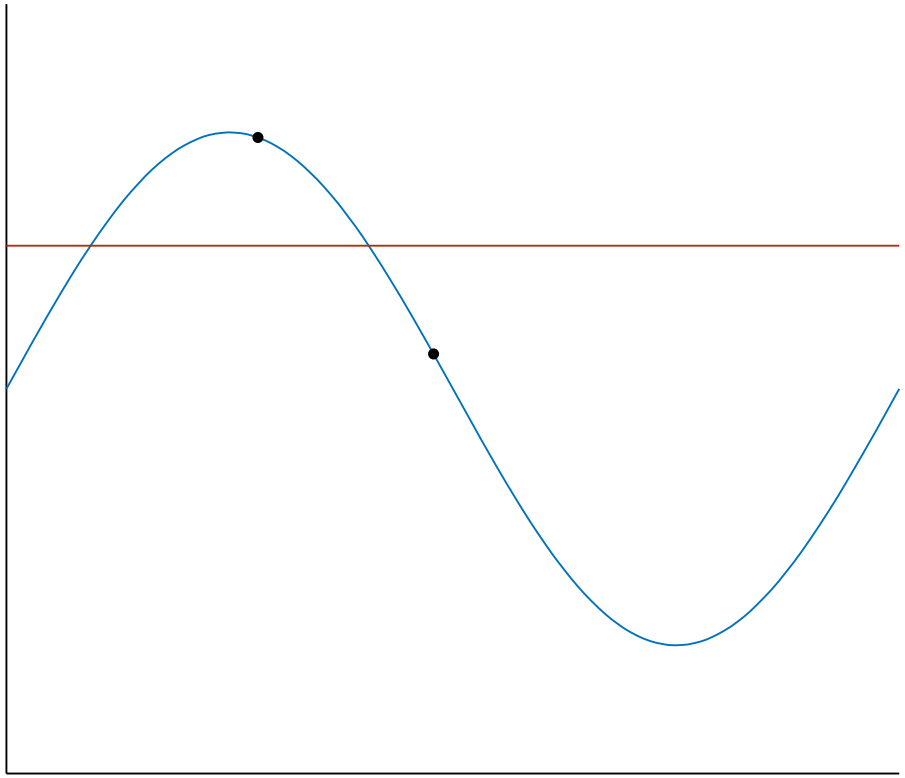
- Fitting a sine function
  - $f(x) = \sin(\pi x)$
  - x is drawn uniformly at random from [0,2]

- Two hypothesis set
  - H_0: $h(x) = b$
  - H_1: $h(x) = ax + b$

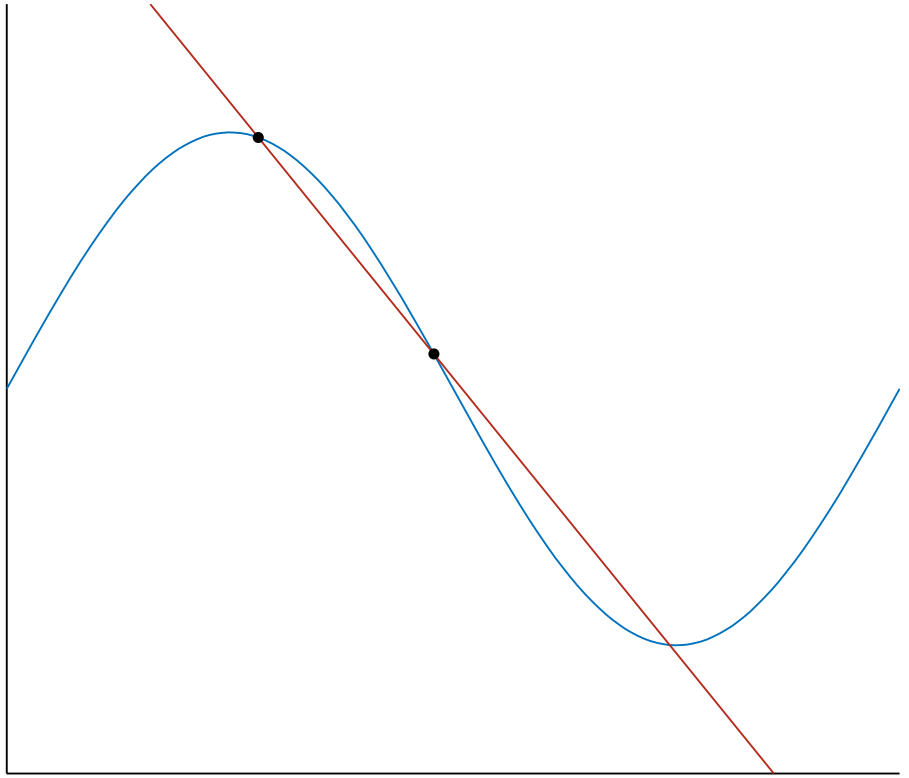
- $N = 2$
- Our algorithm finds g with minimum in-sample error

