Learning Theory

Aarti Singh

Machine Learning 10-315
Apr 20, 2022

Slides courtesy: Carlos Guestrin

Learning Theory

- We have explored **many** ways of learning from data
- But…
  - Can we certify how good is our classifier, really?
  - How much data do I need to make it "good enough"?

PAC Learnability

- True function space, F
- Model space, H

F is ***PAC Learnable*** by a learner using H if

there exists a learning algorithm s.t. for all functions in F, for all distributions over inputs, for all $0 < \varepsilon, \delta < 1$, with probability $> 1-\delta$, the algorithm outputs a model $h \in H$ s.t. $\text{error}_{true}(h) \leq \varepsilon$

in time and samples that are polynomial in $1/\varepsilon$, $1/\delta$.

A simple setting

- Classification
  - m i.i.d. data points
  - **Finite** number of possible classifiers in model class (e.g., dec. trees of depth d)
- Lets consider that a learner finds a classifier *h* that gets zero error in training
  - $\text{error}_{\text{train}}(h) = 0$
- What is the probability that *h* has more than ε true (= test) error?
  - $\text{error}_{\text{true}}(h) \geq \varepsilon$

Even if *h* makes zero errors in training data, may make errors in test

How likely is a bad classifier to get m data points right?

- Consider a bad classifier *h* i.e. $error_{true}(h) \geq \varepsilon$
- Probability that *h* gets one data point right

  $\leq 1- \varepsilon$
- Probability that *h* gets *m* data points right

  $\leq (1- \varepsilon)^m$

How likely is a learner to pick a bad classifier?

- Usually there are many (say k) bad classifiers in model class

  $h_1, h_2, \dots, h_k$ s.t. $error_{true}(h_i) \geq \varepsilon \quad i = 1, \dots, k$

- Probability that learner picks a bad classifier = Probability that some bad classifier gets 0 training error

  Prob(h_1 gets 0 training error OR
  h_2 gets 0 training error OR … OR
  h_k gets 0 training error)

  ≤ Prob(h_1 gets 0 training error) +
  Prob(h_2 gets 0 training error) + … +
  Prob(h_k gets 0 training error)

  $\leq \; k(1-\varepsilon)^m$

Union bound

Loose but works

How likely is a learner to pick a bad classifier?

- Usually there are many many (say k) bad classifiers in the class

$$h_1, h_2, \ldots, h_k \qquad \text{s.t. } error_{true}(h_i) \geq \varepsilon \quad i = 1, \ldots, k$$

- Probability that learner picks a bad classifier

$$\leq \; k\,(1-\varepsilon)^m \quad \leq \quad |H|\,(1-\varepsilon)^m \leq \quad |H|\, e^{-\varepsilon m}$$

→ Size of model class

PAC (Probably Approximately Correct) bound

- ***Theorem [Haussler'88]***: Model class *H* finite, dataset *D* with *m* i.i.d. samples, $0 < \varepsilon < 1$: for any learned classifier *h* that gets 0 training error:

$$P(\text{error}_{true}(h) \geq \epsilon) \leq |H|e^{-m\epsilon} = \delta$$

- Equivalently, with probability $\geq 1 - \delta$

$$\text{error}_{true}(h) \leq \epsilon$$

Important: PAC bound holds for all *h* with 0 training error, but doesn't guarantee that algorithm finds best *h*!!!

Using a PAC bound

$|H|e^{-m\epsilon}$ = δ

- Given ε and δ, yields sample complexity

#training data, m = $\dfrac{\ln|H| + \ln\frac{1}{\delta}}{\epsilon}$

- Given m and δ, yields error bound

error, ϵ = $\dfrac{\ln|H| + \ln\frac{1}{\delta}}{m}$

Poll

Assume m is the minimum number of training examples sufficient to guarantee that with probability $1 - \delta$ a consistent learner using model class H will output a classifier with true error at worst ε.

Then a second learner that uses model space H' will require 2m training examples (to make the same guarantee) if $|H'| = 2|H|$.

A. True B. False

If we double the number of training examples to 2m, the error bound ε will be halved.

C. True D. False

Limitations of Haussler's bound

- Only consider classifiers with 0 training error

  h such that zero error in training, $\text{error}_{\text{train}}(h) = 0$

- Dependence on size of model class |H|

$$m = \frac{\ln |H| + \ln \frac{1}{\delta}}{\epsilon}$$

  what if |H| too big or H is continuous (e.g. linear classifiers)?

PAC bounds for finite model classes

H - Finite model class

e.g. decision trees of depth k

histogram classifiers with binwidth h

With probability ≥ 1-δ,

1) For all h $\in$ H s.t. $\text{error}_{\text{train}}(h) = 0$,

$$\text{error}_{\text{true}}(h) \leq \varepsilon = \frac{\ln|H| + \ln\frac{1}{\delta}}{m}$$

Haussler's bound

What if our classifier does not have zero error on the training data?

