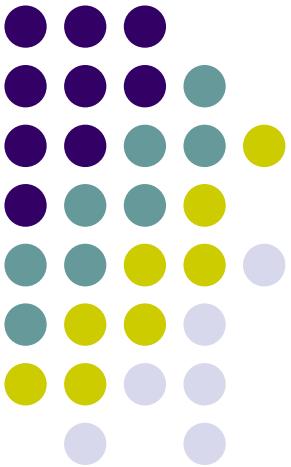
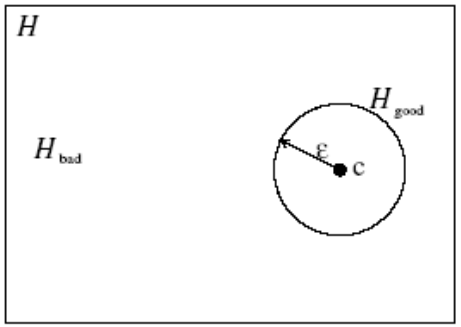
Machine Learning

10-701, Fall 2016

Computational Learning Theory



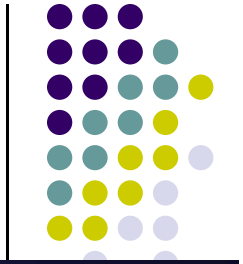
Eric Xing



Lecture 9, October 5, 2016

Reading: Chap. 7 T.M book

Generalizability of Learning



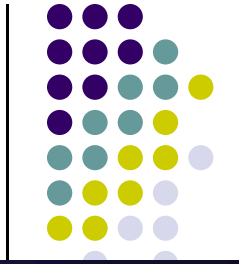
- In machine learning it's really generalization error that we care about, but most learning algorithms fit their models to the training set.

- Why should doing well on the training set tell us anything about generalization error? Specifically, can we relate error on training set to generalization error?

$\epsilon_S(h) \;?\; \epsilon(h)$

- Are there conditions under which we can actually prove that learning algorithms will work well?

Complexity of Learning



- The complexity of leaning is measured mainly along two axis: Information and computation.

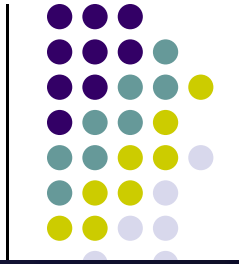
  The Information complexity is concerned with the generalization performance of learning;

  - *How many training examples are needed?*
  - *How fast do learner's estimate converge to the true population parameters? etc.*

  The Computational complexity concerns the computation resources applied to the training data to extract from it learner's predictions.

It seems that when an algorithm improves with respect to one of these measures it deteriorates with respect to the other.

What General Laws Constrain Inductive Learning?

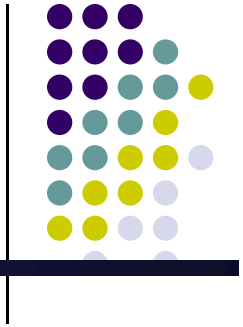


- Sample Complexity
  - How many training examples are sufficient to learn target concept?
- Computational Complexity
  - Resources required to learn target concept?
- Want theory to relate:
  - Training examples
    - Quantity
    - Quality — m
    - How presented
  - Complexity of hypothesis/concept space H
  - Accuracy of approx to target concept — ε
  - Probability of successful learning — δ

$C = h(x) - c(x)$

These results only useful wrt O(...) !

Prototypical concept learning task



Binary classification

- Everything we'll say here generalizes to other, including regression and multi-class classification, problems.

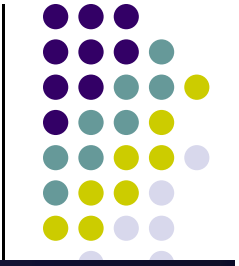
- Given:
  - Instances *X*: Possible days, each described by the attributes *Sky, AirTemp, Humidity, Wind, Water, Forecast*
  - Target function *c*: *EnjoySport* : X → {0, 1}
  - Hypotheses space *H*: Conjunctions of literals. E.g.

