Machine Learning

Lecture 3
Computational Learning Theory

Based on lecture of
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Learning Theory

- Theorems that characterize classes of learning problems or specific algorithms in terms of computational complexity or ***sample complexity***, i.e. the number of training examples necessary or sufficient to learn hypotheses of a given accuracy.
- Complexity of a learning problem depends on:
  - Size or expressiveness of the hypothesis space.
  - Accuracy to which target concept must be approximated.
  - Probability with which the learner must produce a successful hypothesis.
  - Manner in which training examples are presented, e.g. randomly or by query to an oracle.

Types of Results

- **Learning in the limit**: Is the learner guaranteed to converge to the correct hypothesis in the limit as the number of training examples increases indefinitely?
- **Sample Complexity**: How many training examples are needed for a learner to construct (with high probability) a highly accurate concept?
- **Computational Complexity**: How much computational resources (time and space) are needed for a learner to construct (with high probability) a highly accurate concept?
  - High sample complexity implies high computational complexity, since learner at least needs to read the input data.
- **Mistake Bound**: Learning incrementally, how many training examples will the learner misclassify before constructing a highly accurate concept.

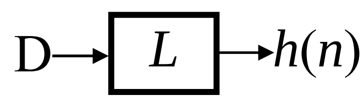
Learning in the Limit

- Given a continuous stream of examples where the learner predicts whether each one is a member of the concept or not and is then is told the correct answer, does the learner eventually converge to a correct concept and never make a mistake again.
- No limit on the number of examples required or computational demands, but must eventually learn the concept exactly, although do not need to explicitly recognize this convergence point.
- By simple enumeration, concepts from any known finite hypothesis space are learnable in the limit, although typically requires an exponential (or doubly exponential) number of examples and time.
- Class of total recursive (Turing computable) functions is not learnable in the limit.

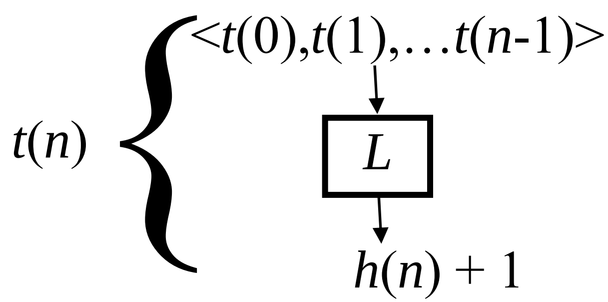
Unlearnable Problem

- Identify the function underlying an ordered sequence of natural numbers ($t:\mathcal{N}\rightarrow\mathcal{N}$), guessing the next number in the sequence and then being told the correct value.
- For any given learning algorithm *L*, there exists a function *t*(*n*) that it cannot learn in the limit.

Given the learning algorithm *L* as a Turing machine:



Construct a function it cannot learn:



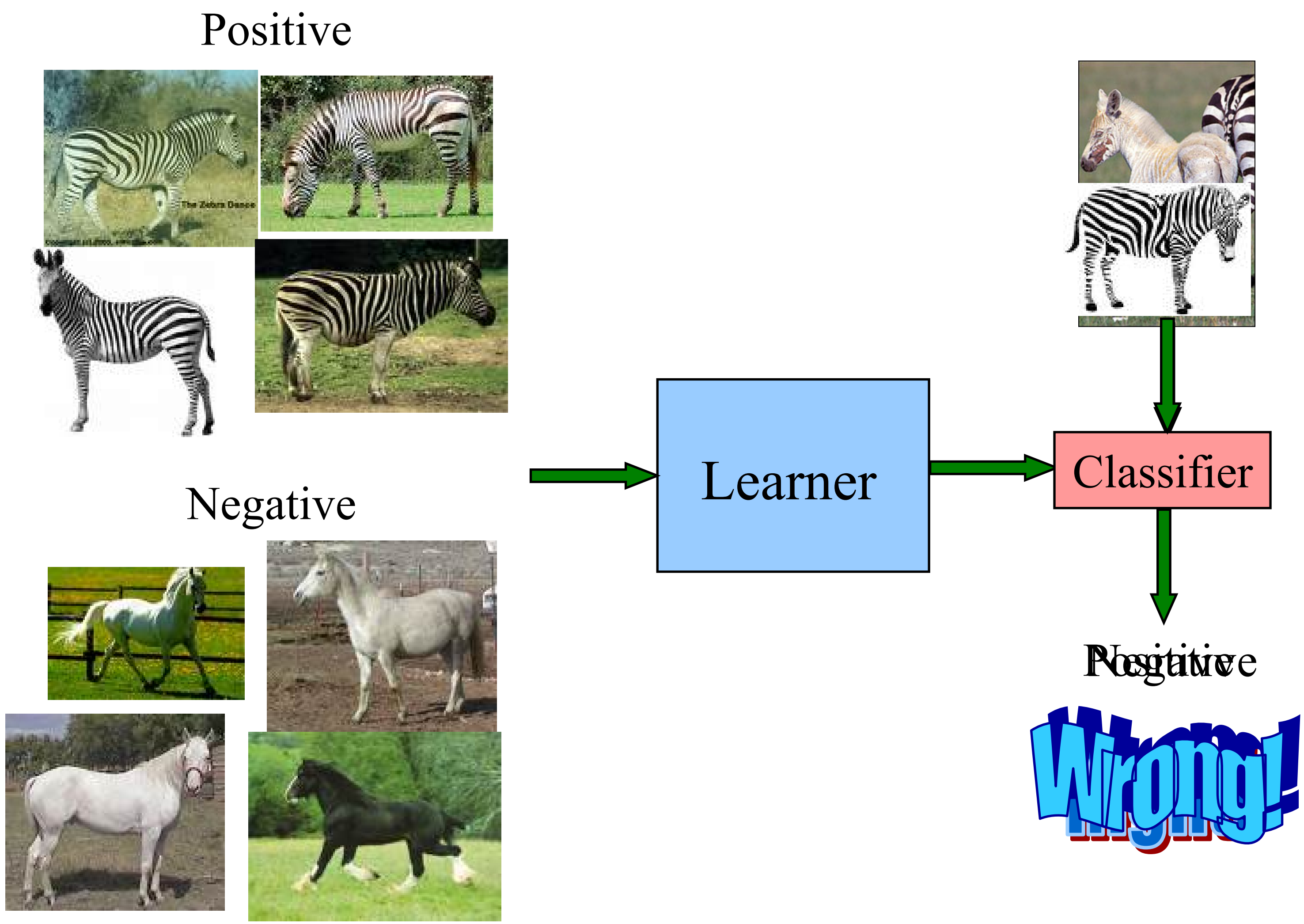
Example Trace

Oracle:	1	3	6	11	…..
Learner:	0	2	5	10	
h:	natural	pos int	odd int	$h(n)=h(n-1)+n+1$	

Learning in the Limit vs. PAC Model

- Learning in the limit model is too strong.
  - Requires learning correct exact concept
- Learning in the limit model is too weak
  - Allows unlimited data and computational resources.
- PAC Model
  - Only requires learning a ***Probably Approximately Correct*** Concept: Learn a decent approximation most of the time.
  - Requires polynomial sample complexity and computational complexity.

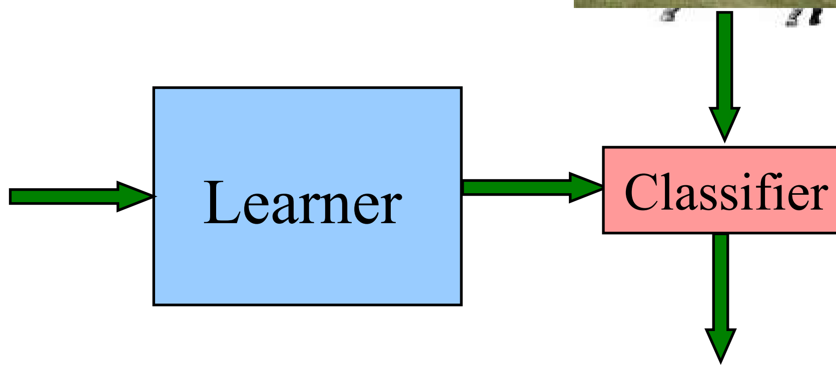
Cannot Learn Exact Concepts from Limited Data, Only Approximations



Cannot Learn Even Approximate Concepts from Pathological Training Sets

Positive

Negative



Positive
Negative

Wrong!

