CSE 417T
Introduction to Machine Learning

Lecture 6
Instructor: Chien-Ju (CJ) Ho
Recap
Dealing with Infinite Hypothesis Set: $M \rightarrow \infty$

• Most of the practical cases involve $M \rightarrow \infty$

• Instead of # hypothesis, counting “effective” # hypothesis

• Dichotomy
  • Informally, consider it as “data-dependent” hypothesis
  • Characterized by both $H$ and $N$ data points $(\vec{x}_1, ..., \vec{x}_N)$
    $$H(\vec{x}_1, ..., \vec{x}_N) = \{ h(\vec{x}_1), ..., h(\vec{x}_N) | h \in H \}$$
  • The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, ..., \vec{x}_N$

• Growth function
  • Largest number of dichotomies $H$ can induce across all possible data sets of size $N$
    $$m_H(N) = \max_{(\vec{x}_1, ..., \vec{x}_N)} |H(\vec{x}_1, ..., \vec{x}_N)|$$
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 $(\vec{x}_1, ..., \vec{x}_N)$ 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 $H$
    • $k$ 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

<table>
<thead>
<tr>
<th>Break Points</th>
<th>VC Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positive Rays</td>
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</tr>
<tr>
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<td>2D Perceptron</td>
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$$m_H(N)$$

<table>
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<th>N=1</th>
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#### Positive Rays

- Predict +1
- Predict -1

#### Positive Intervals

- Predict +1
- Predict -1

#### Convex Sets

- Predict +1
- Predict -1

#### 2D Perceptron

- Predict +1
- Predict -1
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<td>1</td>
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<tr>
<td>Positive Intervals</td>
<td></td>
<td>2</td>
<td>4</td>
<td>7</td>
<td>11</td>
<td>16</td>
<td>(k = 3, 4, 5, \ldots)</td>
<td>2</td>
</tr>
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<td>Convex Sets</td>
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<td>2</td>
<td>4</td>
<td>8</td>
<td>16</td>
<td>32</td>
<td>None</td>
<td>(\infty)</td>
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<td></td>
<td>2</td>
<td>4</td>
<td>8</td>
<td>14</td>
<td>?</td>
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<td>3</td>
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### Diagrams

**Positive Rays**

- Predict 1
- Predict -1

**Positive Intervals**

- Predict 1
- Predict -1

**Convex Sets**

- Predict 1
- Predict -1

**2D Perceptron**

- Predict 1
- Predict -1
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
    
    $$m_H(N) \leq \sum_{i=0}^{k-1} \binom{N}{i}$$
Bounding Growth Functions using Break Points

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

• 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 $m_H(N) \leq N^{d_{vc}} + 1$. 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 treat $\delta$ as a constant, 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.
Bounding Growth Functions using Break Points

• Theorem statement:
  • If there is no break point for $H$, then $m_H(N) = 2^N$ for all $N$.
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  • 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. 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
  • $m_H(N) \leq \sum_{i=0}^{d_{vc}} \binom{N}{i}$
  • $m_H(N) \leq N^{d_{vc}} + 1$
  • $m_H(N) = O(N^{d_{vc}})$
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

<table>
<thead>
<tr>
<th>$\tilde{x}_1$</th>
<th>$\tilde{x}_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>+1</td>
<td>-1</td>
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<tr>
<td>-1</td>
<td>+1</td>
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</table>
Proof Intuitions

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

<table>
<thead>
<tr>
<th>$\tilde{x}_1$</th>
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<th>$\tilde{x}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>1</td>
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<tr>
<td>+1</td>
<td>+1</td>
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<tr>
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<tr>
<td>-1</td>
<td>+1</td>
<td>+1</td>
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Can you add an additional dichotomy?
Proof Intuitions

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

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<td>+1</td>
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$(\vec{x}_1, \vec{x}_2, \vec{x}_3)$ 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

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

A recursive definition:

\[ B(N, k) \leq B(N - 1, k) + B(N - 1, k - 1) \]

No 2 points can be shattered

Prove the bound by **induction**.
Bounding Growth Function 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
    $$m_H(N) \leq \sum_{i=0}^{k-1} \binom{N}{i}$$

• 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”

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<td>$k = 2,3,4,...$</td>
<td>1</td>
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<td>Some $H$</td>
<td>2</td>
<td>4</td>
<td>8</td>
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<td>$&lt;32$</td>
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VC Bound with VC Dimension

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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 $\epsilon$ 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 $N \geq \frac{8}{\epsilon^2} \ln \left( \frac{4(1+(2N)^{d_{vc}})}{\delta} \right)$

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

What we want to minimize

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

How well \( g \) approximates \( f \) in training data

How well \( g \) generalizes
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 $e(h(\vec{x}), f(\vec{x})) = \mathbb{I}[h(\vec{x}_n) \neq f(\vec{x}_n)]$

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

• 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: $E_{out}(g) = \mathbb{E}_{\vec{x}}[e(h(\vec{x}_n), f(\vec{x}_n))] = \mathbb{E}_{\vec{x}}[(g(\vec{x}) - f(\vec{x}))^2]$

• 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 $m_H(N)$]

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

Define $\bar{g}(\tilde{x}) = \mathbb{E}_D[g^{(D)}(\tilde{x})]$.

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

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

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

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

- Bias-Variance Decomposition

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

$X$: a random variable
$\mu$: the mean of $X$

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

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

• 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

\[ H_0: h(x) = b \]
\[ H_1: h(x) = ax + b \]

Bias of \( \bar{g}(\hat{x}) \) \( \approx 0.50 \)
Variance of \( g_D(\hat{x}) \) \( \approx 0.25 \)
\( E_D[E_{out}(g_D)] \) \( \approx 0.75 \)

Bias of \( \bar{g}(\hat{x}) \) \( \approx 0.21 \)
Variance of \( g_D(\hat{x}) \) \( \approx 1.74 \)
\( E_D[E_{out}(g_D)] \) \( \approx 1.95 \)
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 $\tilde{g}(\tilde{x}) \approx 0.50$
Variance of $g_D(\tilde{x}) \approx 0.25$
$E_D[E_{out}(g_D)] \approx 0.75$

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

Bias of $\tilde{g}(\tilde{x}) \approx 0.21$
Variance of $g_D(\tilde{x}) \approx 1.74$
$E_D[E_{out}(g_D)] \approx 1.95$
What if we increase $N$ to 5?

$H_0: h(x) = b$

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

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

Variance of $g_D(\bar{x}) \approx 0.10$

$\mathbb{E}_D[E_{out}(g_D)] \approx 0.60$

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

Variance of $g_D(\bar{x}) \approx 0.21$

$\mathbb{E}_D[E_{out}(g_D)] \approx 0.42$
Discussion

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

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

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

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

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

• 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

Simple Model

Complex Model

Expected Error

Number of Data Points, $N$

$E_{out}$

$E_{in}$

$E_{out}$

$E_{in}$
Learning Curves

VC Analysis

Expected Error

generalization error

$E_{\text{out}}$

in-sample error

$E_{\text{in}}$

Number of Data Points, $N$

Bias-Variance Analysis

Expected Error

variance

$E_{\text{out}}$

bias

$E_{\text{in}}$

Number of Data Points, $N$