    (?, Cold, High, ?, ?, EnjoySport)
  - Training examples *S*: iid positive and negative examples of the target function

    $(x_1, c(x_1)), \ldots (x_m, c(x_m))$

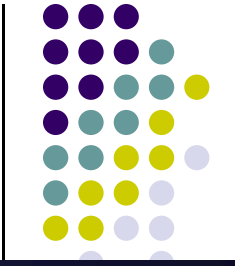
- Determine:
  - A hypothesis *h* in *H* such that *h(x)* is "good" w.r.t *c(x)* for all *x* in *S*?
  - A hypothesis *h* in *H* such that *h(x)* is "good" w.r.t *c(x)* for all *x* in the true dist $\mathcal{D}$?

Two Basic Competing Models



PAC framework	Agnostic framework
Sample labels are consistent with some h in H	*No prior restriction on the sample labels*
Learner's hypothesis required to meet *absolute* upper bound on its error	*The required upper bound on the hypothesis error is only* relative *(to the best hypothesis in the class)*

Sample Complexity



- How many training examples are sufficient to learn the target concept?

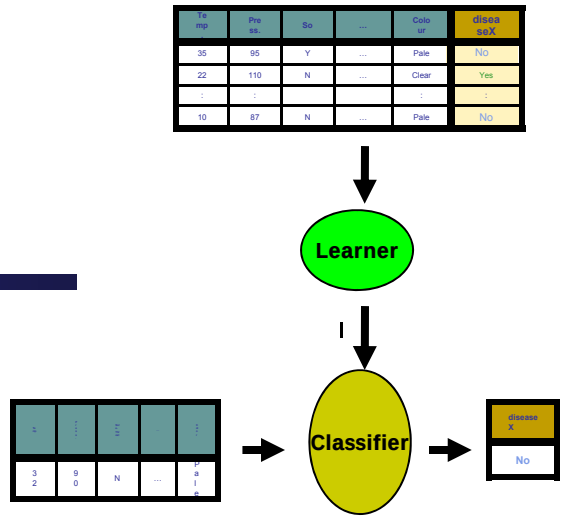
- Training scenarios:

1 If learner proposes instances, as queries to teacher
   - Learner proposes instance x, teacher provides *c(x)*

2 If teacher (who knows *c*) provides training examples
   - teacher provides sequence of examples of form (*x*, *c(x)*)

3 If some random process (e.g., nature) proposes instances
   - instance *x* generated randomly, teacher provides *c(x)*

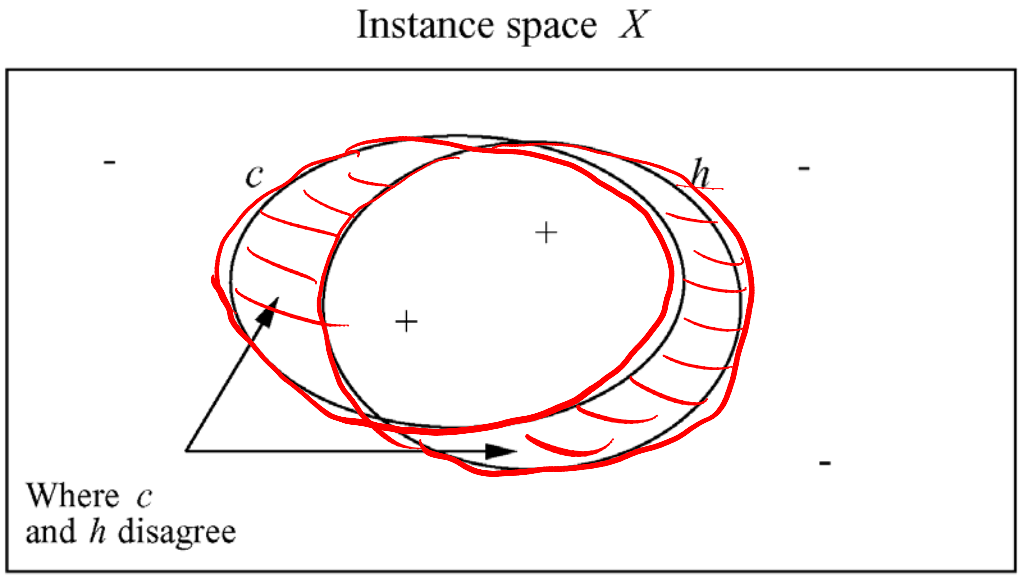
Protocol



- Given:
  - set of examples X
  - fixed (unknown) distribution D over X
  - set of hypotheses H
  - set of possible target concepts C
- Learner observes sample $S = \{ \langle x_i, c(x_i) \rangle \}$
  - instances x_i drawn from distr. D
  - labeled by target concept $c \in C$

