Generalization and Overfitting

Sample Complexity Results for Supervised Classification

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Today's focus: Sample Complexity for Supervised Classification (Function Approximation)

- Statistical Learning Theory (Vapnik)
- PAC (Valiant)

Recommended readings:

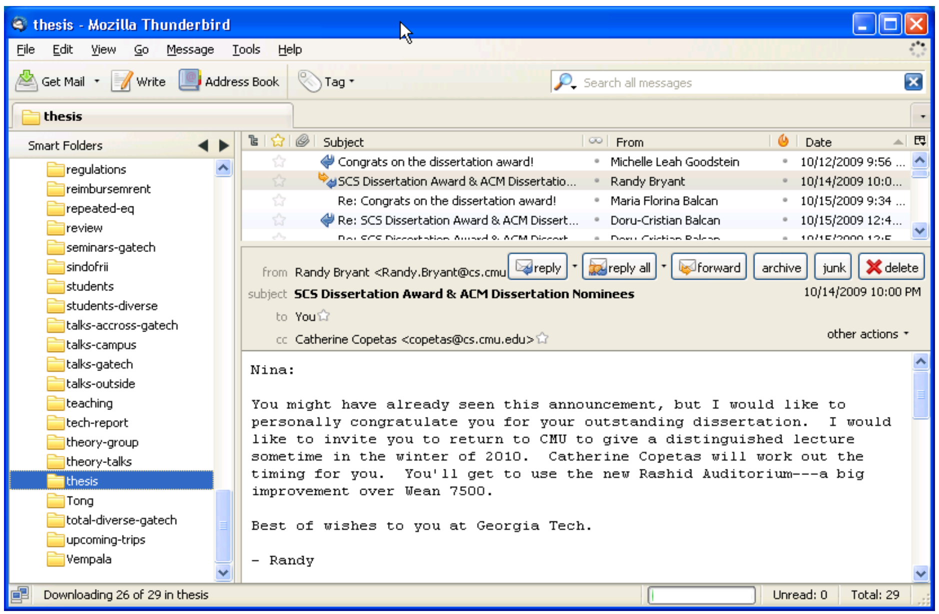
- Mitchell: Ch. 7
- Shalev-Shwartz& Ben-David: Chapters 2,3,4

Supervised Classification

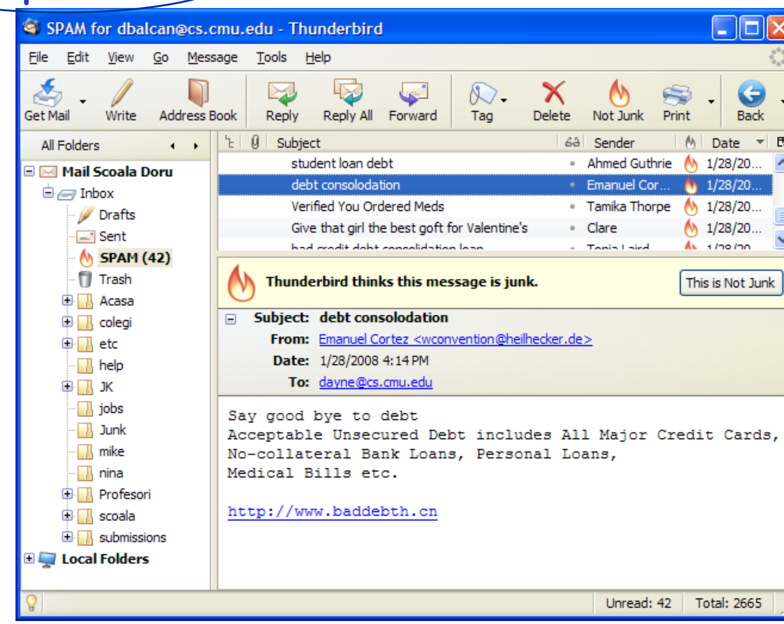
Decide which emails are spam and which are important.

Supervised classification

Not spam



spam



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

Example: Supervised Classification

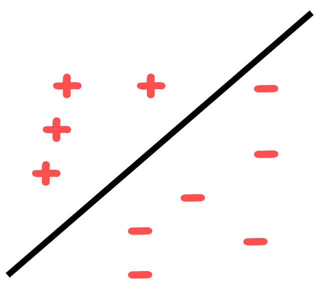
Represent each message by features. (e.g., keywords, spelling, etc.)

