More Learning Theory

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Based on the slides of Vibhav Gogate and David Sontag

Last Time

- Probably approximately correct (PAC)
  - The only reasonable expectation of a learner is that with high probability it learns a close approximation to the target concept
  - Specify two small parameters, $0 < \epsilon, 0 < \delta < 1$
    - ϵ is the error of the approximation
    - $(1 - \delta)$ is the probability that, given M i.i.d. samples, our learning algorithm produces a classifier with error at most ϵ

Learning Theory

- We use the observed data in order to learn a classifier
- Want to know how far the learned classifier deviates from the (unknown) underlying distribution
  - With too few samples, we will with high probability learn a classifier whose true error is quite high even though it may be a perfect classifier for the observed data
  - As we see more samples, we pick a classifier from the hypothesis space with low training error & hope that it also has low true error
    - Want this to be true with high probability – can we bound how many samples that we need?

Haussler, 1988

- What we proved last time:

  Theorem: For a finite hypothesis space, H, with M i.i.d. samples, and $0 < \epsilon < 1$, the probability that any consistent classifier has true error larger than ϵ is at most $|H|e^{-\epsilon M}$

- We can turn this into a sample complexity bound

Sample Complexity

- Let δ be an upper bound on the desired probability of not ϵ-exhausting the sample space
  - The probability that the version space is not ϵ-exhausted is at most $|H|e^{-\epsilon M} \leq \delta$
  - Solving for M yields

$$M \geq -\frac{1}{\epsilon}\ln\frac{\delta}{|H|}$$
$$= \left(\ln|H| + \ln\frac{1}{\delta}\right)/\epsilon$$

PAC Bounds

Theorem: For a finite hypothesis space H, M i.i.d. samples, and $0 < \epsilon < 1$, the probability that true error of any of the best classifiers (i.e., lowest training error) is larger than its training error plus ϵ is at most $|H|e^{-2M\epsilon^2}$

- Sample complexity (for desired $\delta \geq |H|e^{-2M\epsilon^2}$)

$$M \geq \left(\ln|H| + \ln\frac{1}{\delta}\right)/2\epsilon^2$$

PAC Bounds

- If we require that the previous error is bounded above by a fixed δ, then with probability $(1-\delta)$, for all $h \in H$

$$\epsilon_h \leq \underbrace{\epsilon_h^{train}}_{\text{“bias”}} + \underbrace{\sqrt{\frac{1}{2M}\left(\ln|H| + \ln\frac{1}{\delta}\right)}}_{\text{“variance”}}$$

- Follows from Chernoff bound

$$|H|e^{-2M\epsilon^2} \leq \delta$$

$$\sum_{h\in H} p\left(\epsilon_h - \epsilon_h^{train} \geq \epsilon\right) \leq |H|e^{-2M\epsilon^2} \leq \delta$$

PAC Bounds

- If we require that the previous error is bounded above by δ, then with probability $(1-\delta)$, for all $h \in H$

$$\epsilon_h \leq \epsilon_h^{train} + \sqrt{\frac{1}{2M}\left(\ln|H| + \ln\frac{1}{\delta}\right)}$$

"bias" "variance"

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PAC Bounds

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"bias" "variance"

- For small $|H|$
  - High bias (may not be enough hypotheses to choose from)
  - Low variance

PAC Bounds

- If we require that the previous error is bounded above by δ, then with probability $(1-\delta)$, for all $h \in H$

$$\underbrace{\epsilon_h \leq \epsilon_h^{train}}_{\text{"bias"}} + \underbrace{\sqrt{\frac{1}{2M}\left(\ln|H| + \ln\frac{1}{\delta}\right)}}_{\text{"variance"}}$$

“bias” “variance”

- For large $|H|$
  - Low bias (lots of good hypotheses)
  - High variance

PAC Learning

- Given:
  - Set of data X
  - Hypothesis space H
  - Set of target concepts C
  - Training instances from unknown probability distribution over X of the form $(x, c(x))$
- Goal:
  - Learn the target concept $c \in \mathrm{C}$

PAC Learning

- Given:
  - A concept class C over n instances from the set X
  - A learner L with hypothesis space H
  - Two constants, $\epsilon, \delta \in (0, \frac{1}{2})$
- C is said to be PAC learnable by L using H iff for all distributions over X, learner L by sampling n instances, will with probability at least $1 - \delta$ outputs a hypothesis $h \in \mathrm{H}$ such that
  - $\epsilon_h \leq \epsilon$
  - Running time is polynomial in $\frac{1}{\epsilon}, \frac{1}{\delta}, n, size(c)$

VC Dimension

- Our analysis for the finite case was based on $|H|$
  - If H isn't finite, this translates into infinite sample complexity
  - We can derive a different notion of complexity for infinite hypothesis spaces by considering only the number of points that can be correctly classified by some member of H
  - We will only consider the binary classification case for now

VC Dimension

- What is the largest number of data points in 1-D that can be correctly classified by a linear separator (regardless of their assigned labels)?
  - 2 points:

Yes!

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VC Dimension

- What is the largest number of data points in 1-D that can be correctly classified by a linear separator (regardless of their assigned labels)?
  - 3 points:

Yes!

VC Dimension

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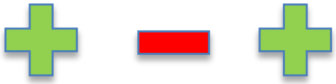
  - 3 points:



NO!

VC Dimension

- What is the largest number of data points in 1-D that can be correctly classified by a linear separator (regardless of their assigned labels)?

  - 3 points:

NO!

