Learning Theory

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Based on the slides of Vibhav Gogate, David Sontag and Nick Rouzzi

Learning Theory

- So far, we've been focused only on algorithms for finding the best hypothesis in the hypothesis space
  - **Generalization**: How do we know that the learned hypothesis will perform well on the test set?
  - **Generalization Bounds:** How many samples do we need to make sure that we learn a good hypothesis?

Learning Theory

- If the training data is linearly separable, we saw that perceptron/SVMs will always perfectly classify the training data
  - This does not mean that it will perfectly classify the test data
  - Intuitively, if the true distribution of samples is linearly separable, then seeing more data should help us do better

Problem Complexity

- Complexity of a learning problem depends on
  - Size/expressiveness of the hypothesis space (Loosely number of parameters)
  - Accuracy to which a target concept must be approximated
  - Probability with which the learner must produce a successful hypothesis
  - Manner in which training examples are presented, e.g. randomly or by query to an oracle

Problem Complexity

- Measures of complexity
  - Sample complexity
    - How much data you need in order to (with high probability) learn a good hypothesis
  - Computational complexity
    - Amount of time and space required to accurately solve (with high probability) the learning problem
    - Higher sample complexity means higher computational complexity

PAC Learning

- 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, ϵ and δ, and require that with probability at least $(1-\delta)$ a system learn a concept with error at most ϵ

Consistent Learners

- Imagine a simple setting
  - The hypothesis space is finite (i.e., $|H| = c$)
  - The true distribution of the data is $p(\vec{x})$, no noisy labels
  - We learned a perfect classifier on the training set, let's call it $h \in \mathrm{H}$
    - A learner is said to be consistent if it always outputs a perfect classifier (assuming that one exists)
  - Want to compute the (expected) error of the classifier

Notions of Error

- Training error of $h \in H$
  - The error on the training data
  - Number of samples incorrectly classified divided by the total number of samples
- True error of $h \in H$
  - The error over all possible future random samples
  - Probability, with respect to the data generating distribution, that h misclassifies a random data point

$$p(h(x) \neq y)$$

Learning Theory

- Assume that there exists a hypothesis in H that perfectly classifies all data points and that $|H|$ is finite
- The version space (set of consistent hypotheses) is said to be ϵ-exhausted if and only if every consistent hypothesis has true error less than ϵ
  - Want enough samples to guarantee that every consistent hypothesis has error at most ϵ

Learning Theory

- Let $\left(x^{(1)}, y^{(1)}\right), \ldots, (x^{(M)}, y^{(M)})$ be M labelled data points sampled independently according to p
- Let C_m^h be a random variable that indicates whether or not the m^{th} data point is correctly classified
- The probability that h misclassifies the m^{th} data point is

$$p\left(C_m^h = 0\right) = \sum_{(x,y)} p(x, y)\, 1_{h(x) \neq y} = \epsilon_h$$

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This is the true error of hypothesis h

Learning Theory

- Probability that all data points classified correctly?

- Probability that a hypothesis $h \in \mathrm{H}$ whose true error is at least ϵ correctly classifies the m data points is then

Learning Theory

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$$p\left(C_1^h = 1, \ldots, C_M^h = 1\right) = \prod_{m=1}^{M} p(C_m^h = 1) = (1 - \epsilon_h)^M$$

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Learning Theory

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- Probability that a hypothesis $h \in \mathrm{H}$ whose true error is at least ϵ correctly classifies the m data points is then

$$p\left(C_1^h = 1, \dots, C_M^h = 1\right) \le (1 - \epsilon)^M \le e^{-\epsilon M}$$

for $\epsilon \le 1$

The Union Bound

- Let $H_{BAD} \subseteq H$ be the set of all hypotheses that have true error at least ϵ

- From before for each $h \in H_{BAD}$,

$$p(h \text{ correctly classifies all } M \text{ data points}) \leq e^{-\epsilon M}$$

- So, the probability that *some* $h \in H_{BAD}$ correctly classifies all of the data points is

$$\begin{aligned} p\left(\bigvee_{h \in H_{BAD}} \left(C_1^h = 1, \dots, C_M^h = 1\right)\right) &\leq \sum_{h \in H_{BAD}} p\left(C_1^h = 1, \dots, C_M^h = 1\right) \\ &\leq |H_{BAD}| e^{-\epsilon M} \\ &\leq |H| e^{-\epsilon M} \end{aligned}$$

Haussler, 1988

- What we just proved:

  - **Theorem:** For a finite hypothesis space, H, with M i.i.d. samples, and $0 < \epsilon < 1$, the probability that the version space is not ϵ-exhausted is at most $|H|e^{-\epsilon M}$

- We can turn this into a **sample complexity bound**

Haussler, 1988

- What we just proved:
  - **Theorem:** For a finite hypothesis space, H, with M i.i.d. samples, and $0 < \epsilon < 1$, the probability that there exists a hypothesis in H that is consistent with the data but 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
  - That is, the probability that the version space is not ϵ-exhausted is at most $|H|e^{-\epsilon M} \leq \delta$
- Solving for M yields

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

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This is sufficient, but not necessary (union bound is quite loose)

Decision Trees

- Suppose that we want to learn an arbitrary Boolean function given n Boolean features
- Hypothesis space consists of all decision trees
  - Size of this space $= ?$
- How many samples are sufficient?

Decision Trees

- Suppose that we want to learn an arbitrary Boolean function given n Boolean features
- Hypothesis space consists of all decision trees
  - Size of this space $= 2^{2^n} =$ number of Boolean functions on n inputs
- How many samples are sufficient?

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

Generalizations

- How do we handle situations with no perfect classifier?
  - Pick the hypothesis with the lowest error on the training set
- What do we do if the hypothesis space isn't finite?
  - Infinite sample complexity?
  - Coming soon…

Chernoff Bounds

- Chernoff bound: Suppose $Y_1, \ldots, Y_M$ are i.i.d. random variables taking values in $\{0, 1\}$ such that $E_p[Y_i] = y$. For $\epsilon > 0$,

$$p\left(\left|y - \frac{1}{M}\sum_m Y_m\right| \geq \epsilon\right) \leq 2e^{-2M\epsilon^2}$$

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- Applying this to $1 - C_1^h, \dots, 1 - C_M^h$ gives

$$p\left(\left|\epsilon_h - \frac{1}{M}\sum_m (1 - C_m^h)\right| \geq \epsilon\right) \leq 2e^{-2M\epsilon^2}$$

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$$p\left(\epsilon_h - \frac{1}{M}\sum_m (1 - C_m^h) \geq \epsilon\right) \leq e^{-2M\epsilon^2}$$

This is the training error

PAC Bounds

- **Theorem:** For a finite hypothesis space H finite, 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 δ, then with probability $(1 - \delta)$, for all $h \in H$

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

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

PAC Bounds

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