  (Learner does NOT know $c(.)$, D)
- Learner outputs $h \in H$ estimating c
  - h is evaluated by performance on subsequent instances drawn from D
- For now:
  - $C = H$ (so $c \in H$)
  - Noise-free data

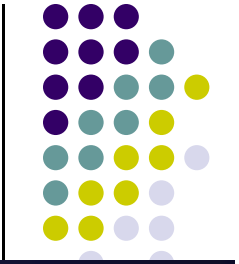
True error of a hypothesis



- Definition: The *true error* (denoted $\varepsilon_D(h)$) of hypothesis h with respect to target concept c and distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

$$\epsilon_{\mathcal{D}}(h) \equiv Pr_{x \in \mathcal{D}}[c(x) \neq h(x)]$$

Two notions of error



- *Training error* (a.k.a., empirical risk or empirical error) of hypothesis h with respect to target concept c
  - How often $h(x) \neq c(x)$ over training instance from $\mathcal{S}$

$$\hat{\epsilon}_{\mathcal{S}}(h) \equiv Pr_{x \in \mathcal{S}}[c(x) \neq h(x)] \equiv \frac{\sum_{x \in \mathcal{S}} \delta(c(x) \neq h(x))}{|\mathcal{S}|}$$

- *True error* of (a.k.a., generalization error, test error) hypothesis *h* with respect to *c*
  - How often $h(x) \neq c(x)$ over future random instances drew iid from $\mathcal{D}$

$$\epsilon_{\mathcal{D}}(h) \equiv Pr_{x \in \mathcal{D}}[c(x) \neq h(x)]$$

Can we bound

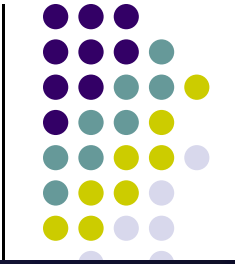
$\hat{\epsilon}_{\mathcal{D}}(h)$

in terms of

$\hat{\epsilon}_{\mathcal{S}}(h)$

??

The Union Bound

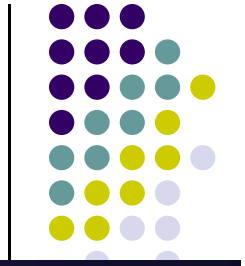


- Lemma. (The union bound). Let A_1;A_2, … , A_k be k different events (that may not be independent). Then

$$P(A_1 \cup A_2 \cup \ldots \cup A_k) \leq P(A_1) + P(A_2) + \ldots + P(A_k)$$

  - In probability theory, the union bound is usually stated as an axiom (and thus we won't try to prove it), but it also makes intuitive sense: The probability of any one of k events happening is at most the sums of the probabilities of the k different events.

Hoeffding inequality



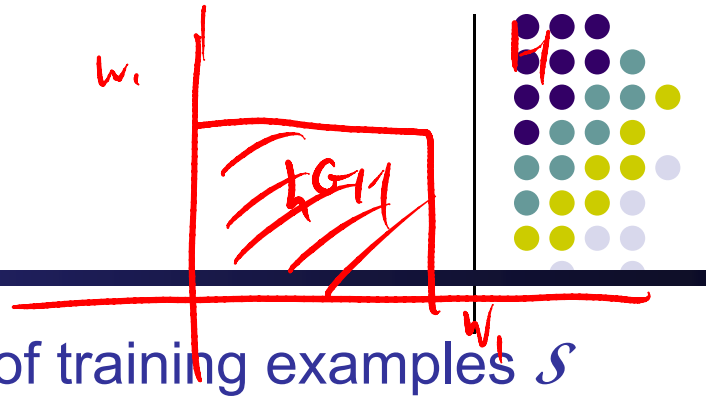
- Lemma. (Hoeding inequality) Let $Z_1,...,Z_m$ be m independent and identically distributed (iid) random variables drawn from a Bernoulli(ϕ) distribution, i.e., $P(Z_i = 1) = \phi$, and $P(Z_i = 0) = 1 - \phi$.