PAC Learning

- The only reasonable expectation of a learner is that with ***high probability*** it learns a ***close approximation*** to the target concept.
- In the PAC model, we specify two small parameters, ε and δ, and require that with probability at least (1 – δ) a system learn a concept with error at most ε.

Formal Definition of PAC-Learnable

- Consider a concept class C defined over an instance space X containing instances of length n, and a learner, L, using a hypothesis space, H. C is said to be ***PAC-learnable*** by L using H iff for all $c \in C$, distributions D over X, $0<\varepsilon<0.5$, $0<\delta<0.5$; learner L by sampling random examples from distribution D, will with probability at least $1-\delta$ output a hypothesis $h \in H$ such that $\text{error}_D(\text{h}) \leq \varepsilon$, in time polynomial in $1/\varepsilon$, $1/\delta$, n and size(c).
- Example:
  - *X*: instances described by *n* binary features
  - *C*: conjunctive descriptions over these features
  - *H*: conjunctive descriptions over these features
  - *L*: most-specific conjunctive generalization algorithm (Find-S)
  - *size(c)*: the number of literals in *c* (i.e. length of the conjunction).

Issues of PAC Learnability

- The computational limitation also imposes a polynomial constraint on the training set size, since a learner can process at most polynomial data in polynomial time.
- How to prove PAC learnability:
  - First prove sample complexity of learning C using H is polynomial.
  - Second prove that the learner can train on a polynomial-sized data set in polynomial time.
- To be PAC-learnable, there must be a hypothesis in H with arbitrarily small error for every concept in C, generally $C \subseteq H$.

Consistent Learners

- A learner *L* using a hypothesis *H* and training data *D* is said to be a consistent learner if it always outputs a hypothesis with zero error on *D* whenever *H* contains such a hypothesis.
- By definition, a consistent learner must produce a hypothesis in the version space for *H* given *D*.
- Therefore, to bound the number of examples needed by a consistent learner, we just need to bound the number of examples needed to ensure that the version-space contains no hypotheses with unacceptably high error.

ε-Exhausted Version Space

- The version space, $VS_{H,D}$, is said to be ***ε-exhausted*** iff every hypothesis in it has true error less than or equal to ε.
- In other words, there are enough training examples to guarantee than any consistent hypothesis has error at most ε.
- One can never be sure that the version-space is ε-exhausted, but one can bound the probability that it is not.
- **Theorem 7.1** (Haussler, 1988): If the hypothesis space *H* is finite, and *D* is a sequence of $m \geq 1$ independent random examples for some target concept *c*, then for any $0 \leq \varepsilon \leq 1$, the probability that the version space $VS_{H,D}$ is ***not*** ε-exhausted is less than or equal to:

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

Proof

- Let $H_{\text{bad}}=\{h_1,\ldots h_k\}$ be the subset of H with error > ε. The VS is not ε-exhausted if any of these are consistent with all *m* examples.
- A single $h_i \in H_{\text{bad}}$ is consistent with ***one*** example with probability:

$$P(\text{consist}(h_i, e_i)) \leq (1-\varepsilon)$$

- A single $h_i \in H_{\text{bad}}$ is consistent with ***all*** *m* independent random examples with probability:

$$P(\text{consist}(h_i, D)) \leq (1-\varepsilon)^m$$

- The probability that ***any*** $h_i \in H_{\text{bad}}$ is consistent with all *m* examples is:

$$P(\text{consist}(H_{bad}, D)) = P(\text{consist}(h_1, D) \vee \cdots \vee \text{consist}(h_k, D))$$

Proof (cont.)