	"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

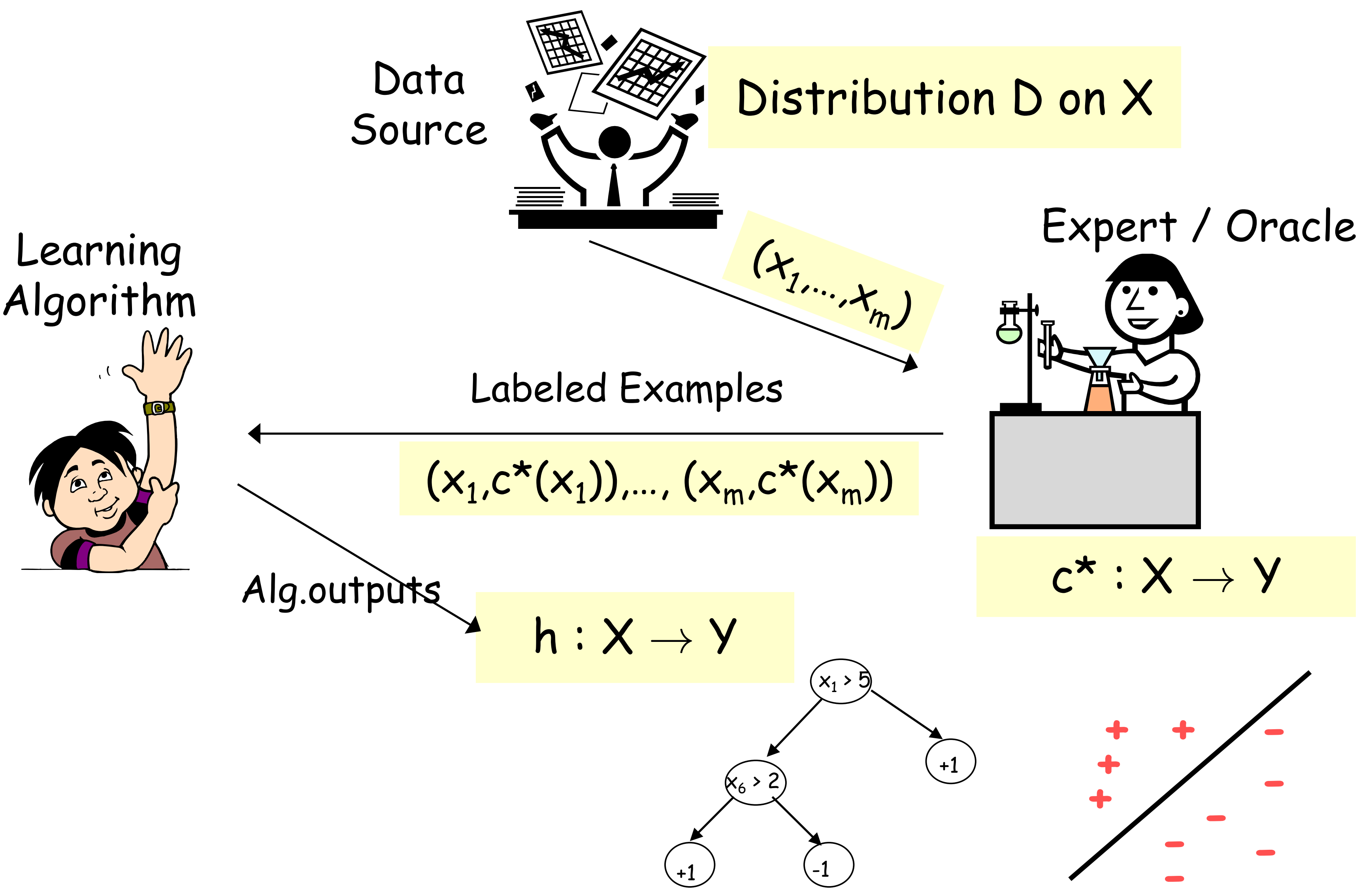
(Labeled) Data

Confidence for rule effectiveness on future data.