  Let $\hat{\phi} = (1/m)\sum_{i=1}^{m} Z_i$ be the mean of these random variables, and let any $\gamma > 0$ be fixed. Then

$$P(|\phi - \hat{\phi}| > \gamma) \leq 2\exp(-2\gamma^2 m)$$

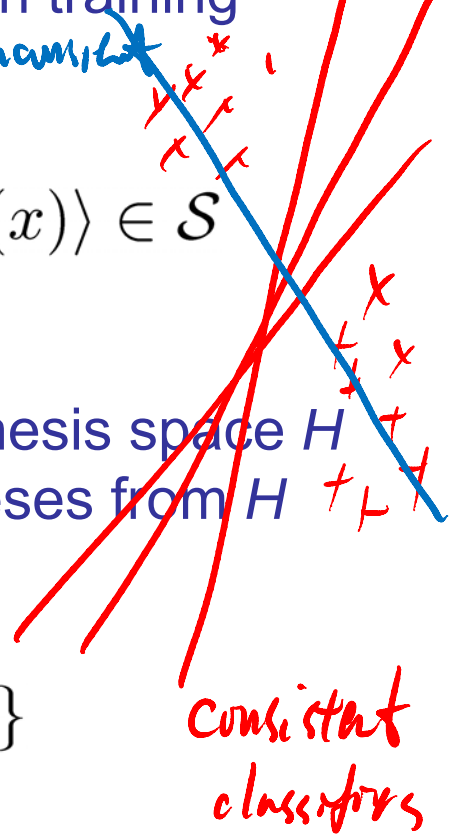
  - This lemma (which in learning theory is also called the Chernoff bound) says that if we take $\hat{\phi}$ — the average of m Bernoulli(ϕ) random variables — to be our estimate of ϕ , then the probability of our being far from the true value is small, so long as m is large.

Version Space



- A hypothesis h is consistent with a set of training examples $\mathcal{S}$ of target concept c if and only if h(x)=c(x) for each training example $\langle x_i, c(x_i) \rangle$ *in* $\mathcal{S}$

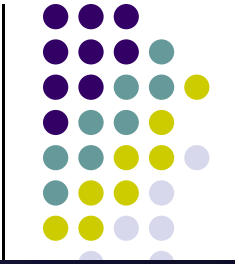
$$Consistent(h, \mathcal{S}) \models \quad h(x) = c(x), \forall \langle x, c(x) \rangle \in \mathcal{S}$$



- The version space, $VS_{H,\mathcal{S}}$, with respect to hypothesis space H and training examples $\mathcal{S}$ is the subset of hypotheses from H consistent with all training examples in $\mathcal{S}$.

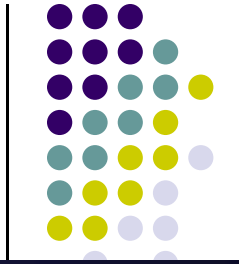
$$VS_{H,\mathcal{S}} \equiv \{h \in H | Consistent(h, \mathcal{S})\}$$

Consistent Learner



- A learner is ***consistent*** if it outputs hypothesis that perfectly fits the training data
  - This is a quite reasonable learning stragety
- Every consistent learning outputs a hypothesis belonging to the version space
- We want to know how such hypothesis generalizes

Probably Approximately Correct



Goal:

PAC-Learner produces hypothesis $\hat{h}$ that

is approximately correct,

$err_D(\hat{h}) \approx 0$

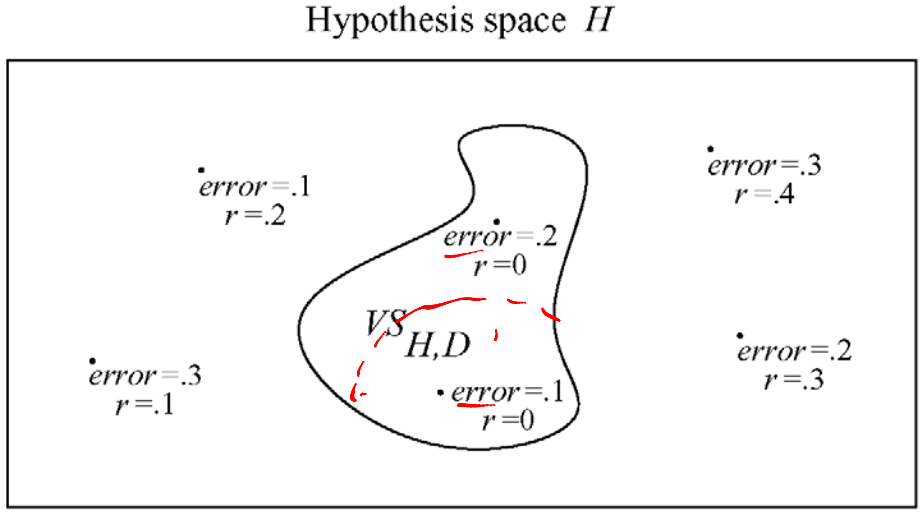
with high probability

$P(\ err_D(\hat{h}) \approx 0\ ) \approx 1$

- Double "hedging"
  - approximately
  - probably

Need both!

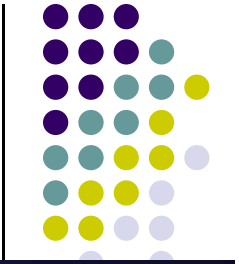
Exhausting the version space



- Definition: The version space $VS_{H,S}$ is said to be ε-exhausted with respect to c and S, if every hypothesis h in $VS_{H,S}$ has **true error** less than ε with respect to c and $\mathcal{D}$.

$$\forall h \in VS_{H,S}, \qquad \hat{\epsilon}_{\mathcal{D}}(h) < \epsilon$$

How many examples will ε-exhaust the VS



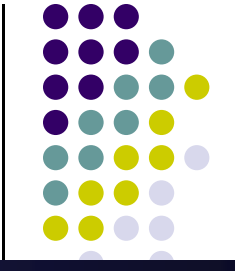
Theorem: [Haussler, 1988].

- If the hypothesis space *H* is finite, and *S* is a sequence of m ≥ 1 independent random examples of some target concept *c*, then for any 0 ≤ ε ≤ 1/2, the probability that the version space with respect to *H* and *S* is **not** ε-exhausted (with respect to *c*) is less than

$$|H|e^{-\epsilon m}$$

- This bounds the probability that any consistent learner will output a hypothesis *h* with ε(*h*) ≥ ε

Proof



From an ϵ-exhausted VS, a consistent learner output $h \in H$

① the prob of h making an error on $x_i \in S$. (① this event did not happen)

i.e.: $p(h(x_i) \neq c(x_i), x_i \in S) > \epsilon$

② then the prob of h not commit a error on $x_i \in S$ (this has happened!!)

i.e.: $p(h(x_i) = c(x_i), x_i \in S) < 1-\epsilon$

③ the prob of h being correct on all examples $x_i \in S$ $\forall i$

$p(h(x_i) = c(x_i) \ \forall i \in S) < (1-\epsilon)^m \approx e^{-m\epsilon}$ (this also happend)

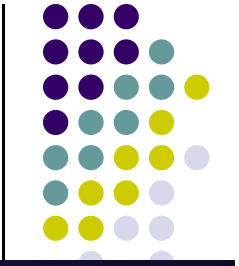
call this event $\{h x_i = c(x_i), \forall i \in S\} \equiv \epsilon_h$

$P(\epsilon_h) \leq e^{-m\epsilon}$ $h \in H$

④ the prob of existing $h \in H$, s.t. ϵ_h is true

$P(\epsilon_{h_1} \vee \epsilon_{h_2} \vee \cdots \vee \epsilon_{h_{|H|}}) \leq \sum_{i=1}^{|H|} P(\epsilon_{h_i}) = \sum_{i=1}^{|H|} e^{-m\epsilon} = |H| e^{-m\epsilon}$

