Generalization, Overfitting, Sample Complexity.

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February 25th, 2019

- Recommended reading: Mitchell: Ch. 7
  - Suggested exercises: 7.1, 7.2, 7.7

Admin

Midterm: in class, March 4th.

Closed book.

Allowed to bring one sheet of notes (front and back).

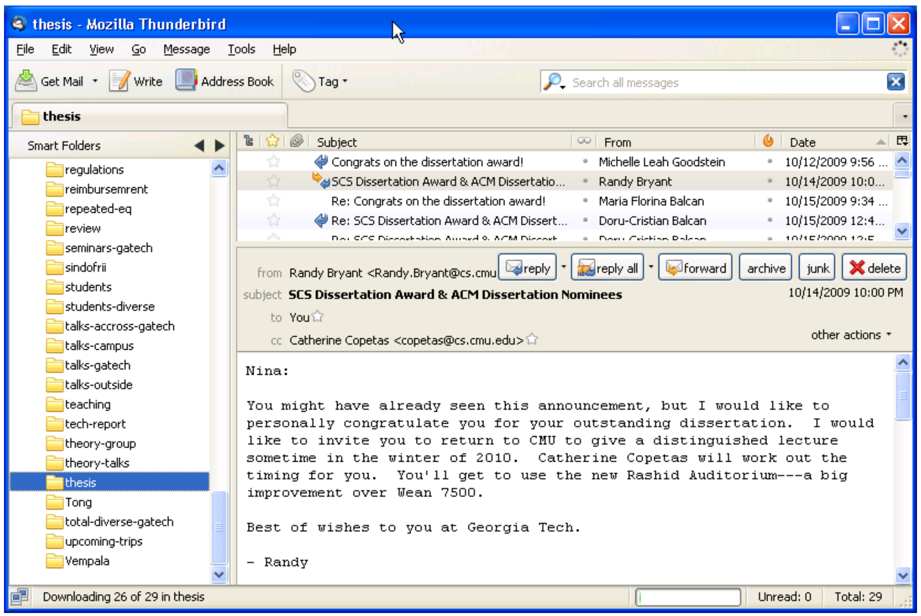
Supervised Classification

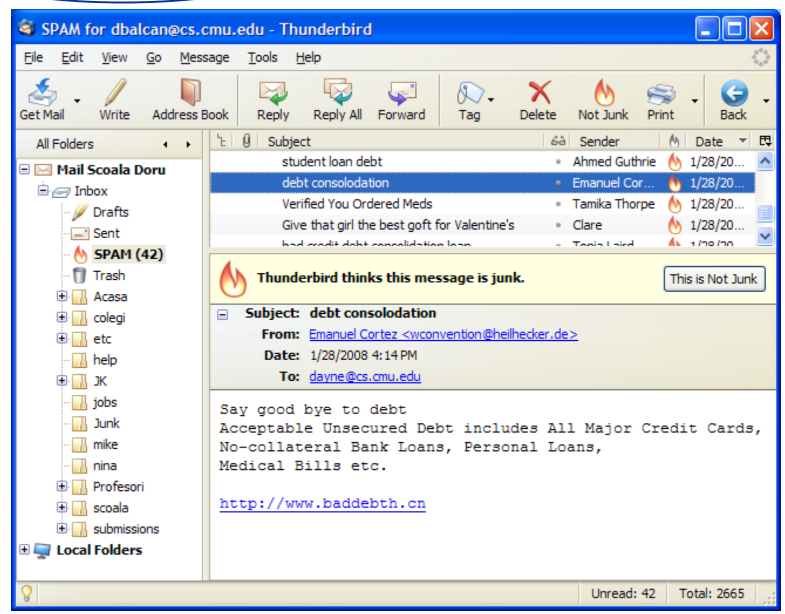
Decide which emails are spam and which are important.

Supervised classification

Not spam

spam





Goal: use emails seen so far to produce good prediction rule for future data.

Example: Supervised Classification

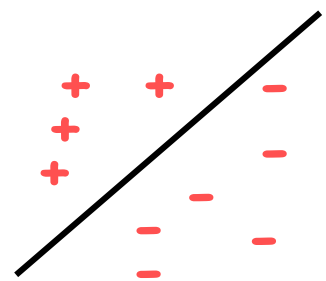
Represent each message by features. (e.g., keywords, spelling, etc.)

