CSE 417T
Introduction to Machine Learning

Lecture 5

Instructor: Chien-Ju (CJ) Ho

Logistics: HW1

- Due: **Feb 19 (Friday), 2020**
  - http://chienjuho.com/courses/cse417t/hw1.pdf
  - Strongly encouraged to work on it before the drop deadline
  - 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.

- (Optional) Python session
  - See Piazza post

Logistics: Office Hours

- TA office hours

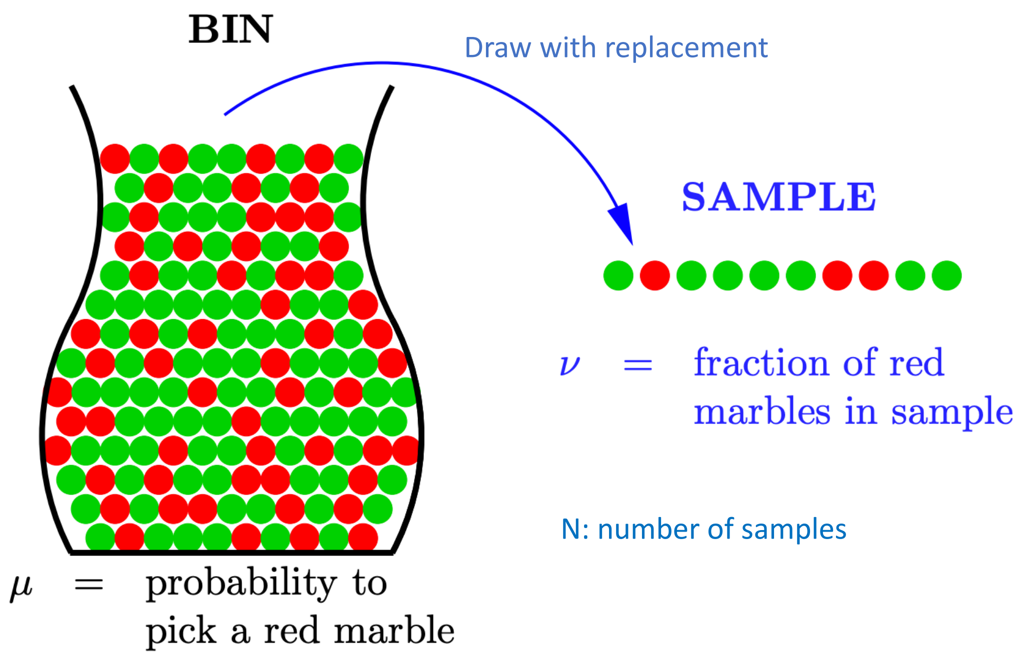
Monday	10:00 AM to 11:20 AM (Oliver)	02:30 PM to 03:50 PM (Guanghui)	
Tuesday	02:30 PM to 03:50 PM (Quentin)	05:00 PM to 06:20 PM (Victoria)	
Wednesday	04:30 PM to 05:50 PM (Amrit)	08:00 PM to 09:20 PM (Cecilia)	
Thursday	10:00 AM to 11:20 AM (Aaron)	02:30 PM to 03:50 PM (Matthew)	
Friday	08:00 AM to 09:20 AM (Shohaib)	12:00 PM-1:20 PM (Tong)	04:10 PM to 05:30 PM (Flora)

- My office hour: after Tuesday’s class till 2pm

- Remote via Zoom
- Please follow **Piazza** for zoom links and potential updates
- 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



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

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 $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$
  - $\boldsymbol{E_{in}(h)} \overset{\text{def}}{=} \frac{1}{N}\sum_{n=1}^{N} \mathbb{1}[h(\vec{x}_n) \neq f(\vec{x}_n)]$ [In-sample error, analogy to ν]
  - $\boldsymbol{E_{out}(h)} \overset{\text{def}}{=} \Pr_{\vec{x}\sim P(\vec{x})}[h(\vec{x}) \neq f(\vec{x})]$ [Out-of-sample error, analogy to μ]

- Learning bounds
  - Fixed h (verification)

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

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

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

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

- Most of the practical cases involve $M \to \infty$

- Instead of # hypothesis, counting "effective" # hypothesis
- <u>Dichotomies</u>
  - Informally, consider a dichotomy as "data-dependent" hypothesis
  - Characterized by both H and N data points $(\vec{x}_1, \dots, \vec{x}_N)$

