Computational Learning Theory

Reading: Andrew’s lecture notes Part VI Learning theory
《机器学习》Chap. 12

Generalizability of Learning

- In machine learning it's really the 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?
- Are there conditions under which we can actually prove that learning algorithms will work well?

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?
- What 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

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

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)*

Probably Approximately Correct

- Goal:
  - PAC-Learner produces hypothesis $\hat{h}$

    that is approximately correct

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

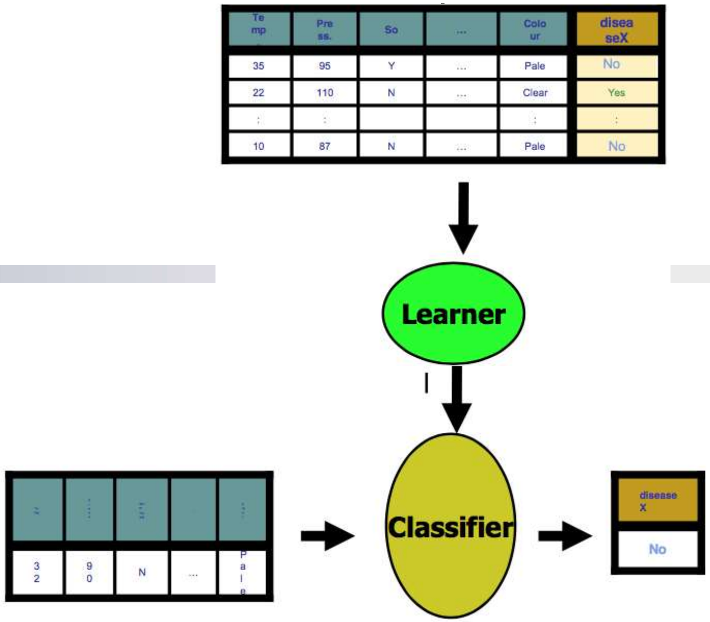
    with high probability

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

- Double "hedging"
  - approximately
  - probably

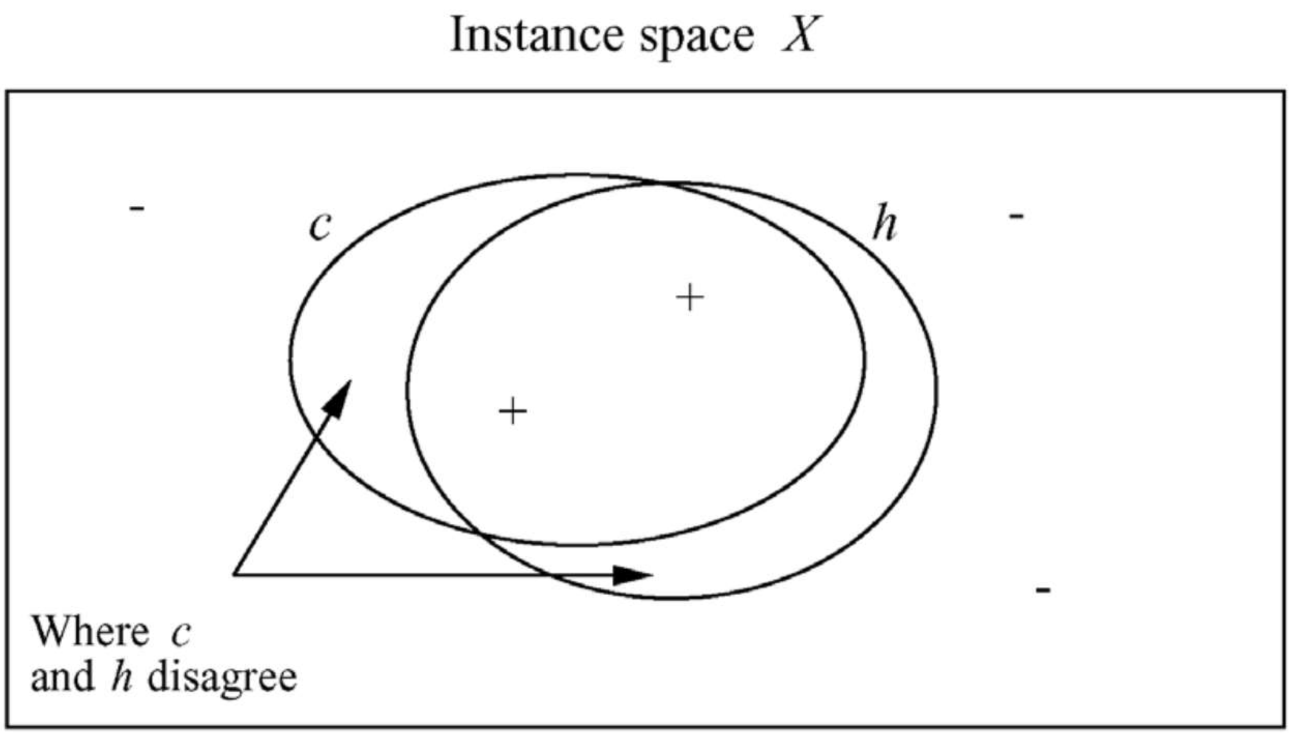
Need both !