What it means



- [Haussler, 1988]: probability that the version space is not ε-exhausted after *m* training examples is at most $|H|e^{-\varepsilon m}$

$$Pr(\exists h \in H,\ s.t.\ (error_{train}(h) = 0) \wedge (error_{true}(h) > \epsilon)\ ) \leq |H|e^{-\epsilon m}$$

Suppose we want this probability to be at most δ

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

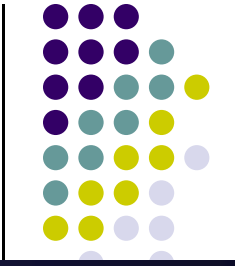
1. How many training examples suffice?

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

2. If $error_{train}(h) = 0$ then with probability at least (1-δ):

$$error_{true} \leq \frac{1}{m}(\ln|H| + \ln(1/\delta))$$

Learning Conjunctions of Boolean Literals



- How many examples are sufficient to assure with probability at least (1 - δ) that

  every h in $VS_{H,S}$ satisfies $\varepsilon_{\mathcal{D}}(h) \leq \varepsilon$

- Use our theorem:

$$m \geq \frac{1}{\varepsilon}(\ln|H| + \ln(1/\delta))$$

- Suppose H contains conjunctions of constraints on up to n boolean attributes (i.e., n boolean literals).

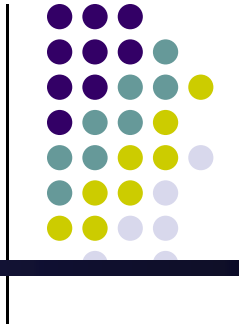
  Then $|H| = 3^n$, and

$$m \geq \frac{1}{\varepsilon}(\ln 3^n + \ln(1/\delta))$$

or

$$m \geq \frac{1}{\varepsilon}(n \ln 3 + \ln(1/\delta))$$

PAC Learnability

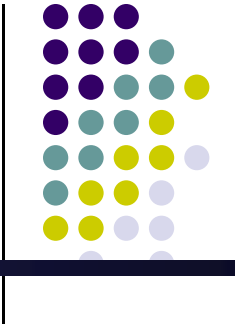


A learning algorithm is PAC learnable if it

- Requires no more than polynomial computation per training example, and
- no more than polynomial number of samples

Theorem: conjunctions of Boolean literals is PAC learnable

How about *EnjoySport*?



$$m \geq \frac{1}{\varepsilon}(\ln|H| + \ln(1/\delta))$$

- If H is as given in *EnjoySport* then $|H| = 729$, and

$$m \geq \frac{1}{\varepsilon}(\ln 729 + \ln(1/\delta))$$

- if want to assure that with probability 95%, *VS* contains only hypotheses with $\varepsilon_S(h) \leq .1$, then it is sufficient to have m examples, where

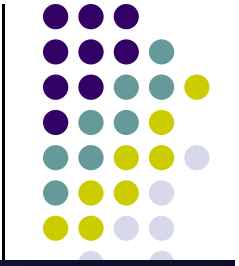
$$m \geq \frac{1}{.1}(\ln 729 + \ln(1/.05))$$

$$m \geq 10(\ln 729 + \ln 20)$$

$$m \geq 10(6.59 + 3.00)$$

$$m \geq 95.9$$

PAC-Learning



- Learner L can draw labeled instance $\langle x, c(x) \rangle$ in unit time, $x \in X$ of length *n* drawn from distribution $\mathcal{D}$, labeled by target concept $c \in C$

Def'n: Learner L PAC-learns class C using hypothesis space H

if

1. for any target concept $c \in C$,

   any distribution $\mathcal{D}$, any ε such that $0 < \varepsilon < 1/2$, δ such that $0 < \delta < 1/2$,

   L returns $h \in H$ s.t.

   w/ prob. $\geq 1 - \delta$, $\quad err_D(h) < \varepsilon$

2. L's run-time (and hence, sample complexity)

   is poly(|x|, size(c), $1/\varepsilon$, $1/\delta$)