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

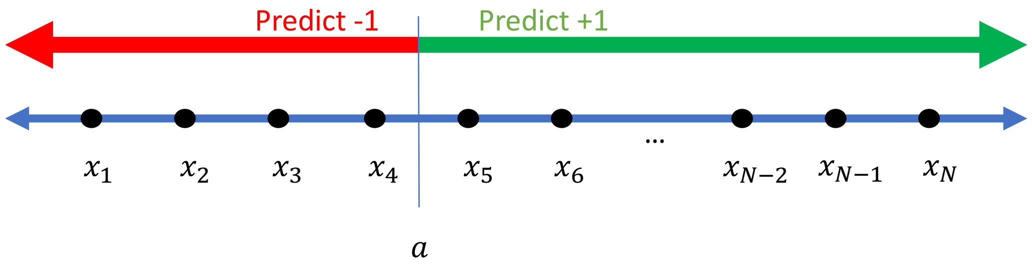
  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \dots, \vec{x}_N$

- <u>Growth function</u>
  - Largest number of dichotomies H can induce across all possible data sets of size N

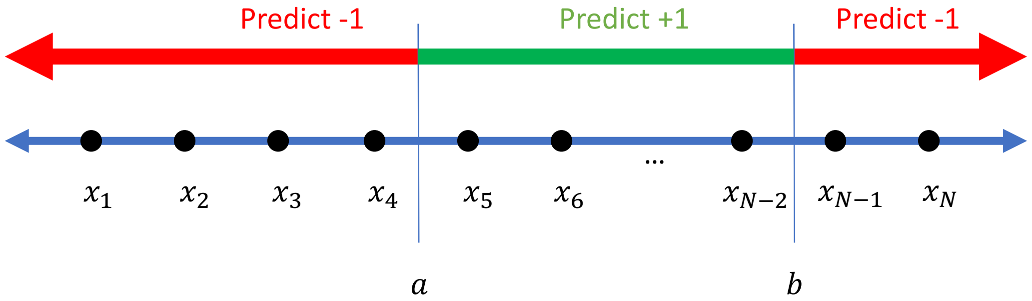
$$m_H(N) = \max_{(\vec{x}_1, \dots, \vec{x}_N)} |H(\vec{x}_1, \dots, \vec{x}_N)|$$

Examples on Growth Functions

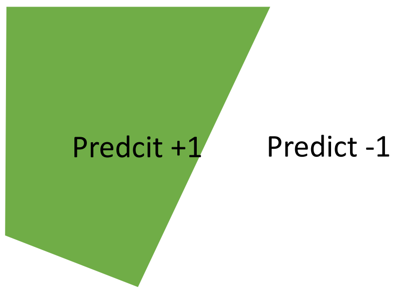
- H = Positive rays
  - $m_H(N) = N + 1$



- H = Positive intervals
  - $m_H(N) = \binom{N+1}{2} + 1 = \frac{N^2}{2} + \frac{N}{2} + 1$



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



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

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

- VC Generalization Bound (VC Inequality, 1971)

  With prob at least $1-\delta$

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

Today’s Lecture

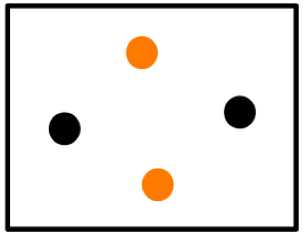
The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

Let me know if you spot errors.

Bounding Growth Function

- What we know so far
  - H = Positive rays: $m_H(N) = N + 1$
  - H = Positive intervals: $m_H(N) = \binom{N+1}{2} + 1$
  - H = 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** $(\vec{x}_1, \ldots, \vec{x}_N)$ if $|H(\vec{x}_1, \ldots, \vec{x}_N)| = 2^N$
    - H can induce all label combinations for $(\vec{x}_1, \ldots, \vec{x}_N)$
  - 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:

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

Practice

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

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

  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \ldots, \vec{x}_N$
- Growth function
  - Largest number of dichotomies H can induce across all possible data sets of size N

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

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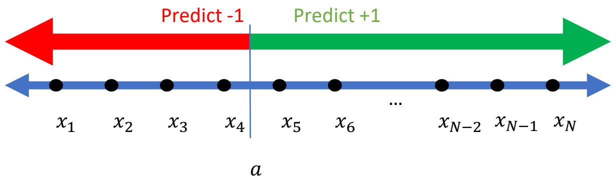
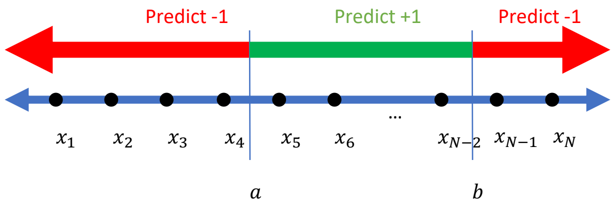
- What is the break point for