	"money"	"pills"	"Mr."	bad spelling	known-sender	spam?	
	Y	N	Y	Y	N	Y	
	N	N	N	Y	Y	N	
	N	Y	N	N	N	Y	
example	Y	N	N	N	Y	N	label
	N	N	Y	N	Y	N	
	Y	N	N	Y	N	Y	
	N	N	Y	N	N	N	

Reasonable RULES:

Predict SPAM if unknown AND (money OR pills)

Predict SPAM if 2money + 3pills –5 known > 0



Linearly separable

Two Core Aspects of Machine Learning

Algorithm Design. How to optimize?

Computation

Automatically generate rules that do well on observed data.

- E.g.: logistic regression, SVM, Adaboost, etc.

Confidence Bounds, Generalization

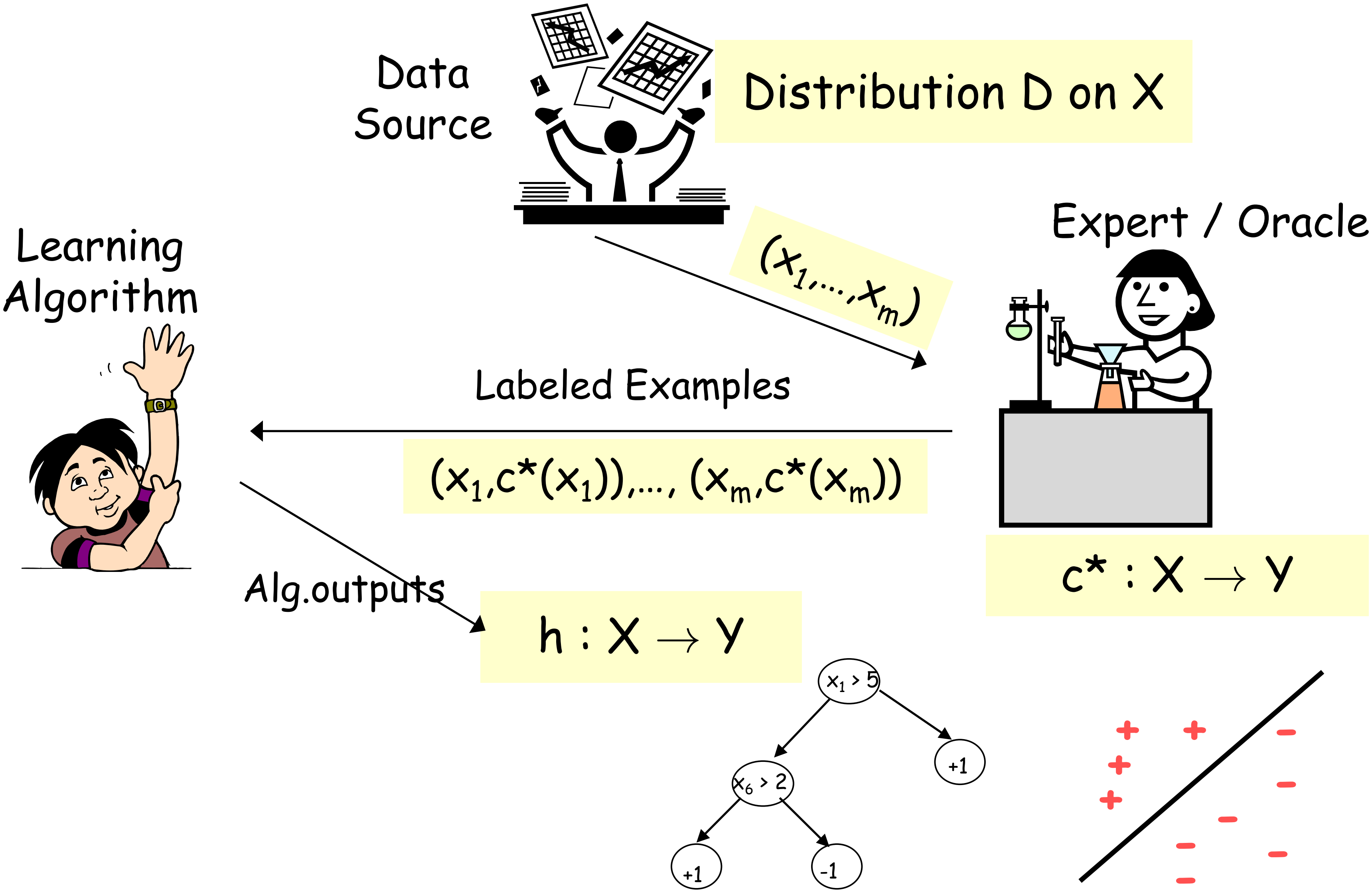
(Labeled) Data

Confidence for rule effectiveness on future data.