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 = { $< x^{(i)}, c(x^{(i)}) >$ }
  - instances $x^{(i)}$ drawn from distribution D
  - labeled by target concept c $\in$ C
- 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 to target concept c and distribution D is the probability that h will misclassify an instance drawn at random according to D.

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

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 S

符号函数

$$\hat{\varepsilon}_S(h) \equiv Pr_{x \in S}[c(x) \neq h(x)] \equiv \frac{\sum_{x \in S} \boxed{\delta}(c(x) \neq h(x))}{|S|}$$

- 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 i.i.d. from D

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

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

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

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

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

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

- 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 S of target concept c if and only if h(x) = c(x) for each training example $< x^{(i)},\ c(x^{(i)}) >$ in S

$$Consistent(h, S) \models \quad h(x) = c(x),\ \forall < x, c(x) > \in S$$

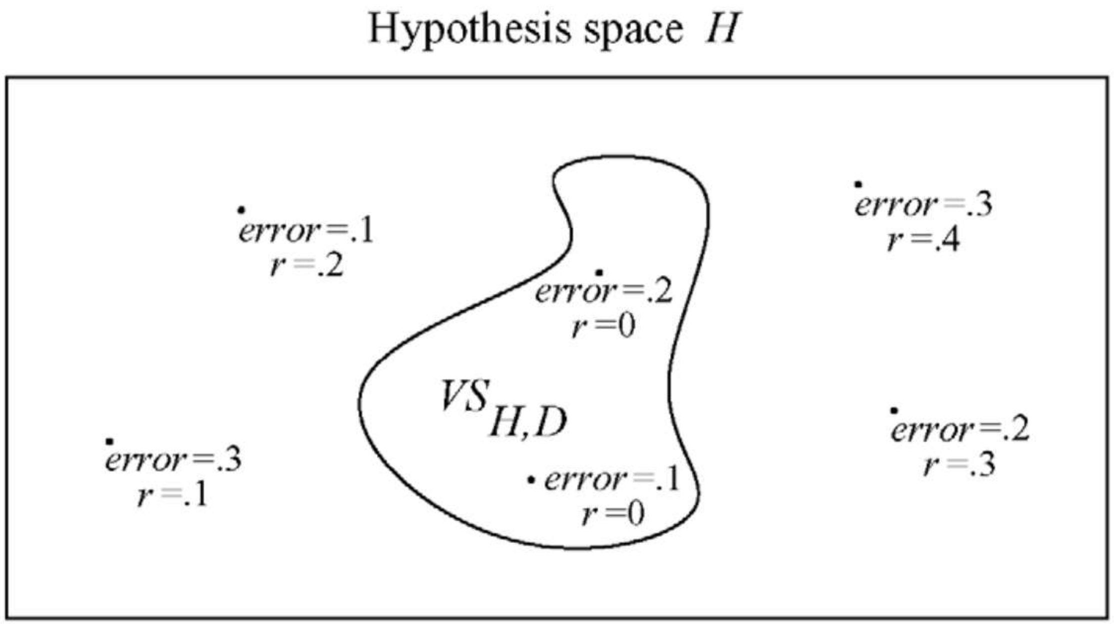
- The version space, $VS_{H,S}$, with respect to hypothesis space H and training examples S is the subset of hypotheses from H consistent with all training examples in S.

