15-859(B) Machine Learning Theory

Lecture 5: uniform convergence, tail inequalities, VC-dimension I

Avrim Blum

02/01/12

Today's focus: sample complexity

- We are given sample $S = \{(x,y)\}$.
  - Assume x's come from some fixed probability distribution D over instance space.
  - View labels y as being produced by some target function f.
- Alg does optimization over S to produce some hypothesis h. Want h to do well on new examples also from D.
- How big does S have to be to get this kind of guarantee?

Basic sample complexity bound recap

- If $|S| \geq (1/\varepsilon)[\ln(|C|) + \ln(1/\delta)]$, then with probability $\geq 1-\delta$, all $h \in C$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

- Argument: fix bad h. Prob of consistency at most $(1-\varepsilon)^{|S|}$. Set to $\delta/|C|$ and use union bound.
- So, if the target concept is in C, and we have an algorithm that can find consistent functions, then we only need this many examples to achieve the PAC guarantee.

Today: two issues

- If $|S| \geq (1/\varepsilon)[\ln(|C|) + \ln(1/\delta)]$, then with probability $\geq 1-\delta$, all $h \in C$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

1. Look at more general notions of "uniform convergence".
2. Replace $\ln(|C|)$ with better measures of complexity.

Uniform Convergence

- Our basic result only bounds the chance that a bad hypothesis looks perfect on the data. What if there is no perfect $h \in C$?
- Without making any assumptions about the target function, can we say that whp all $h \in C$ satisfy $|err_D(h) - err_S(h)| \leq \varepsilon$?
  - Called "uniform convergence".
  - Motivates optimizing over S, even if we can't find a perfect function.
- To prove bounds like this, need some good tail inequalities.

Tail inequalities

Tail inequality: bound probability mass in tail of distribution.

- Consider a hypothesis h with true error p.
- If we see m examples, then the expected fraction of mistakes is p, and the standard deviation σ is $(p(1-p)/m)^{1/2}$.
- A convenient rule for iid Bernoulli trials, in our notation, is: $\Pr[|err_D(h) - err_S(h)| > 1.96\sigma] < 0.05$.
  - If we want 95% confidence that true and observed errors differ by only ε, only need $(1.96)^2 p(1-p)/\varepsilon^2 < 1/\varepsilon^2$ examples. [worst case is when p=1/2]
- Chernoff and Hoeffding bounds extend to case where we want to show something is really unlikely, so can rule out lots of hypotheses.

Chernoff and Hoeffding bounds

Consider coin of bias p flipped m times. Let $\#$ be the observed # heads. Let $\varepsilon, \alpha \in [0,1]$.

Hoeffding bounds:

- $\Pr[\#/m > p + \varepsilon] \leq e^{-2m\varepsilon^2}$, and
- $\Pr[\#/m < p - \varepsilon] \leq e^{-2m\varepsilon^2}$.

Chernoff bounds:

- $\Pr[\#/m > p(1+\alpha)] \leq e^{-mp\alpha^2/3}$, and
- $\Pr[\#/m < p(1-\alpha)] \leq e^{-mp\alpha^2/2}$.

E.g,

- $\Pr[\# > 2(\text{expectation})] \leq e^{-(\text{expectation})/3}$.
- $\Pr[\# < (\text{expectation})/2] \leq e^{-(\text{expectation})/8}$.

Typical use of bounds

Thm: If $|S| \geq (1/(2\varepsilon^2))[\ln(|C|) + \ln(2/\delta)]$, then with probability $\geq 1-\delta$, all $h \in C$ have $|err_D(h) - err_S(h)| < \varepsilon$.

- Proof: Just apply Hoeffding.
  - Chance of failure at most $2|C|e^{-2|S|\varepsilon^2}$.
  - Set to δ. Solve.
- So, whp, best on sample is ε-best over D.
  - Note: this is worse than previous bound ($1/\varepsilon$ has become $1/\varepsilon^2$), because we are asking for something stronger.
  - Can also get bounds "between" these two.