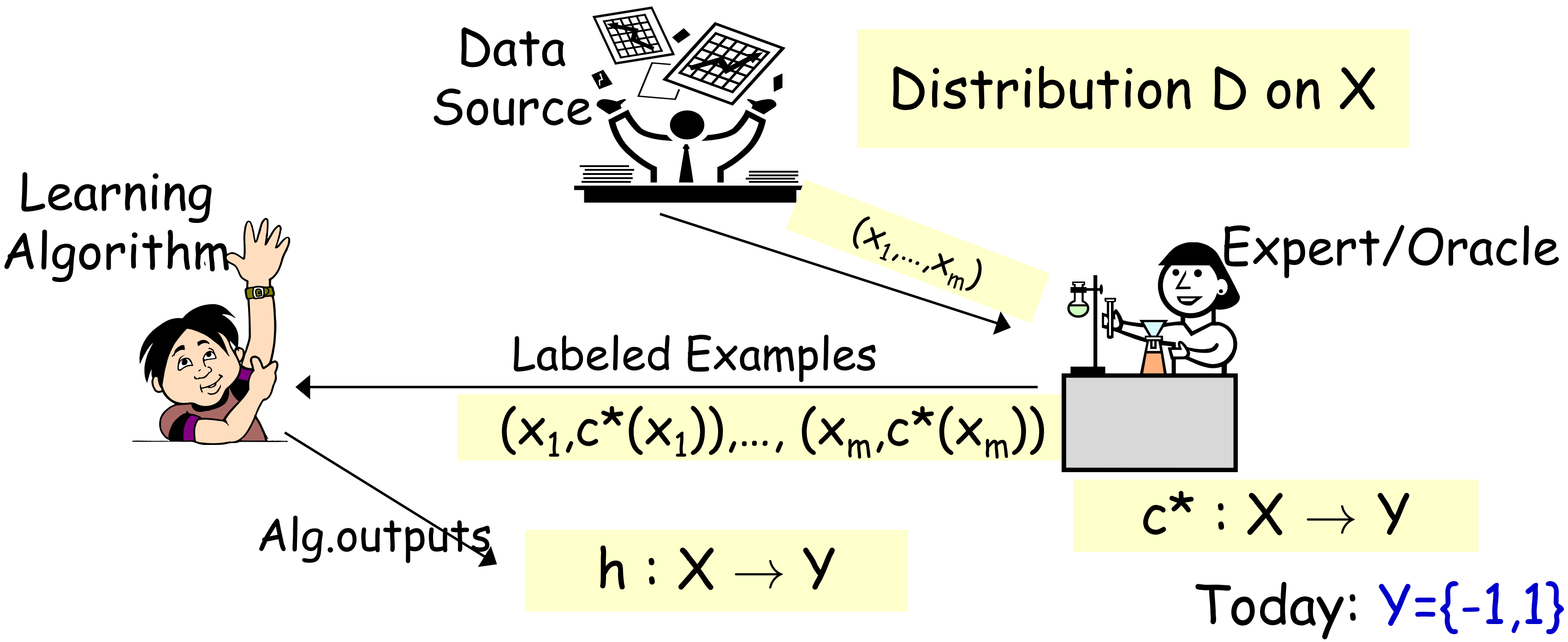
- Very well understood: Occam's bound, VC theory, etc.

- 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.

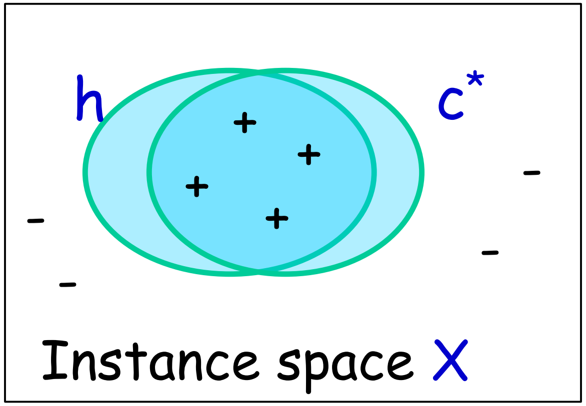
PAC/SLT models for Supervised Learning

- 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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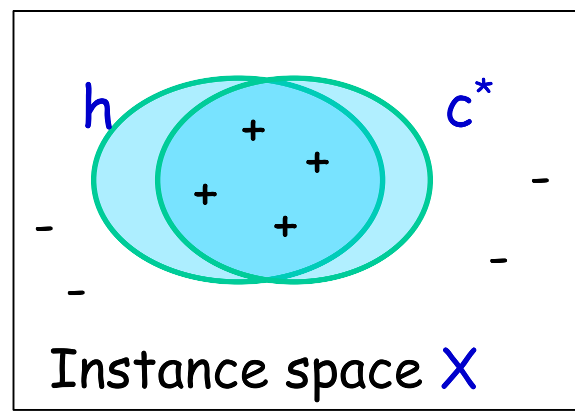

Bias: Fix hypotheses space H.

(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

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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

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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 $h \in H$ s.t. $err_S(h) = 0$ we have

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

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/ε,1/δ,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:

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

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.