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

Consistent Learner

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

Exhausting the Version Space



$(r = \text{training error}, \ error = \text{true error})$

- 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 D.

$$\forall h \in VS_{H,S}, \qquad \hat{\varepsilon}_D(h) < \varepsilon$$

How Many Examples Will ε-exhaust the VS

- Theorem: [Haussler, 1988].
  - If the hypothesis space H is finite, and S is a sequence of $m \geq 1$ independent random examples of some target concept c, then for ANY $0 \leq \varepsilon \leq 1/2$, the probability that the version space with respect to H and S is not ε-exhausted (with respect to c) is less than

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

  - This bounds the probability that any consistent learner will output a hypothesis h with $\varepsilon(h) \geq \varepsilon$

What It Means

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

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

Suppose we want this probability to be at most δ

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

1. How many training examples suffice ? $m \geq \frac{1}{\varepsilon}\left(ln|H| + ln(\frac{1}{\delta})\right)$

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

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

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

PAC-Learning

- Learner L can draw labeled instance <x, c(x)> in unit time, $x \in X$ of length n drawn from distribution 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 D,
   any ε such that 0 < ε < 1/2, δ such that 0 < δ < 1/2,
   L returns $h \in H$ s.t. w/ prob. ≥ 1 - δ $err_D(h) < \varepsilon$
2. L's run-time (and hence, sample complexity)
   is $poly(|x|, size(c), 1/\varepsilon, 1/\delta)$

- Sufficient:

1. Only poly(…) training instances — $|H| = 2^{poly()}$ $m \geq \frac{1}{\varepsilon}\left(ln|H| + ln(\frac{1}{\delta})\right)$
2. Only poly(…) time per instance …

Often C = H

Example 1:

If |H| = 973, and

$$m \geq \frac{1}{\epsilon}(\ln 973 + \ln\left(\frac{1}{\delta}\right))$$

If want to assure that with probability 95%, *VS* contains only hypotheses with $\text{error}_{D(h)} \leq 0.1$, then it is sufficient to have *m* examples, where

- $m \geq (1/\ 0.1)(\ln 973+\ln(1/0.05))$

  $= 10(\ln 973+\ln 20) = 10(6.88+3.00) = 98.8$

Example 2: Learning conjunctions of boolean literals

- Let H be the hypothesis space defined by conjunctions of literals based on n boolean attributes possibly with negation

- Question: How many examples are sufficient to assure with probability of at least $(1 - \delta)$ that every h in $VS_{H,D}$ satisfies $error_{D(h)} \leq \epsilon$?

- Answer: $|H| = 3^n$, and using our theorem it follows that

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

Agnostic Learning

- So far, assumed c ∈ H
- Agnostic learning setting: don't assume c ∈ H

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

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

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

$$\hat{h} = argmin_{h \in H} \ \hat{\varepsilon}_S(h)$$

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

$$\hat{\theta} = argmin_\theta \ \hat{\varepsilon}_S(h_\theta)$$

  - We think of ERM as the most "basic" learning algorithm, and it will be this algorithm that we focus on in the remaining.
  - In out 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 classifier 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 $\hat{\varepsilon}(h)$ 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: $Z_j = 1\{h_i(x^{(j)}) \neq c(x^{(j)})\}$

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

- Hoeffding inequality

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

  - 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 $\hat{\varepsilon}(h_i)$ will be close to $\varepsilon(h_i)$ (with high probability) for just only one particular h_i. We want to prove that this will be true for simultaneously for all $h_i \in H$

- For k hypothesis:

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

- This means:

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

Uniform Convergence, cont.

- In the discussion above, what we did was, for particular values of m and γ, given a bound on the probability that for some $h_i \in H$

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

- 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 to make a guarantee ?

$$P(\exists h \in H,\ |\varepsilon(h) - \hat{\varepsilon}(h)| > \gamma) \leq 2ke^{-2\gamma^2 m}$$

- We find that if $m \geq \frac{1}{2\gamma^2} \, log \frac{2k}{\delta}$

  then with probability at least 1- δ, we have that $\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma$ 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.