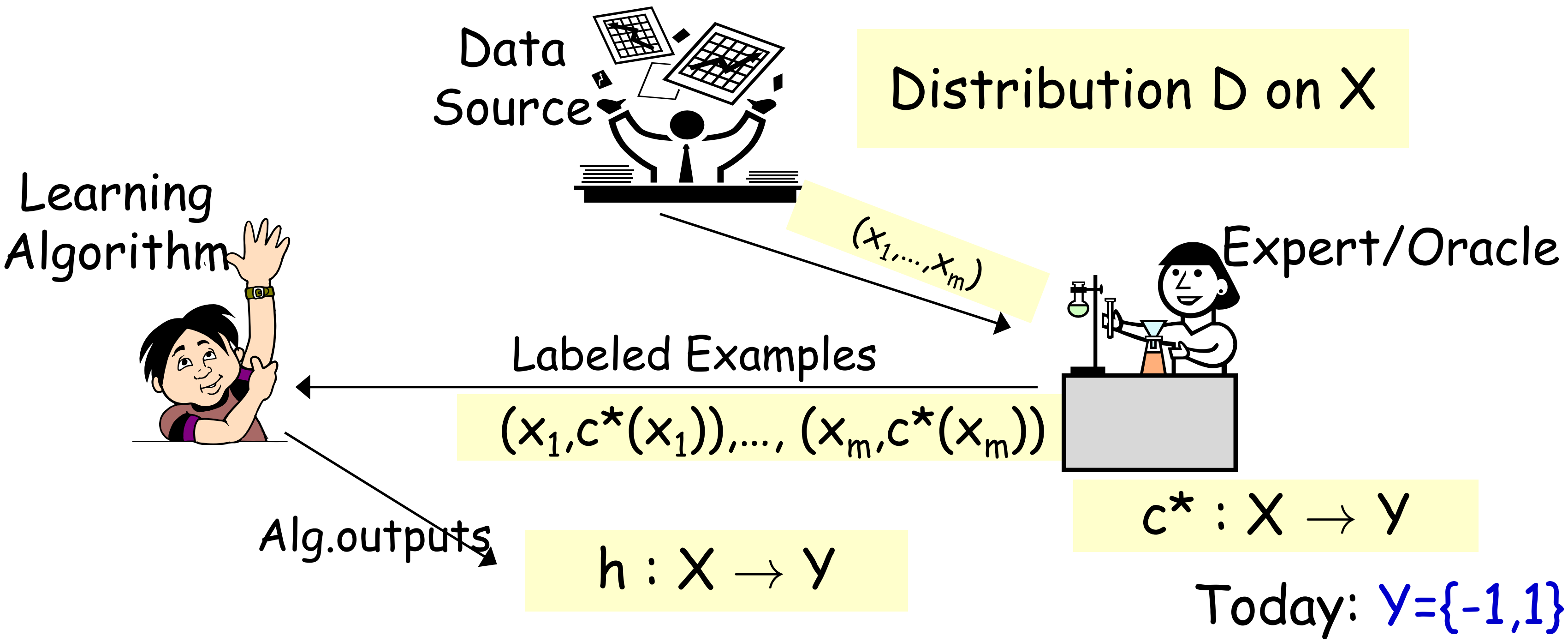
- Very well understood: Occam's bound, VC theory, etc.

- Note: to talk about these we need a precise model.

PAC/SLT models for Supervised Learning



PAC/SLT models for Supervised Learning



- Algo sees training sample S: $(x_1,c^*(x_1)),\ldots, (x_m,c^*(x_m))$, x_i independently and identically distributed (i.i.d.) from D; labeled by c^*

- Does optimization over S, finds hypothesis h (e.g., a decision tree).
- Goal: h has small error over D.