Example of Bias-Variance Decomposition

$H_0: h(x) = b$

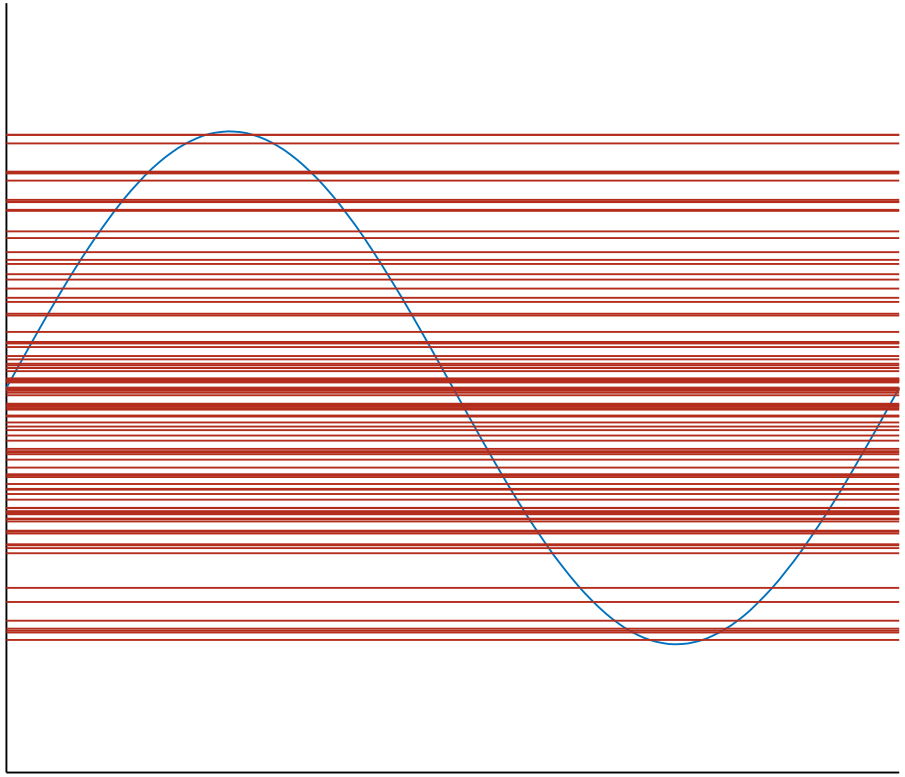


$H_1: h(x) = ax + b$

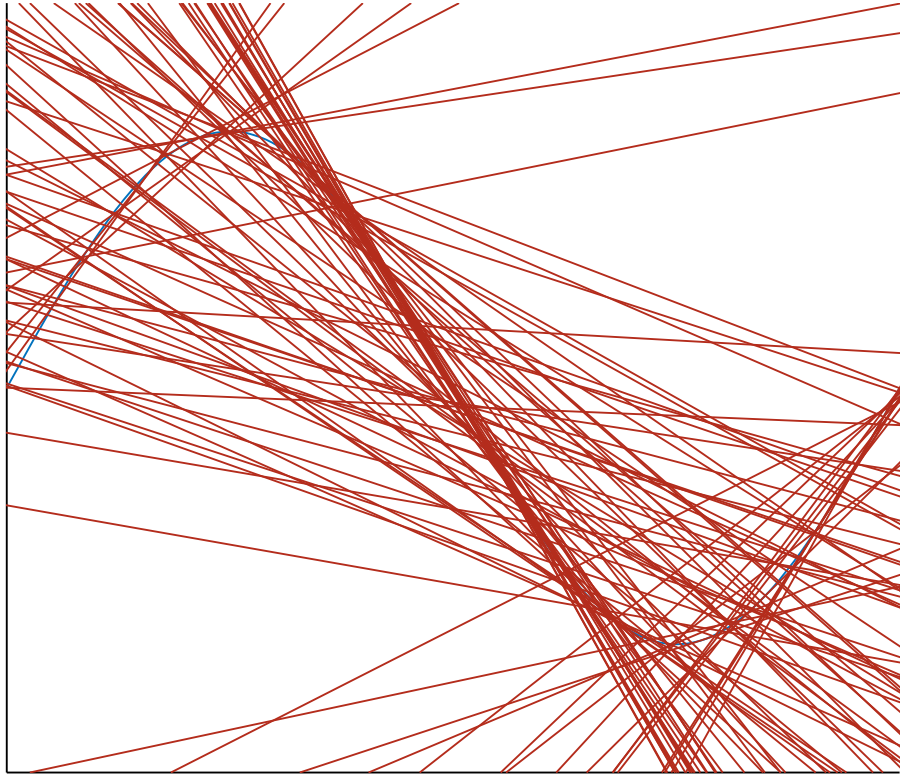


Example of Bias-Variance Decomposition

$H_0: h(x) = b$

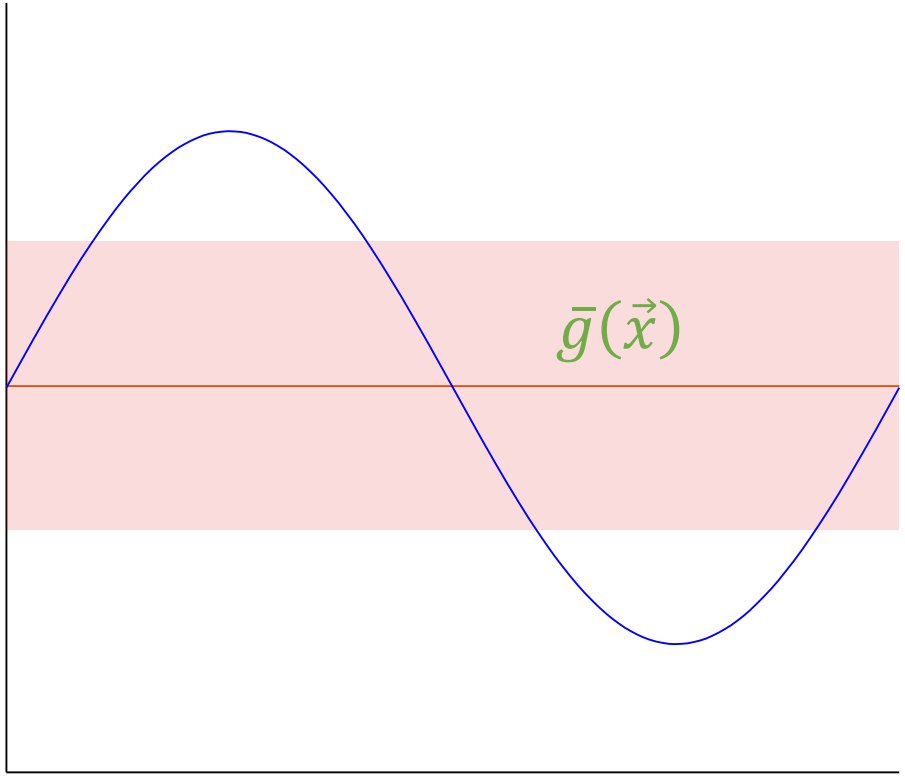