Example: Conjunctions of Boolean Literals

- Let H be the space of all pure conjunctive formulae over n Boolean attributes.
- Recall, $|H|=3^n$
- From the previous result, we get:

$$m \geq \frac{1}{2\varepsilon^2} \ln \frac{2|H|}{\delta} = n \frac{1}{2\varepsilon^2} \ln \frac{6}{\delta}$$

- This is linear in n!

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 $h_i \in H$

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

- Define $h^* = argmin_{h \in H} \; \varepsilon(h)$ to be the best possible hypothesis in H.

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

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

Summary

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

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

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

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

What If H is Not Finite ?

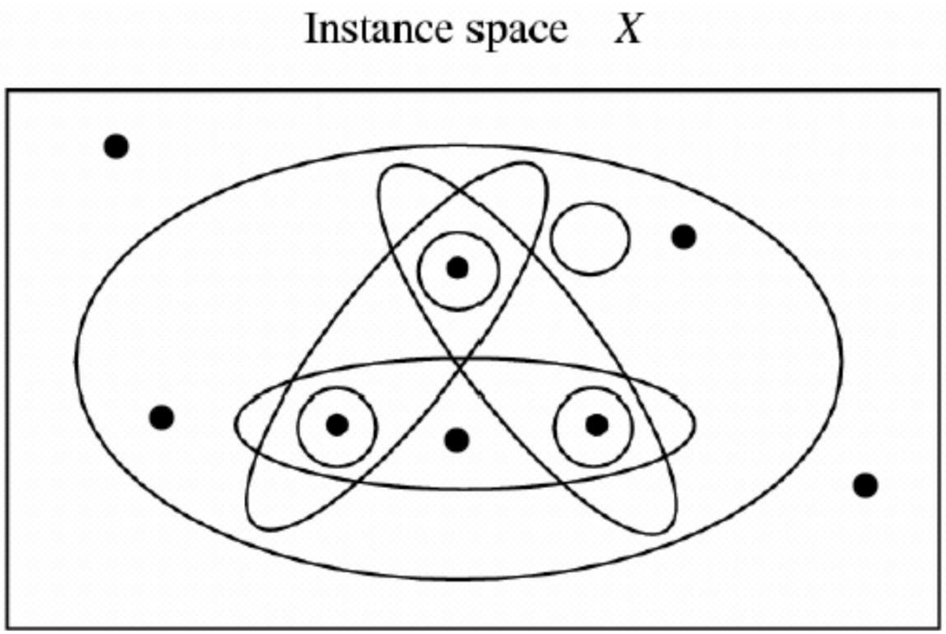
- Can’t use our result for infinite H
- Need some other measure of complexity for H — Vapnik-Chervonenkis (VC) dimension !

How do we characterize "power"?

- Different machines have different amounts of "power"
- Tradeoff between:
  - More power: Can model more complex classifiers but might overfit
  - Less power: Not going to overfit, but restricted in what it can model
- How do we characterize the amount of power ?

The Vapnik-Chervonenkis Dimension

- Definition: The Vapnik-Chervonenkis dimension, VC(H), of hypothesis space H defined over instance space X is the size of the largest finite subset of X shattered by H. If arbitrarily large finite sets of X can be shattered by H, then VC(H) $\equiv \infty$.



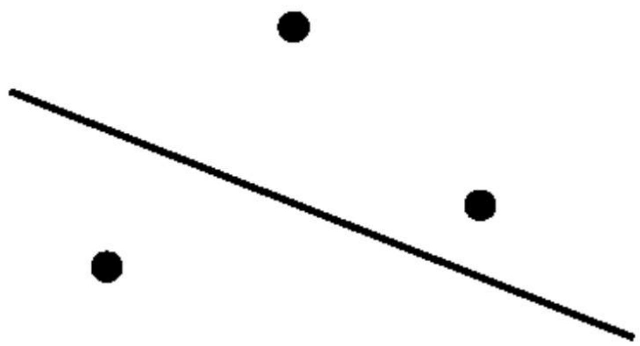
Definition:

Given a set $S = \{x(1), \ldots, x(d)\}$ of points $x(i) \in X$, we say that H shatters S if H can realize any labeling on S.