PAC/SLT models for Supervised Learning

- X – feature or instance space; distribution D over X

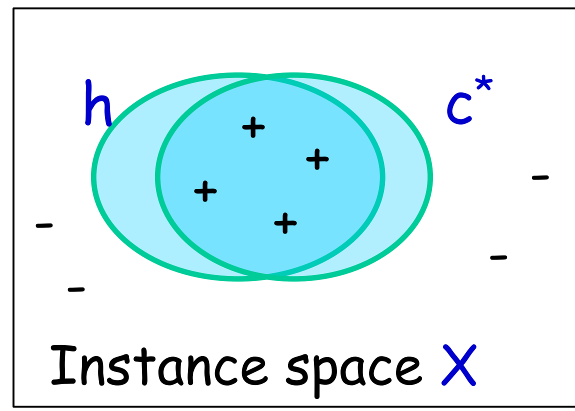
  e.g., $X = R^d$ or $X = \{0,1\}^d$

- Algo sees training sample S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$, x_i i.i.d. from D
  - labeled examples - assumed to be drawn i.i.d. from some distr. D over X and labeled by some target concept c^*
  - labels $\in \{-1,1\}$ - binary classification

- Algo does optimization over S, find hypothesis h.

- Goal: h has small error over D.

$$err_D(h) = \Pr_{x \sim D}(h(x) \neq c^*(x))$$



Need a bias: no free lunch.

PAC/SLT models for Supervised Learning

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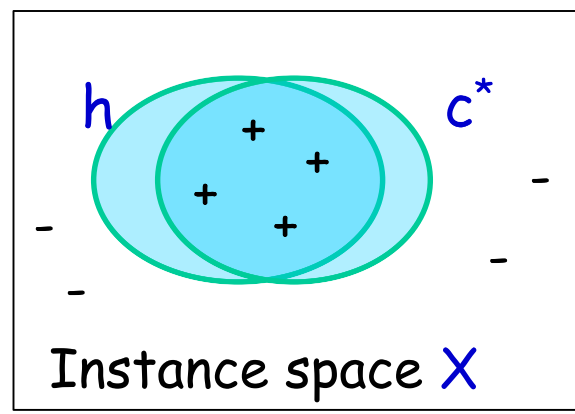

Bias: Fix hypotheses space H.

(whose complexity is not too large).

Realizable: $c^* \in H$.

Agnostic: c^* “close to” H.

PAC/SLT models for Supervised Learning

- Algo sees training sample S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$, x_i i.i.d. from D
- Does optimization over S, find hypothesis $h \in H$.
- Goal: h has small error over D.

True error: $err_D(h) = \Pr_{x\sim D}(h(x) \neq c^*(x))$

How often $h(x) \neq c^*(x)$ over future instances drawn at random from D

- But, can only measure:

Training error: $err_S(h) = \frac{1}{m}\sum_i I\big(h(x_i) \neq c^*(x_i)\big)$

How often $h(x) \neq c^*(x)$ over training instances

Sample complexity: bound $err_D(h)$ in terms of $err_S(h)$

Sample Complexity for Supervised Learning

Consistent Learner

- Input: S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$
- Output: Find h in H consistent with the sample (if one exits).

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Contrapositive: if the target is in H, and we have an algo that can find consistent fns, then we only need this many examples to get generalization error $\leq \epsilon$ with prob. $\geq 1-\delta$

Sample Complexity for Supervised Learning

Consistent Learner

- Input: S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$
- Output: Find h in H consistent with the sample (if one exits).

Theorem

Bound inversely linear in ϵ

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Bound only logarithmic in |H|

- ϵ is called error parameter
  - D might place low weight on certain parts of the space
- δ is called confidence parameter
  - there is a small chance the examples we get are not representative of the distribution

Sample Complexity for Supervised Learning

Consistent Learner

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Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Example: H is the class of conjunctions over $X = \{0,1\}^n$. $|H| = 3^n$

E.g., $h = x_1 \overline{x_3} x_5$ or $h = x_1 \overline{x_2} x_4 x_9$

Then $m \geq \frac{1}{\epsilon}\left[n \ln 3 + \ln\left(\frac{1}{\delta}\right)\right]$ suffice

$n = 10, \epsilon = 0.1, \delta = 0.01$ then $m \geq 156$ suffice

Sample Complexity for Supervised Learning

Consistent Learner

- Input: S: $(x_1,c^*(x_1)),\ldots,(x_m,c^*(x_m))$
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Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Example: H is the class of conjunctions over $X = \{0,1\}^n$.