$H_1: h(x) = ax + b$



Example of Bias-Variance Decomposition

$H_0: h(x) = b$

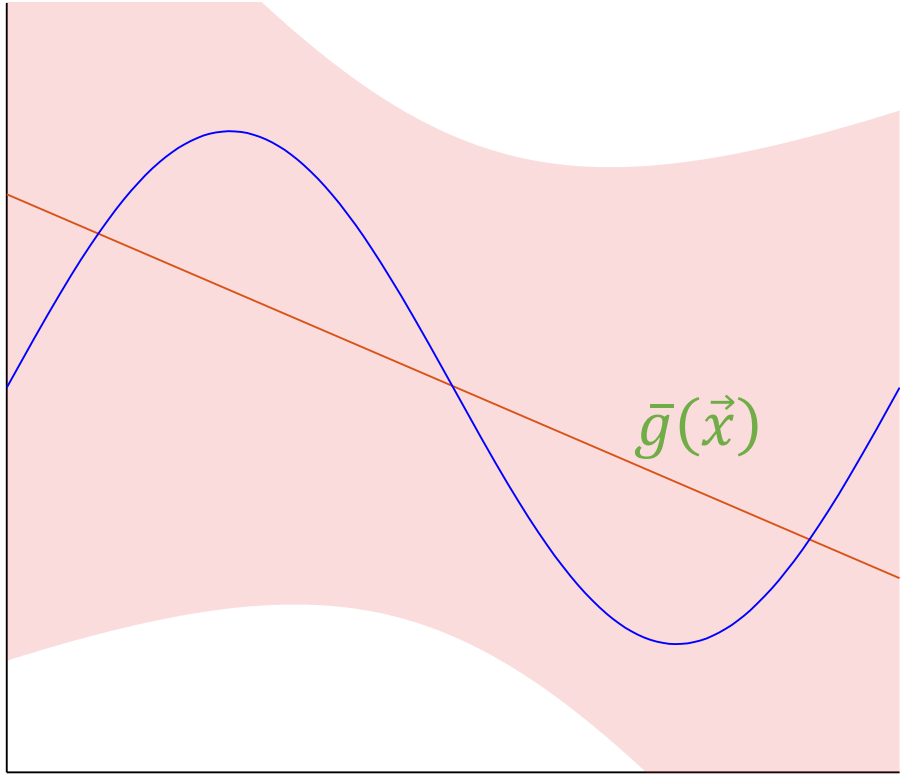


Bias of $\bar{g}(\vec{x}) \approx 0.50$

Variance of $g_{\mathcal{D}}(\vec{x}) \approx 0.25$

