We have explored many ways of learning from data.

But...

- How good is our classifier, really?
- How much data do I need to make it “good enough”?
A simple setting...

- Classification
  - N data points
  - Finite number of possible hypothesis (e.g., dec. trees of depth d)
- A learner finds a hypothesis \( h \) that is **consistent** with training data
  - Gets zero error in training – \( \text{error}_{\text{train}}(h) = 0 \)
- What is the probability that \( h \) has more than \( \varepsilon \) true error?
  - \( \text{error}_{\text{true}}(h) \geq \varepsilon \)

How likely is a bad hypothesis to get \( N \) data points right?

- Hypothesis \( h \) that is **consistent** with training data → got \( N \) i.i.d. points right
  - \( h \) “bad” if it gets all this data right, but has high true error
- Prob. \( h \) with \( \text{error}_{\text{true}}(h) \geq \varepsilon \) gets one data point right

- Prob. \( h \) with \( \text{error}_{\text{true}}(h) \geq \varepsilon \) gets \( N \) data points right
But there are many possible hypothesis that are consistent with training data

How likely is learner to pick a bad hypothesis

- Prob. $h$ with $\text{error}_{\text{true}}(h) \geq \varepsilon$ gets $N$ data points right

- There are $k$ hypothesis consistent with data
  - How likely is learner to pick a bad one?
Union bound

- $P(A \text{ or } B \text{ or } C \text{ or } D \text{ or } ...)$

How likely is learner to pick a bad hypothesis

- Prob. a particular $h$ with $\text{error}_{\text{true}}(h) \geq \varepsilon$ gets $N$ data points right

- There are $k$ hypothesis consistent with data
  - How likely is it that learner will pick a bad one out of these $k$ choices?
Generalization error in finite hypothesis spaces [Haussler ‘88]

**Theorem:** Hypothesis space $H$ finite, dataset $D$ with $N$ i.i.d. samples, $0 < \varepsilon < 1$: for any learned hypothesis $h$ that is consistent on the training data:

$$P(error_{true}(h) > \varepsilon) \leq |H|e^{-N\varepsilon}$$

Using a PAC bound

Typically, 2 use cases:

- 1: Pick $\varepsilon$ and $\delta$, give you $N$
- 2: Pick $N$ and $\delta$, give you $\varepsilon$
Summary: Generalization error in finite hypothesis spaces [Haussler ‘88]

**Theorem:** Hypothesis space $H$ finite, dataset $D$ with $N$ i.i.d. samples, $0 < \epsilon < 1$: for any learned hypothesis $h$ that is consistent on the training data:

$$P(error_{true}(h) > \epsilon) \leq |H|e^{-N\epsilon}$$

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

Limitations of Haussler ‘88 bound

- Consistent classifier
- Size of hypothesis space
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 $\text{error}_{\text{train}}(h)$ in training set?

Simpler question: What’s the expected error of a hypothesis?

- The error of a hypothesis is like estimating the parameter of a coin!

- Chernoff bound: for $N$ i.i.d. coin flips, $x^1, \ldots, x^N$, where $x^i \in \{0, 1\}$. For $0 < \epsilon < 1$:

$$P \left( \theta - \frac{1}{N} \sum_{j=1}^{N} x^j > \epsilon \right) \leq e^{-2N\epsilon^2}$$
Using Chernoff bound to estimate error of a single hypothesis

\[ P \left( \theta - \frac{1}{N} \sum_{j=1}^{N} x^j > \epsilon \right) \leq e^{-2N\epsilon^2} \]

But we are comparing many hypothesis: **Union bound**

For each hypothesis \( h_i \):

\[ P (error_{true}(h_i) - error_{train}(h_i) > \epsilon) \leq e^{-2N\epsilon^2} \]

What if I am comparing two hypothesis, \( h_1 \) and \( h_2 \)?
Generalization bound for $|H|$ hypothesis

**Theorem**: Hypothesis space $H$ finite, dataset $D$ with $N$ i.i.d. samples, $0 < \varepsilon < 1$ : for any learned hypothesis $h$:

$$P(error_{true}(h) - error_{train}(h) > \varepsilon) \leq e^{-2N\varepsilon^2}$$

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PAC bound and Bias-Variance tradeoff

$$P(error_{true}(h) - error_{train}(h) > \varepsilon) \leq e^{-2N\varepsilon^2}$$

or, after moving some terms around, with probability at least $1-\delta$:

$$error_{true}(h) \leq error_{train}(h) + \sqrt{\ln |H| + \ln \frac{1}{\delta}}$$

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**Important**: PAC bound holds for all $h$, but doesn’t guarantee that algorithm finds best $h$!!!
What about the size of the hypothesis space?

\[ N \geq \frac{\ln |H| + \ln \frac{1}{\delta}}{2\epsilon^2} \]

- How large is the hypothesis space?

Boolean formulas with \( m \) binary features

\[ N \geq \frac{\ln |H| + \ln \frac{1}{\delta}}{2\epsilon^2} \]
Number of decision trees of depth $k$

Recursive solution

Given $m$ attributes

$H_k = \text{Number of decision trees of depth } k$

$H_0 = 2$

$H_{k+1} = (\# \text{choices of root attribute}) \times$

$\quad (\# \text{possible left subtrees}) \times$

$\quad (\# \text{possible right subtrees})$

$= m \times H_k \times H_k$

Write $L_k = \log_2 H_k$

$L_0 = 1$

$L_{k+1} = \log_2 m + 2L_k$

So $L_k = (2^k - 1) (1 + \log_2 m) + 1$

PAC bound for decision trees of depth $k$

$$N \geq \frac{2^k \log m + \ln \frac{1}{\delta}}{\epsilon^2}$$

- Bad!!!
  - Number of points is exponential in depth!

- But, for $N$ data points, decision tree can’t get too big…

Number of leaves never more than number data points
Number of Decision Trees with k Leaves

- Number of decision trees of depth $k$ is really really big:
  - $\ln |H|$ is about $2^k \log m$

- Decision trees with up to $k$ leaves:
  - $|H|$ is about $m^k k^{2k}$
    - A very loose bound

PAC bound for decision trees with $k$ leaves – Bias-Variance revisited

$$\ln |H_{\text{DTs \; k \; leaves}}| \leq 2k(\ln m + \ln k)$$

$$\text{error}_{\text{true}}(h) \leq \text{error}_{\text{train}}(h) + \sqrt{\frac{2k(\ln m + \ln k) + \ln \frac{1}{\delta}}{2N}}$$
What did we learn from decision trees?

- Bias-Variance tradeoff formalized

\[ \text{error}_{\text{true}}(h) \leq \text{error}_{\text{train}}(h) + \sqrt{\frac{2k(ln m + ln k) + ln \frac{1}{\delta}}{2N}} \]

- Moral of the story:
  Complexity of learning not measured in terms of size hypothesis space, but in maximum number of points that allows consistent classification.
  - Complexity \( N \) – no bias, lots of variance
  - Lower than \( N \) – some bias, less variance

What about continuous hypothesis spaces?

- Continuous hypothesis space:
  - \( |H| = \infty \)
  - Infinite variance???

- As with decision trees, only care about the maximum number of points that can be classified exactly!
  - Called VC dimension… see readings for details
What you need to know

- Finite hypothesis space
  - Derive results
  - Counting number of hypothesis
  - Mistakes on Training data

- Complexity of the classifier depends on number of points that can be classified exactly
  - Finite case – decision trees
  - Infinite case – VC dimension

- Bias-Variance tradeoff in learning theory

- Remember: will your algorithm find best classifier?