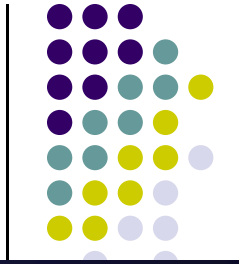
- Sufficient:

  1. Only poly(…) training instances – $|H| = 2^{poly()}$
  2. Only poly time / instance …

  Often C = H

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

Agnostic Learning



So far, assumed $c \in H$

Agnostic learning setting: don't assume $c \in H$

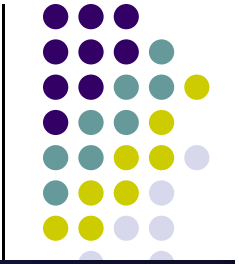
- What do we want then?
  - The hypothesis *h* that makes fewest errors on training data
- What is sample complexity in this case?

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

derived from Hoeffding bounds:

$$\Pr[error_D(h) > error_S(h) + \varepsilon] \leq e^{-2m\varepsilon^2}$$

Empirical Risk Minimization Paradigm



- Choose a *Hypothesis Class* H of subsets of X.
- For an input sample S, find some h in H that fits S "well".
- For a new point x, predict a label according to its membership in h.

$$\hat{h} = \arg\min_{h \in H} \hat{\epsilon}_S(h)$$

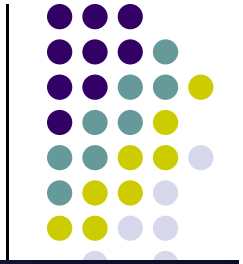
- Example:
  - Consider linear classification, and let $h_\theta(x) = 1\{\theta^T x \geq 0\}$

    Then $H = \{h_\theta \ : \ h_\theta(x) = 1\{\theta^T x \geq 0\}, \ \theta \in R^{n+1}\}$

$$\hat{\theta} = \arg\min_\theta \hat{\epsilon}_S(h_\theta)$$

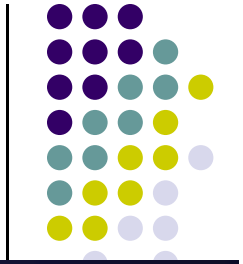
  - We think of ERM as the most "basic" learning algorithm, and it will be this algorithm that we focus on in the remaining.
  - In our study of learning theory, it will be useful to abstract away from the specific parameterization of hypotheses and from issues such as whether we're using a linear classier or an ANN

The Case of Finite H



- H = $\{h_1, \ldots, h_k\}$ consisting of k hypotheses.
- We would like to give guarantees on the generalization error of $\hat{h}$.
- First, we will show that $\hat{\epsilon}(h)$ is a reliable estimate of $\varepsilon(h)$ for all h.
- Second, we will show that this implies an upper-bound on the generalization error of $\hat{h}$.

Misclassification Probability



- The outcome of a binary classifier can be viewed as a Bernoulli random variable Z : $Z = 1\{h_i(x) \neq c(x)\}$

- For each sample: $Z_j = 1\{h_i(x_j) \neq c(x_j)\}$

$$\hat{\epsilon}(h_i) = \frac{1}{m}\sum_{j=1}^{m} Z_j$$

- Hoeffding inequality

$$P(|\epsilon(h_i) - \hat{\epsilon}(h_i)| > \gamma) \leq 2\exp(-2\gamma^2 m)$$

  - This shows that, for our particular h_i, training error will be close to generalization error with high probability, assuming m is large.

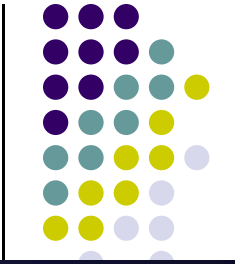
Uniform Convergence

- But we don't just want to guarantee that $\hat{\epsilon}(h_i)$ will be close $\epsilon(h_i)$ (with high probability) for just only one particular h_i. We want to prove that this will be true simultaneously for all $h_i \in H$
- For k hypothesis:

$$\begin{aligned} P(\exists h \in H,\ |\epsilon(h_i) - \hat{\epsilon}(h_i)| > \gamma) &= P(A_1 \cup \ldots \cup A_k) \\ &< \sum_{i=1}^{k} P(A_i) \\ &= \sum_{i=1}^{k} 2\exp(-2\gamma^2 m) \\ &= 2k\exp(-2\gamma^2 m) \end{aligned}$$