$\mathbb{E}_{\mathcal{D}}[E_{out}(g_{\mathcal{D}})] \approx 0.75$

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



Bias of $\bar{g}(\vec{x}) \approx 0.21$

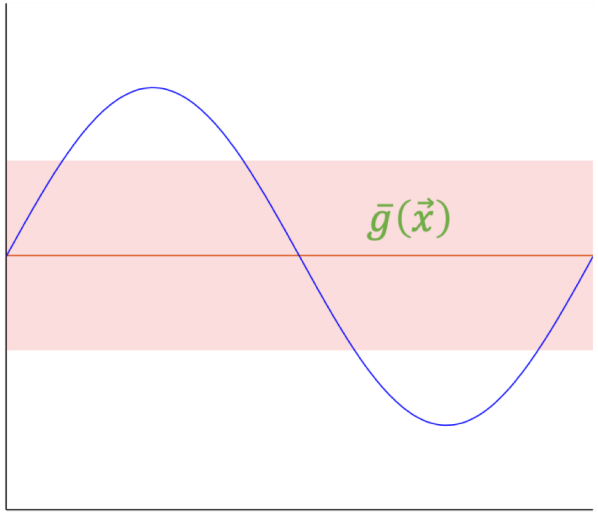
Variance of $g_{\mathcal{D}}(\vec{x}) \approx 1.74$