- A learner with zero training errors may make mistakes in test set
- What about a learner with $error_{train}(h) \neq 0$ in training set?
- The error of a classifier is like estimating the parameter of a coin!

$$error_{true}(h) := P(h(X) \neq Y) \equiv P(H=1) =: \theta$$

$$error_{train}(h) := \frac{1}{m}\sum_i \mathbf{1}_{h(X_i)\neq Y_i} \equiv \frac{1}{m}\sum_i Z_i =: \widehat{\theta}$$

Hoeffding's bound for a single classifier

- Consider *m* i.i.d. flips $x_1,\ldots,x_m$, where $x_i \in \{0,1\}$ of a coin with parameter θ. For $0<\varepsilon<1$:

$$P\left(\left|\theta - \frac{1}{m}\sum_i x_i\right| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

- Central limit theorem:

Hoeffding's bound for a single classifier

- Consider m i.i.d. flips $x_1,\ldots,x_m$, where $x_i \in \{0,1\}$ of a coin with parameter θ. For $0<\varepsilon<1$:

$$P\left(\left|\theta - \frac{1}{m}\sum_i x_i\right| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

- For a single classifier h

$$P\left(|\text{error}_{true}(h) - \text{error}_{train}(h)| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

Hoeffding's bound for |H| classifiers

- For each classifier h_i:

$$P\left(|\text{error}_{true}(h_i) - \text{error}_{train}(h_i)| \geq \epsilon\right) \leq 2e^{-2m\epsilon^2}$$

- What if we are comparing |H| classifiers?

  Union bound

- ***Theorem***: Model class *H* finite, dataset *D* with *m* i.i.d. samples, $0 < \varepsilon < 1$: for any learned classifier $h \in H$:

$$P\left(|\text{error}_{true}(h) - \text{error}_{train}(h)| \geq \epsilon\right) \leq 2|H|e^{-2m\epsilon^2} \leq \delta$$

Important: PAC bound holds for all *h*, but doesn't guarantee that algorithm finds best *h*!!!

Summary of PAC bounds for finite model classes

With probability $\geq 1-\delta$,

1) For all $h \in H$ s.t. $\text{error}_{\text{train}}(h) = 0$,

$$\text{error}_{\text{true}}(h) \leq \varepsilon = \frac{\ln|H| + \ln\frac{1}{\delta}}{m}$$

Haussler's bound

2) For all $h \in H$

$$|\text{error}_{\text{true}}(h) - \text{error}_{\text{train}}(h)| \leq \varepsilon = \sqrt{\frac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$$

Hoeffding's bound

PAC bound and Bias-Variance tradeoff

$$P\left(|\text{error}_{true}(h) - \text{error}_{train}(h)| \geq \epsilon\right) \leq 2|H|e^{-2m\epsilon^2} \leq \delta$$

- Equivalently, with probability $\geq 1 - \delta$

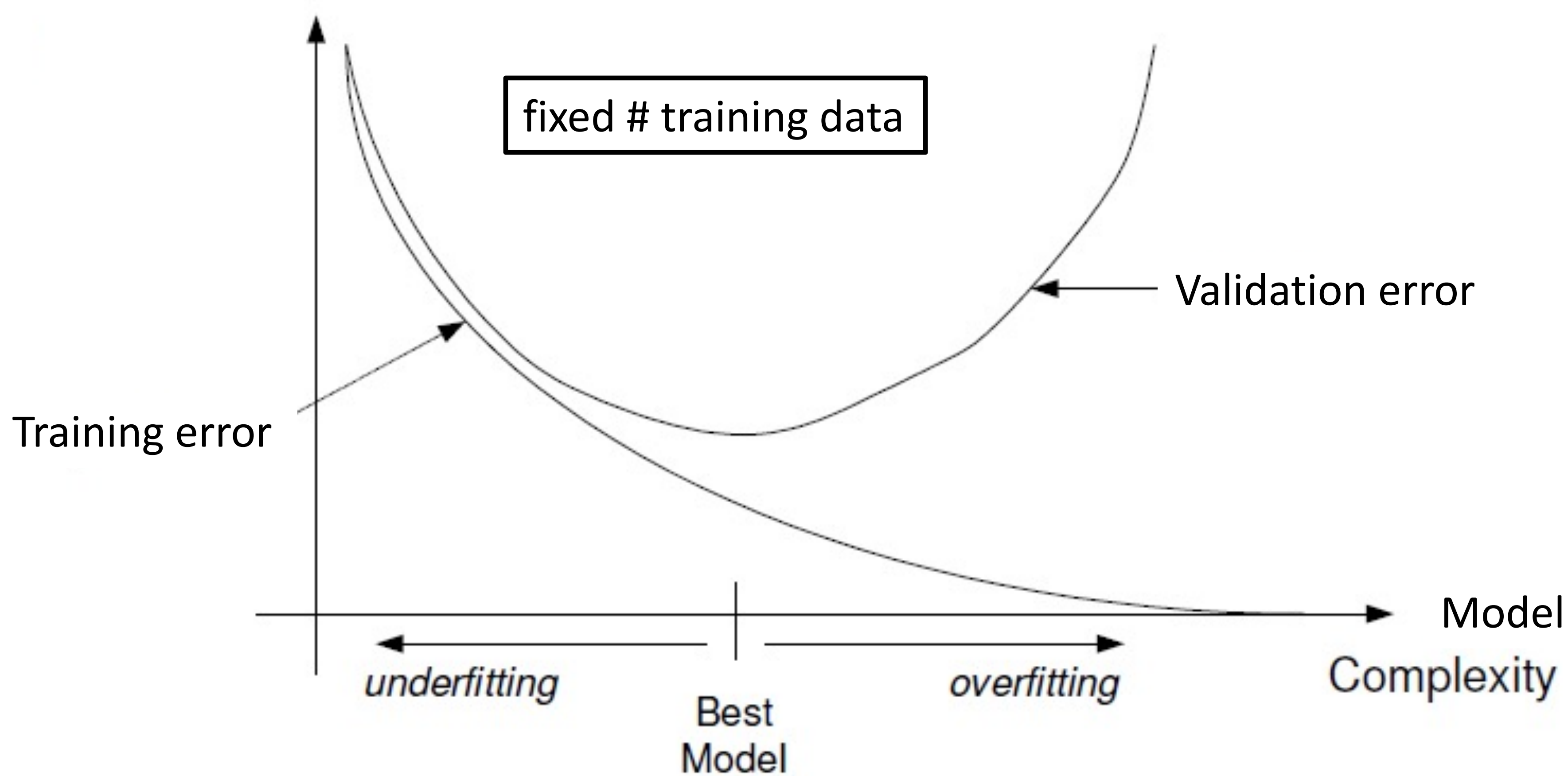
$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$$