Side HWK question: show that any conjunctions can be represented by a small decision tree; also by a linear separator.

Sample Complexity for Supervised Learning

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Proof Assume k bad hypotheses $h_1, h_2, \ldots, h_k$ with $err_D(h_i) \geq \epsilon$

1) Fix h_i. Prob. h_i consistent with first training example is $\leq 1-\epsilon$.

   Prob. h_i consistent with first m training examples is $\leq (1-\epsilon)^m$.

2) Prob. that at least one h_i consistent with first m training examples is $\leq k\,(1-\epsilon)^m \leq |H|(1-\epsilon)^m$.

3) Calculate value of m so that $|H|(1-\epsilon)^m \leq \delta$

3) Use the fact that $1-x \leq e^{-x}$, sufficient to set $|H|(1-\epsilon)^m \leq |H|\, e^{-\epsilon m} \leq \delta$

Sample Complexity: Finite Hypothesis Spaces

Realizable Case

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Probability over different samples
of m training examples

Sample Complexity: Finite Hypothesis Spaces Realizable Case

1) PAC: How many examples suffice to guarantee small error whp.

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

2) Statistical Learning Way:

With probability at least $1-\delta$, for all $\mathrm{h} \in \mathrm{H}$ s.t. $\mathrm{err_S(h)} = 0$ we have

$$\mathrm{err_D(h)} \leq \frac{1}{\mathrm{m}}\left(\ln|\mathrm{H}| + \ln\left(\frac{1}{\delta}\right)\right).$$

Supervised Learning: PAC model (Valiant)

- X - instance space, e.g., $X = \{0,1\}^n$ or $X = R^n$
- $S_l=\{(x_i, y_i)\}$ - labeled examples drawn i.i.d. from some distr. D over X and labeled by some target concept c^*
  - labels $\in \{-1,1\}$ - binary classification

- Algorithm A PAC-learns concept class H if for any target c^* in H, any distrib. D over X, any $\varepsilon, \delta > 0$:
  - A uses at most poly(n,$1/\varepsilon$,$1/\delta$,size(c^*)) examples and running time.
  - With probab. $1-\delta$, A produces h in H of error at $\leq \varepsilon$.

Uniform Convergence

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

- This basic result only bounds the chance that a bad hypothesis looks perfect on the data. What if there is no perfect $h \in H$ (agnostic case)?

- What can we say if $c^* \notin H$?
- Can we say that whp all $h \in H$ 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.

Sample Complexity: Finite Hypothesis Spaces

Realizable Case

Theorem

$$m \geq \frac{1}{\varepsilon}\left[\ln(|H|) + \ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \varepsilon$ have $err_S(h) > 0$.

Agnostic Case

What if there is no perfect h?

Theorem After m examples, with probab. $\geq 1-\delta$, all $h \in H$ have $|err_D(h) - err_S(h)| < \varepsilon$, for

$$m \geq \frac{1}{2\varepsilon^2}\left[\ln(|H|) + \ln\left(\frac{2}{\delta}\right)\right]$$

To prove bounds like this, need some good tail inequalities.

Hoeffding bounds

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

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

Exponentially decreasing tails

- Tail inequality: bound probability mass in tail of distribution (how concentrated is a random variable around its expectation).

Sample Complexity: Finite Hypothesis Spaces Agnostic Case

Theorem After m examples, with probab. $\geq 1 - \delta$, all $h \in H$ have $|err_D(h) - err_S(h)| < \varepsilon$, for

$$m \geq \frac{1}{2\varepsilon^2}\left[\ln(|H|) + \ln\left(\frac{2}{\delta}\right)\right]$$

- Proof: Just apply Hoeffding.
  - Chance of failure at most $2|H|e^{-2|S|\varepsilon^2}$.
  - 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.

What you should know

- Notion of sample complexity.
- Understand reasoning behind the simple sample complexity bound for finite H.