$\mathbb{E}_{\mathcal{D}}[E_{out}(g_{\mathcal{D}})] \approx 1.95$

Peer Discussion

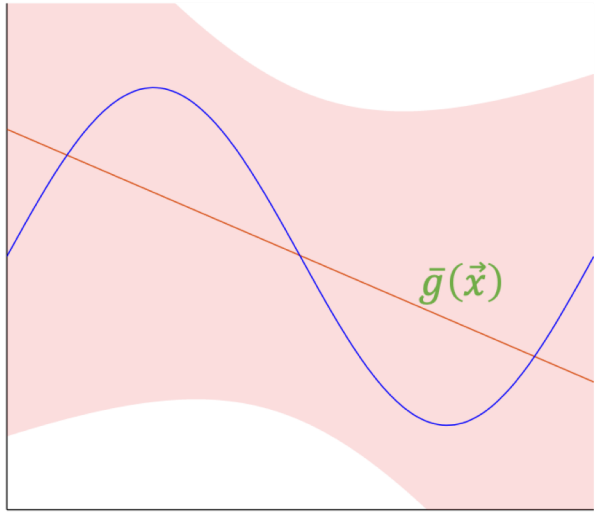
- What do you think will happen to bias and variance when we increase N from 2 to 5?

$H_0: h(x) = b$



Bias of $\bar{g}(\vec{x}) \approx 0.50$
Variance of $g_{\mathcal{D}}(\vec{x}) \approx 0.25$
$\mathbb{E}_{\mathcal{D}}[E_{out}(g_{\mathcal{D}})] \approx 0.75$