- Fixed m

Model class		
complex	small	large
simple	large	small

Training vs. Test Error

With prob $\geq 1-\delta$, $\text{error}_{true}(h) \leq \text{error}_{train}(h) + \sqrt{\dfrac{\ln|H| + \ln\frac{2}{\delta}}{2m}}$



What about the size of the model class?

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

- Sample complexity

$$m = \frac{1}{2\epsilon^2}\left(\ln|H| + \ln\frac{2}{\delta}\right)$$

- How large is the model class?
  - Number of binary decision trees of depth k = 2^{2^k}
    m is exponential in depth k
    BUT given m points, decision tree can't get too big
  - Number of binary decision trees with k leaves = 2^k
    m is linear in number of leaves k

What did we learn from decision trees?

- Moral of the story:

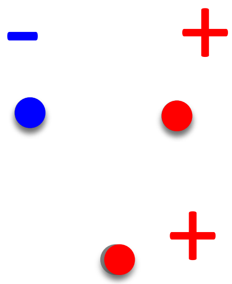
  Complexity of learning not measured in terms of size of model space, but in *number of points* that can be correctly classified

Rademacher Complexity

- Measure complexity by how accurately a model space can match a random labeling of the data.

For each data point i, draw random label

σ_i s.t. $P(\sigma_i = +1) = ½ = P(\sigma_i = -1)$



Then empirical Rademacher complexity of H is

$$\widehat{R}_m(H) = \mathbb{E}_\sigma \left[\sup_{h \in H} \left(\frac{1}{m} \sum_{i=1}^{m} \sigma_i h(X_i) \right) \right]$$

Max correlation possible with random labels

Rademacher Bounds

- With probability ≥ 1-δ,

$$\text{error}_{true}(h) \leq \text{error}_{train}(h) + \widehat{R}_m(H) + 3\sqrt{\frac{\log(2/\delta)}{m}}$$

where empirical Rademacher complexity of H

$$\widehat{R}_m(H) = \mathbb{E}_\sigma \left[\sup_{h \in H} \left(\frac{1}{m} \sum_{i=1}^{m} \sigma_i h(X_i) \right) \right]$$

is purely data-dependent.

Finite model class

- Rademacher complexity can be upper bounded in terms of model class size |H|:

$$\widehat{R}_m(H) \leq \sqrt{\frac{2\ln|H|}{m}}$$

- Often Rademacher bounds are significantly better

Summary of PAC bounds

With probability $\geq 1-\delta$,

1) for all $h \in H$ s.t. $\text{error}_{train}(h) = 0$,

$$\text{error}_{true}(h) \leq \varepsilon = \frac{\ln |H| + \ln \frac{1}{\delta}}{m}$$

2) for all $h \in H$,

$$|\text{error}_{true}(h) - \text{error}_{train}(h)| \leq \varepsilon = \sqrt{\frac{\ln |H| + \ln \frac{1}{\delta}}{2m}}$$

Finite hypothesis space

3) For all $h \in H$,

$$|\text{error}_{true}(h) - \text{error}_{train}(h)| \leq \varepsilon = \widehat{R}_m(H) + 3\sqrt{\frac{\log(2/\delta)}{m}}$$

Infinite hypothesis space