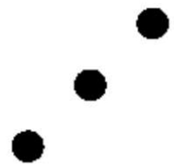
VC Dimension: Examples

- Consider $X = R^2$, want to learn c: X -> {0, 1}

  - What is VC dimension of lines in a plane ?
    H = { ((wx+b)>0 -> y=1) }

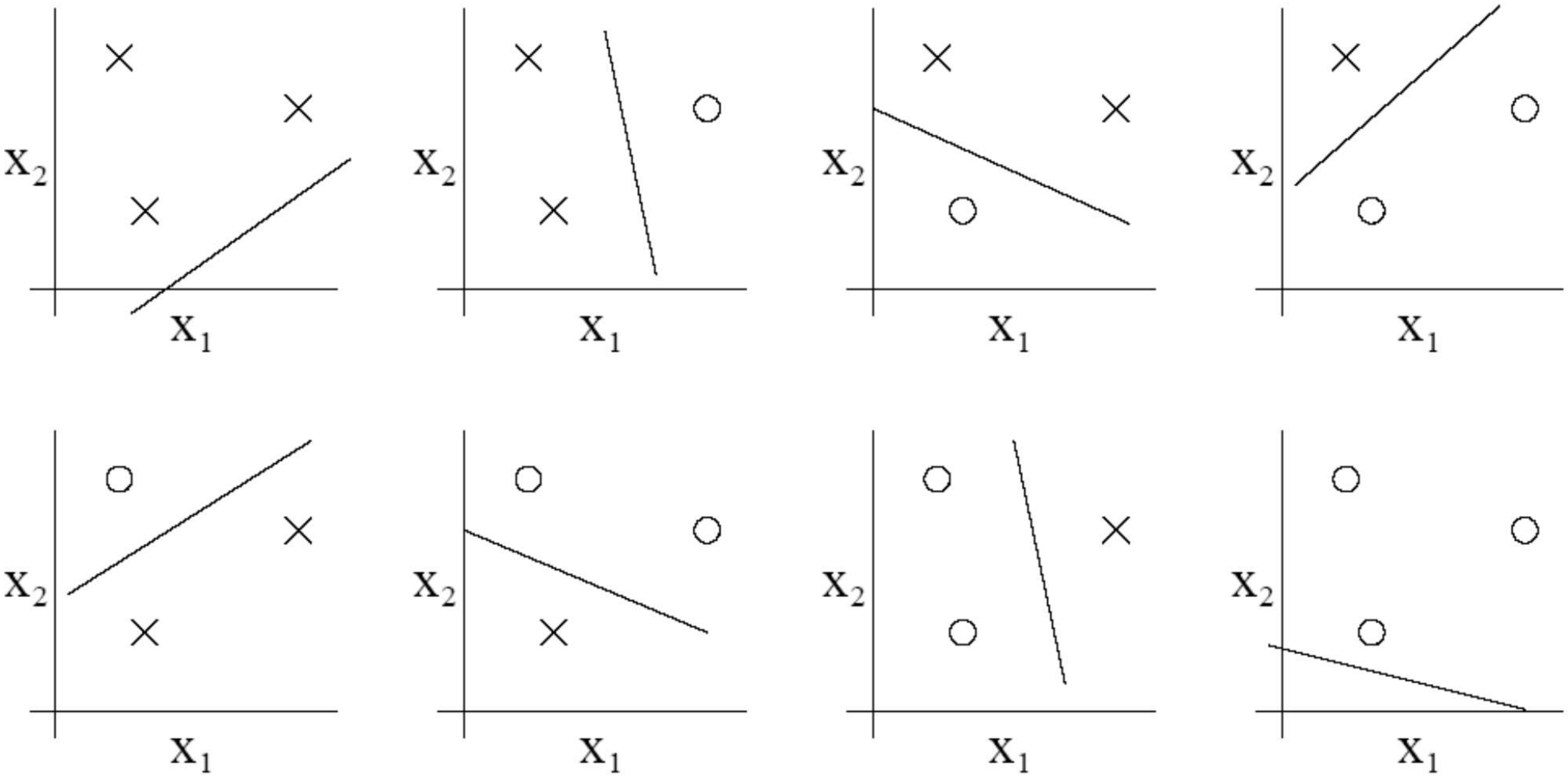


(a)