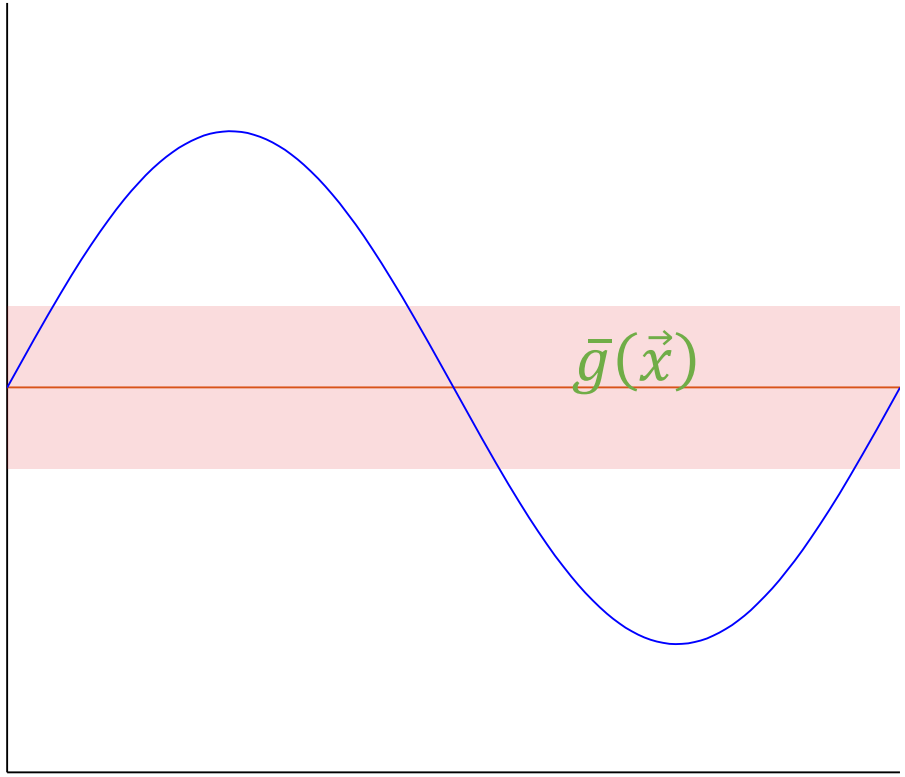
$H_1: h(x) = ax + b$



Bias of $\bar{g}(\vec{x}) \approx 0.21$
Variance of $g_{\mathcal{D}}(\vec{x}) \approx 1.74$
$\mathbb{E}_{\mathcal{D}}[E_{out}(g_{\mathcal{D}})] \approx 1.95$

What if we increase N to 5?

$H_0: h(x) = b$

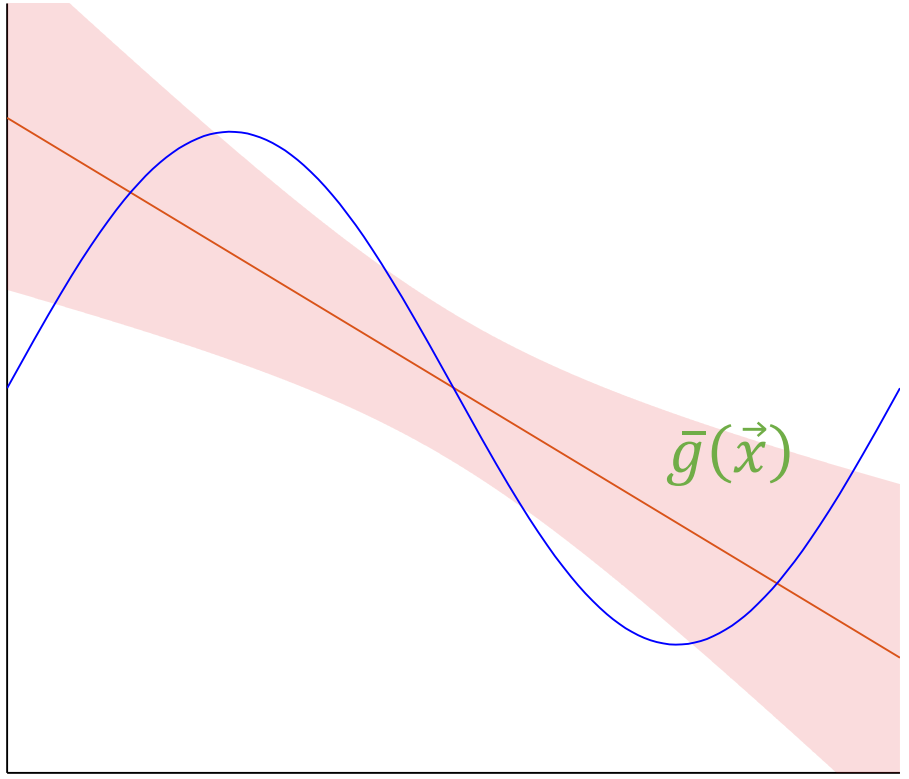


Bias of $\bar{g}(\vec{x}) \approx 0.50$

Variance of $g_{\mathcal{D}}(\vec{x}) \approx 0.10$

$\mathbb{E}_{\mathcal{D}}[E_{out}(g_{\mathcal{D}})] \approx 0.60$

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



Bias of $\bar{g}(\vec{x}) \approx 0.21$

Variance of $g_{\mathcal{D}}(\vec{x}) \approx 0.21$

$\mathbb{E}_{\mathcal{D}}[E_{out}(g_{\mathcal{D}})] \approx 0.42$

Discussion

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

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

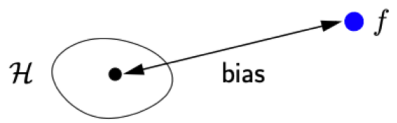
- Increasing the number of data points N
  - Biases roughly stay the same
  - Variances decrease
  - Expected E_{out} decreases