Typical use of bounds

Thm: If $|S| \geq (6/\varepsilon)[\ln(|C|) + \ln(1/\delta)]$, then with prob $\geq 1-\delta$, all $h \in C$ with $err_D(h) > 2\varepsilon$ have $err_S(h) > \varepsilon$, and all $h \in C$ with $err_D(h) < \varepsilon/2$ have $err_S(h) < \varepsilon$.

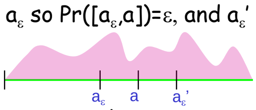
- Proof: apply Chernoff.

Next topic: improving the |C|

- For convenience, let's go back to the question: how big does S have to be so that whp, $err_S(h)=0 \Rightarrow err_D(h) \leq \varepsilon$.

VC-dimension and effective size of C

- If many hypotheses in C are very similar, we shouldn't have to pay so much
- E.g., consider the class $C = \{[0,a]: 0 \leq a \leq 1\}$.
  - Define a_ε so $\Pr([a_\varepsilon, a]) = \varepsilon$, and a_ε' so $\Pr([a, a_\varepsilon']) = \varepsilon$.



  - Enough to get at least one example in each interval. Just need $(1-\varepsilon)^{|S|} \leq \delta/2$.
  - $(1/\varepsilon)\ln(2/\delta)$ examples.
- How can we generalize this notion?

Effective number of hypotheses

Define: C[m] = maximum number of ways to split m points using concepts in C. (Book calls this $\Pi_C(m)$.)

- What is C[m] for "initial intervals"?
- How about linear separators in R^2?

- Thm: For any class C, distribution D, if $|S| = m > (2/\varepsilon)[\log_2(2C[2m]) + \log_2(1/\delta)]$, then with prob. $1-\delta$, all $h \in C$ with error $> \varepsilon$ are inconsistent with data. [Will prove soon]
- I.e., can roughly replace "|C|" with "C[2m]".

Effective number of hypotheses

Define: $C[m]$ = maximum number of ways to split m points using concepts in C. (Book calls this $\Pi_C(m)$.)

- What is C[m] for "initial intervals"?
- How about linear separators in R^2?

- C[m] is sometimes hard to calculate exactly, but can get a good bound using "VC-dimension".
- VC-dimension is roughly the point at which C stops looking like it contains all functions.

Shattering

- Defn: A set of points S is shattered by C if there are concepts in C that split S in all of the $2^{|S|}$ possible ways.
  - In other words, all possible ways of classifying points in S are achievable using concepts in C.
- E.g., any 3 non-collinear points can be shattered by linear threshold functions in 2-D.
- But no set of 4 points in R^2 can be shattered by LTFs.

VC-dimension

- The VC-dimension of a concept class C is the size of the largest set of points that can be shattered by C.
- So, if the VC-dimension is d, that means there exists a set of d points that can be shattered, but there is no set of d+1 points that can be shattered.
- E.g., VC-dim(linear threshold fns in 2-D) = 3.
  - Will later show VC-dim(LTFs in R^n) = n+1.
  - What is the VC-dim of intervals on the real line?
  - How about C = {all 0/1 functions on $\{0,1\}^n$}?

Upper and lower bound theorems

- Theorem 1: For any class C, distribution D, if $m=|S| > (2/\varepsilon)[\log_2(2C[2m]) + \log_2(1/\delta)]$, then with prob. $1-\delta$, all $h\in C$ with error $> \varepsilon$ are inconsistent with data.
- Theorem 2 (Sauer's lemma):
  $$C[m] \le \sum_{i=0}^{VCdim(C)} \binom{m}{i} = O(m^{VCdim(C)})$$
- Corollary 3: can replace bound in Thm 1 with
  $$O\left(\frac{1}{\epsilon}[VCdim(C)\log(1/\epsilon) + \log(1/\delta)]\right)$$
- Theorem 4: For any alg A, there exists a distrib D and target in C such that $|S| < (VCdim(C)-1)/(8\varepsilon) \Rightarrow E[err_D(A)] \ge \varepsilon$.