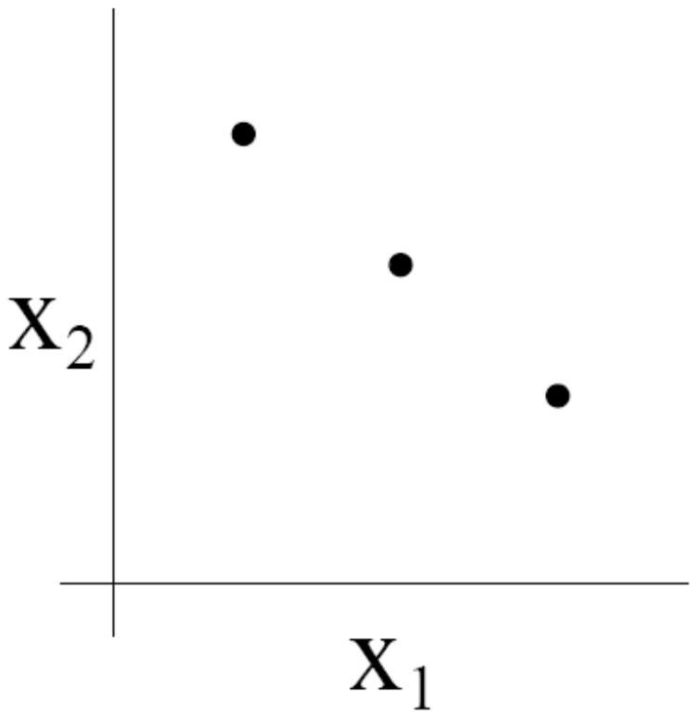
(b)

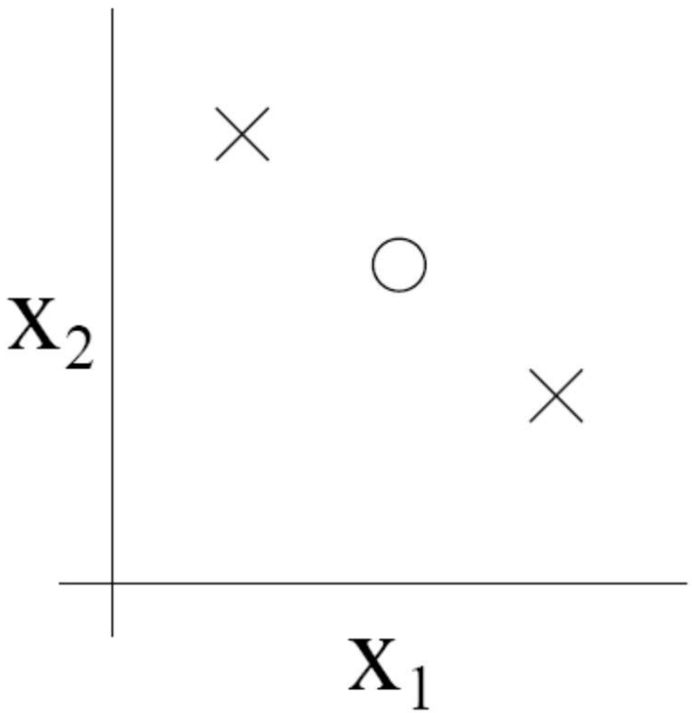
VC Dimension: Examples



- For any of the eight possible labeling of these points, we can find a linear classifier that obtains "zero training error" on them.
- Moreover, it is possible to show that there is no set of 4 points that this hypothesis class can shatter.

VC Dimension: Examples





- The VC dimension of H here is 3 even though there may be sets of size 3 that it cannot shatter.
- Under the definition of the VC dimension, in order to prove that VC(H) is at least d, we need to show only that there is at least one set of size d that H can shatter.

- **Theorem**: Consider some set of m points in R^n. Choose any one of the points as origin. Then the m points can be shattered by oriented hyperplanes if and only if the position vectors of the remaining points are linearly independent.