Discussion

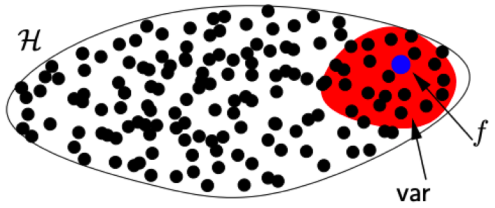
$\text{Bias}(\vec{x})$ $\qquad\qquad$ $\text{Var}(\vec{x})$

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

- Increasing the complexity of H
  - Bias goes down (more likely to approximate f)
  - Variance goes up (The stability of $g^{(D)}$ is worse)



Very small model



Very large model

Discussion

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

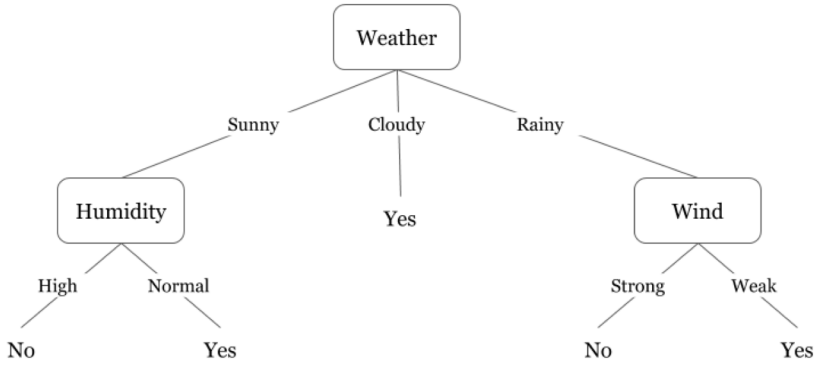
- $\mathbb{E}_D\left[E_{out}\left(g^{(D)}\right)\right] = \mathbb{E}_{\vec{x}}\left[\left(\bar{g}(\vec{x}) - f(\vec{x})\right)^2\right] + \mathbb{E}_{\vec{x}}\left[\mathbb{E}_D\left[\left(g^{(D)}(\vec{x}) - \bar{g}(\vec{x})\right)^2\right]\right]$

- This is a **conceptual** decomposition
  - Both $\bar{g}$ and f are unknown
  - We can't really calculate bias and variance for practical problems