- This means:

$$\begin{aligned} P(\neg\exists h \in H,\ |\epsilon(h_i) - \hat{\epsilon}(h_i)| > \gamma) &= P(\forall h \in H,\ |\epsilon(h_i) - \hat{\epsilon}(h_i)| \leq \gamma) \\ &= 1 - 2k\exp(-2\gamma^2 m) \end{aligned}$$



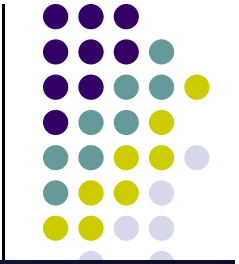
- In the discussion above, what we did was, for particular values of m and γ, given a bound on the probability that:

  for some $h_i \in H$

$$|\epsilon(h_i) - \hat{\epsilon}(h_i)| > \gamma$$

- There are three quantities of interest here: m and γ, and probability of error; we can bound either one in terms of the other two.

Sample Complexity



- How many training examples we need in order make a guarantee?

$$P(\exists h \in H,\ |\epsilon(h) - \hat{\epsilon}(h)| > \gamma) \quad = \quad 2k \exp(-2\gamma^2 m)$$

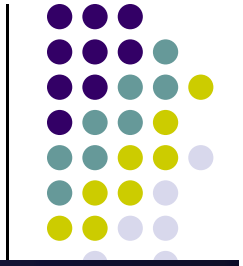
- We find that if

$$m \geq \frac{1}{2\gamma^2} \log \frac{2k}{\delta}$$

then with probability at least $1\text{-}\delta$, we have that $|\epsilon(h_i) - \hat{\epsilon}(h_i)| \leq \gamma$ for all $h_i \in H$

- The key property of the bound above is that the number of training examples needed to make this guarantee is only logarithmic in k, the number of hypotheses in H. This will be important later.

Generalization Error Bound



- Similarly, we can also hold m and δ fixed and solve for γ in the previous equation, and show [again, convince yourself that this is right!] that with probability 1- δ , we have that for all $h_i \in H$

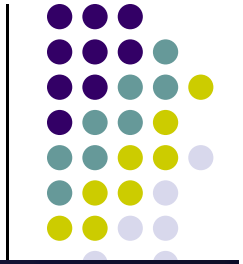
$$|\hat{\epsilon}(h) - \epsilon(h)| \leq \sqrt{\frac{1}{m} \log \frac{2k}{\delta}}$$

- Define $h^* = \arg\min_{h \in H} \epsilon(h)$ to be the best possible hypothesis in H.

$$\begin{aligned} \epsilon(\hat{h}) &\leq \hat{\epsilon}(\hat{h}) + \gamma \\ &\leq \hat{\epsilon}(\hat{h}^*) + \gamma \\ &\leq \epsilon(\hat{h}^*) + 2\gamma \end{aligned}$$

  - If uniform convergence occurs, then the generalization error of $\hat{\epsilon}(h)$ is at most 2γ worse than the best possible hypothesis in H!

Summary



Theorem. Let $|\mathcal{H}| = k$, and let any m, δ be fixed. Then with probability at least $1 - \delta$, we have that

$$\varepsilon(\hat{h}) \leq \left(\min_{h \in \mathcal{H}} \varepsilon(h) \right) + 2\sqrt{\frac{1}{2m} \log \frac{2k}{\delta}}.$$

Corollary. Let $|\mathcal{H}| = k$, and let any δ, γ be fixed. Then for $\varepsilon(\hat{h}) \leq \min_{h \in \mathcal{H}} \varepsilon(h) + 2\gamma$ to hold with probability at least $1 - \delta$, it suffices that

$$\begin{aligned} m &\geq \frac{1}{2\gamma^2} \log \frac{2k}{\delta} \\ &= O\left(\frac{1}{\gamma^2} \log \frac{k}{\delta} \right), \end{aligned}$$