- **Corollary**: The VC dimension of the set of oriented hyperplanes in R^n is n+1.

  Proof: we can always choose n + 1 points, and then choose one of the points as origin, such that the position vectors of the remaining n points are linearly independent, but can never choose n + 2 such points (since no n + 1 vectors in R^n can be linearly independent).

Example: Shattering a circle

- Let H be the set of circles in 2-D such that h(x)=1 iff x is inside the circle.

- How many points can be shattered by H?

3

The VC Dimension and the Number of Parameters

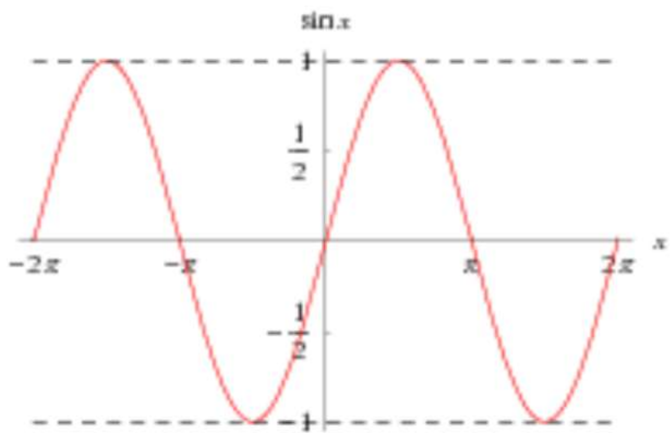
- The VC dimension thus gives concreteness to the notion of the capacity of a given set of h.

- Is it true that learning machines with many parameters would have high VC dimension, while learning machines with few parameters would have low VC dimension ?

An infinite-VC function with just one parameter !

$$f(x,\alpha) \equiv \theta(sin(\alpha x)), \quad x, \alpha \in R$$

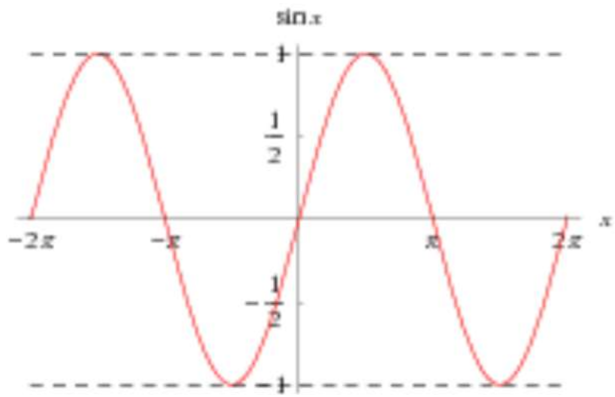
where θ is an indicator function



An Infinite-VC Function with Just One Parameter

- You choose some number *l*, and present me with the task of finding *l* points that can be shattered. I choose them to be

$$x_i = 10^{-i} \quad i = 1, \ldots, l,$$



- You specify any labels you like:

$$y_1, y_2, \ldots, y_l, \quad y_i \in \{-1, 1\}$$

- Then $f(\alpha)$ gives this labeling if I choose α to be

$$\alpha = \pi\left(1 + \sum_{i=1}^{l} \frac{(1-y_i)10^i}{2}\right)$$

- Thus the VC dimension of this machine is infinite.

Sample Complexity from VC Dimension

- How many randomly drawn examples suffice to ε-exhaust $VS_{H,S}$ with probability at least 1 - δ ?

i.e., to guarantee that any hypothesis that perfectly fits the training data is probably 1 - δ approximately (ε) correct on testing data from the same distribution

$$m \geq \frac{1}{\varepsilon}\left(4log_2\frac{2}{\delta} + 8VC(H)log_2\frac{13}{\varepsilon}\right)$$

Compare to our earlier results based on |H|:

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

What You Should Know

- Sample complexity varies with the learning setting
  - Learner actively queries trainer
  - Examples provided at random
- Within the PAC learning setting, we can bound the probability that learner will output hypothesis with given error
  - For ANY consistent learner (case where c in H)
  - For ANY “best fit” hypothesis (agnostic learning, where perhaps c not in H
- VC dimension as measure of complexity of H