- However, it provides an conceptual guidelines in decreasing E_{out}

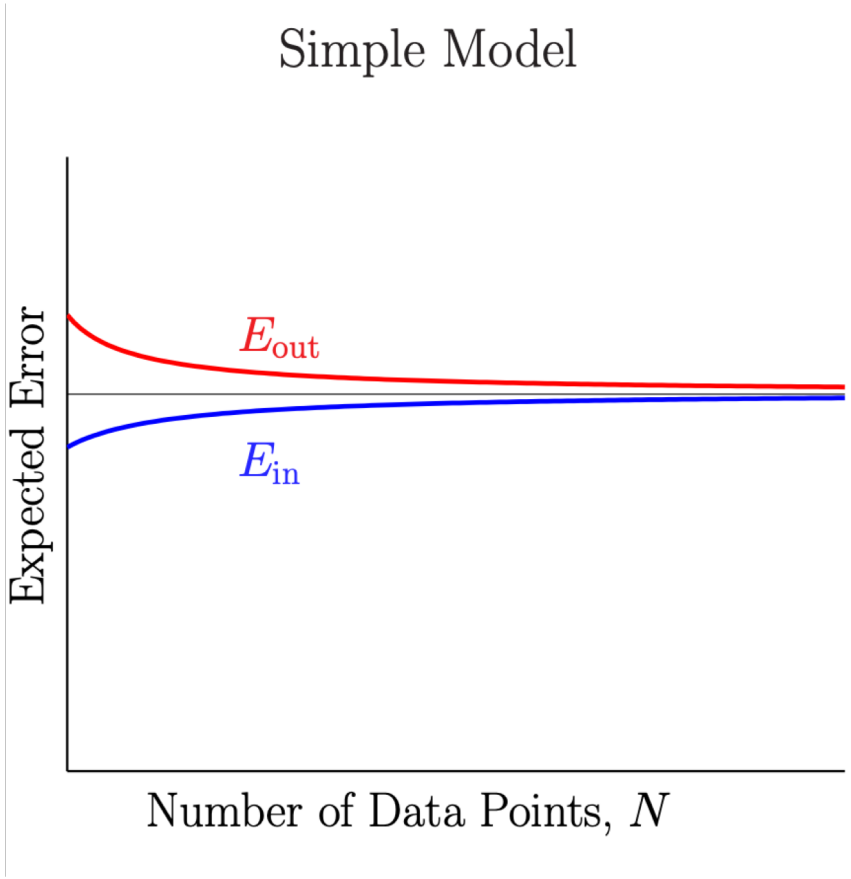
Example

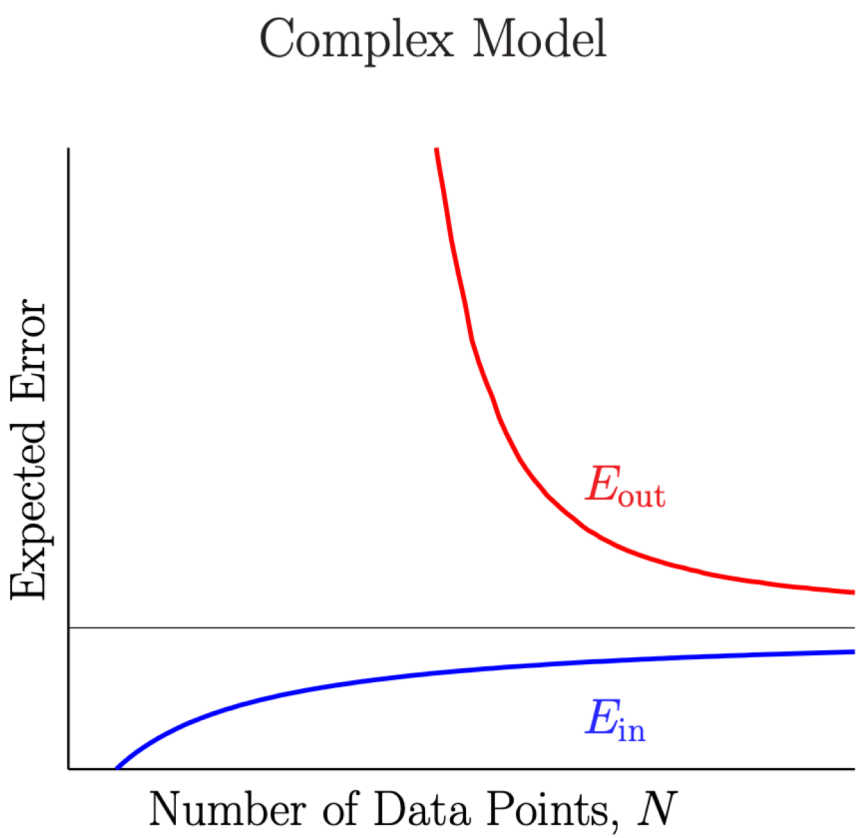
- Will talk about this in the 2nd half of the semester
- Decision tree
  - A low bias but high variance hypothesis set
  - Practical performance is not ideal



- Random forest
  - Trying to reduce the variance while not sacrificing bias
  - Idea: Generate many trees randomly and average them

Learning Curves





Learning Curves