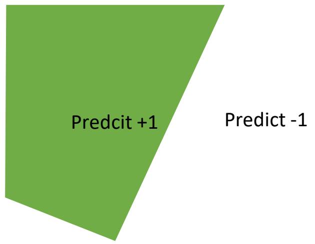
1. Positive Rays



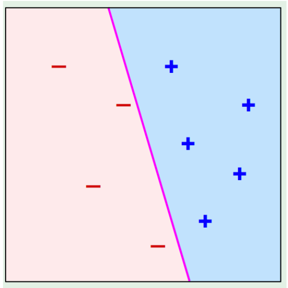
2. Positive Intervals



3. Convex Sets



4. 2-D Perceptron



Practice

- <u>Dichotomies</u>
  - Informally, consider a dichotomy as "data-dependent" hypothesis
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$$H(\vec{x}_1, \dots \vec{x}_N) = \{h(\vec{x}_1), \dots, h(\vec{x}_N) | h \in H\}$$

  - The set of possible prediction combinations $h \in H$ can induce on $\vec{x}_1, \dots, \vec{x}_N$
- <u>Growth function</u>
  - Largest number of dichotomies H can induce across all possible data sets of size N

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- <u>Break point</u>
  - k is a **break point** for H if no data set of size k can be shattered by H

$\boldsymbol{m_H(N)}$

$\boldsymbol{m_H(N)}$		N=1	N=2	N=3	N=4	N=5	Break Points
$N+1$	Positive Rays						
$\frac{N^2}{2} + \frac{N}{2} + 1$	Positive Intervals						
N^2	Convex Sets						
	2D Perceptron						

Practice

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

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

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  - k is a **break point** for H if no data set of size k can be shattered by H

$$\boldsymbol{m_H(N)}$$

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

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

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

- 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
    - $m_H(N) \leq N^{k-1} + 1$ [Can be proven using induction. See LFD Problem 2.5]
    - $m_H(N) = O(N^{k-1})$
    - $m_H(N)$ is polynomial in N

- We can "bound" the growth function without knowing it exactly.
  - Find break point!

Why Break Points?

- 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

- VC Generalization Bound

  With prob at least $1 - \delta$

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

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

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

[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:

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

➕

- 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
    - $m_H(N) \leq N^{k-1} + 1$ [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 there are no break point ($m_H(N) = 2^N$)

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

(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., $m_H(N) = O(N^{k-1})$

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

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
    - $m_H(N) \leq N^{k-1} + 1$ [Can be proven using induction. See LFD Problem 2.5]
    - $m_H(N) = O(N^{k-1})$
    - $m_H(N)$ is polynomial in N

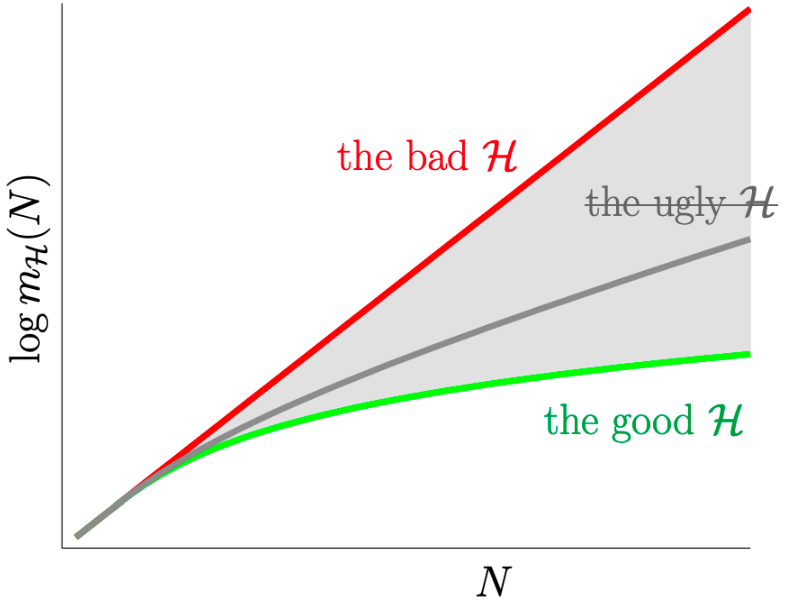
- The growth function of H is either one of the two
  - Without break points, $m_H(N) = 2^N$
  - With some break point, $m_H(N)$ is polynomial in N (it can be bounded more tightly using the theorem)
  - There is nothing in between!