  - 3 points and up: for any collection of three or more there is always some choice of pluses and minuses such that that the points cannot be classified with a linear separator (in one dimension)

VC Dimension

- A set of points is shattered by a hypothesis space H if and only if for every partition of the set of points into positive and negative examples, there exists some consistent $h \in H$

- The Vapnik–Chervonenkis (VC) dimension of H over inputs from X is the size of the ***largest*** finite subset of X shattered by H

VC Dimension

- Common misconception:
  - VC dimension is determined by the **largest shatterable set of points**, not the highest number such that all sets of points that size can be shattered

Cannot be shattered by a line

VC Dimension

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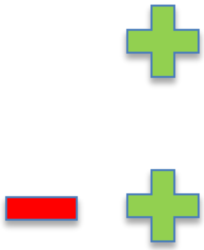
  - VC dimension is determined by the **largest shatterable set of points**, not the highest number such that all sets of points that size can be shattered



Can be shattered by a line (no matter the labels), so VC dimension is at least 3

VC Dimension

- What is the VC dimension of 2-D space under linear separators?
  - It is at least three from the last slide
  - Can some set of four points be shattered?

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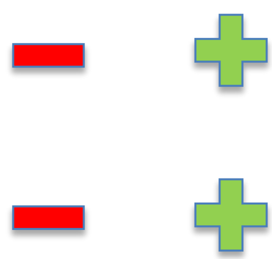

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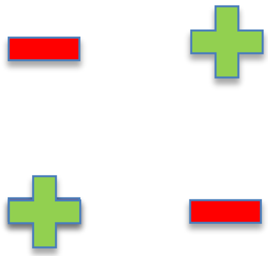


VC Dimension

- What is the VC dimension of 2-D space under linear separators?
  - It is at least three from the last slide
  - Can some set of four points be shattered?

NO! This means that the VC dimension is at most 3

VC Dimension

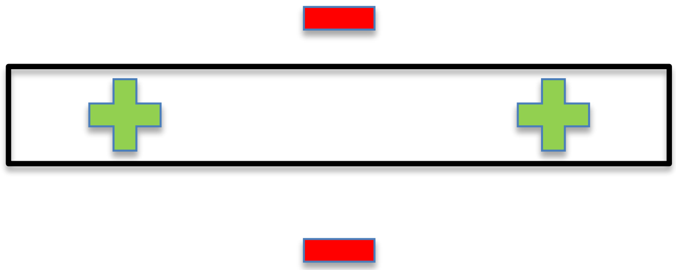
- There exists a set of size $d + 1$ in a $d - dimensional$ space that can be shattered by a linear separator, but not a set of size $d + 2$
- The larger the subset of X that can be shattered, the more expressive the hypothesis space is
- If arbitrarily large finite subsets of X can be shattered, then $VC(H) = \infty$

Axis Parallel Rectangles

- Let X be the set of all points in $\mathbb{R}^2$
- Let H be the set of all axis parallel rectangles in 2-D (inside + outside -)
  - What is $VC(H)$?

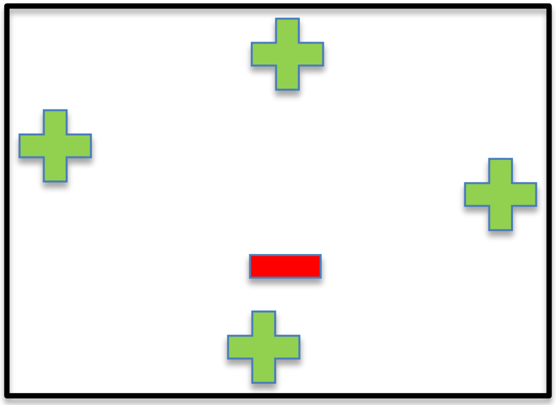
Axis Parallel Rectangles

- Let X be the set of all points in $\mathbb{R}^2$
- Let H be the set of all axis parallel rectangles in 2-D (inside + outside -)
  - $VC(H) \geq 4$



Axis Parallel Rectangles

- Let X be the set of all points in $\mathbb{R}^2$
- Let H be the set of all axis parallel rectangles in 2-D
  - $VC(H) = 4$
  - A rectangle can contain at most 4 extreme points, the fifth point must be contained within the rectangle defined by these points



Examples

- VC dimension of one-level decision trees over real vectors of length 2?

- VC dimension of linear separators through the origin?

- VC dimension of a hypothesis space with exactly one hypothesis in it for binary vectors of length $n \geq 1$?

Examples

- VC dimension of one-level decision trees over real vectors of length 2?
  - Three
- VC dimension of linear separators through the origin?
- VC dimension of a hypothesis space with exactly one hypothesis in it for binary vectors of length $n \geq 1$?

Examples

- VC dimension of one-level decision trees over real vectors of length 2?
  - Three
- VC dimension of linear separators through the origin?
  - Two
- VC dimension of a hypothesis space with exactly one hypothesis in it for binary vectors of length $n \geq 1$?

Examples

- VC dimension of one-level decision trees over real vectors of length 2?
  - Three
- VC dimension of linear separators through the origin?
  - Two
- VC dimension of a hypothesis space with exactly one hypothesis in it for binary vectors of length $n \geq 1$?
  - Zero

PAC Bounds with VC Dimension

- VC dimension can be used to construct PAC bounds

$$M \geq \frac{1}{\epsilon}\left(4\ln\frac{2}{\delta} + 8 \cdot VC(H)\ln\frac{13}{\epsilon}\right)$$

- Then, with probability at least $(1-\delta)$ every $h \in H$ satisfies

$$\epsilon_h \leq \epsilon_h^{train} + \sqrt{\frac{1}{M}\left(VC(H)\left(\ln\left(\frac{2M}{VC(H)}\right) + 1\right) + \ln\frac{4}{\delta}\right)}$$

- These bounds (and the preceding discussion) only work for binary classification, but there are generalizations