- Bad hypothesis set

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

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

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



VC Dimension

- 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	$k = 2,3,4,\ldots$	
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	?	$k = 4,5,6,\ldots$	

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	$m_H(N)$						
	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

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

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

Discussion on the VC Theory

All models are wrong

but some are useful

George E.P. Box

Discussion on the VC Theory

- VC Bound

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

- 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)

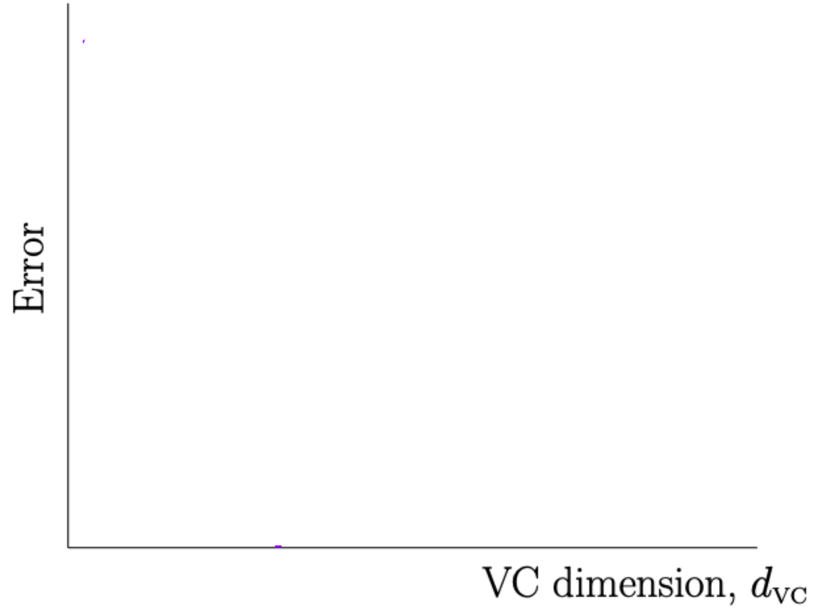
$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{VC}\frac{\ln N}{N}}\right)$$

- 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

Discussion on the VC Theory

- 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

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



Discussion on the VC Theory

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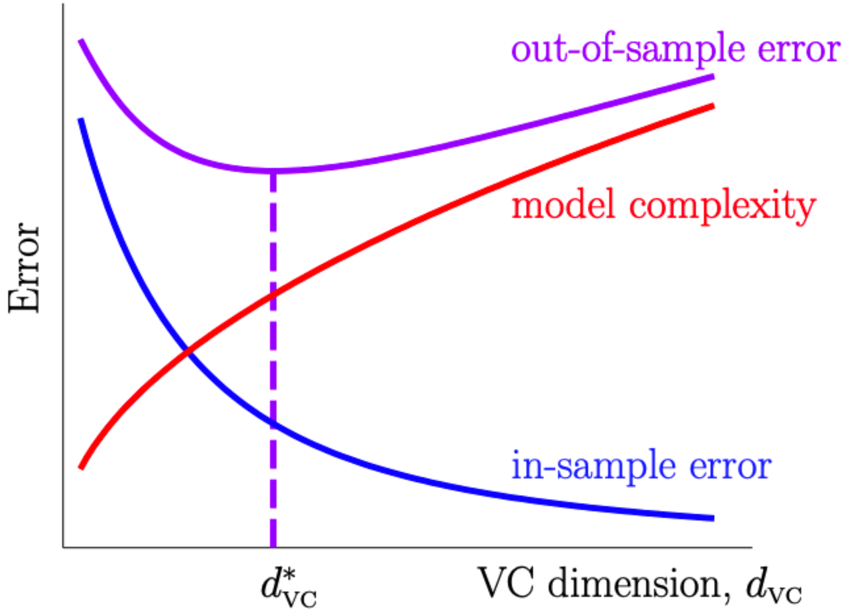

Sample Complexity

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

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

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

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

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