- Since the probability of a disjunction of events is ***at most*** the sum of the probabilities of the individual events:

$$P(\text{consist}(H_{bad}, D)) \leq |H_{bad}|(1-\varepsilon)^m$$

- Since: $|H_{\text{bad}}| \leq |H|$ and $(1-\varepsilon)^m \leq e^{-\varepsilon m}$, $0 \leq \varepsilon \leq 1$, $m \geq 0$

$$P(\text{consist}(H_{bad}, D)) \leq |H| e^{-\varepsilon m}$$

Q.E.D

Sample Complexity Analysis

- Let δ be an upper bound on the probability of ***not*** exhausting the version space. So:

$$P(\text{consist}(H_{bad}, D)) \leq |H| e^{-\varepsilon m} \leq \delta$$

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

$$-\varepsilon m \leq \ln(\frac{\delta}{|H|})$$

$$m \geq \left(-\ln \frac{\delta}{|H|}\right) / \varepsilon \quad \text{(flip inequality)}$$

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

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

Sample Complexity Result

- Therefore, any consistent learner, given at least:

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

examples will produce a result that is PAC.
- Just need to determine the size of a hypothesis space to instantiate this result for learning specific classes of concepts.
- This gives a ***sufficient*** number of examples for PAC learning, but ***not*** a ***necessary*** number. Several approximations like that used to bound the probability of a disjunction make this a gross over-estimate in practice.

Sample Complexity of Conjunction Learning

- Consider conjunctions over n boolean features. There are 3^n of these since each feature can appear positively, appear negatively, or not appear in a given conjunction. Therefore $|H|= 3^n$, so a sufficient number of examples to learn a PAC concept is:

$$\left(\ln\frac{1}{\delta}+\ln 3^n\right)/\varepsilon = \left(\ln\frac{1}{\delta}+n\ln 3\right)/\varepsilon$$

- Concrete examples:
  - δ=ε=0.05, n=10 gives 280 examples
  - δ=0.01, ε=0.05, n=10 gives 312 examples
  - δ=ε=0.01, n=10 gives 1,560 examples
  - δ=ε=0.01, n=50 gives 5,954 examples
- Result holds for any consistent learner.

Sample Complexity of Learning Arbitrary Boolean Functions

- Consider any boolean function over n boolean features such as the hypothesis space of DNF or decision trees. There are $2^{2^\wedge n}$ of these, so a sufficient number of examples to learn a PAC concept is:

$$\left(\ln\frac{1}{\delta}+\ln 2^{2^n}\right)/\,\varepsilon=\left(\ln\frac{1}{\delta}+2^n\ln 2\right)/\,\varepsilon$$

- Concrete examples:
  - δ=ε=0.05, n=10 gives 14,256 examples
  - δ=ε=0.05, n=20 gives 14,536,410 examples
  - δ=ε=0.05, n=50 gives 1.561×10^{16} examples

Other Concept Classes

- k-term DNF: Disjunctions of at most k unbounded conjunctive terms: $T_1 \vee T_2 \vee \cdots \vee T_k$
  - $\ln(|H|)=O(kn)$
- k-DNF: Disjunctions of any number of terms each limited to at most k literals: $((L_1 \wedge L_2 \wedge \cdots \wedge L_k) \vee (M_1 \wedge M_2 \wedge \cdots \wedge M_k) \vee \cdots$
  - $\ln(|H|)=O(n^k)$
- k-term CNF: Conjunctions of at most k unbounded disjunctive clauses: $C_1 \wedge C_2 \wedge \cdots \wedge C_k$
  - $\ln(|H|)=O(kn)$
- k-CNF: Conjunctions of any number of clauses each limited to at most k literals: $((L_1 \vee L_2 \vee \cdots \vee L_k) \wedge (M_1 \vee M_2 \vee \cdots \vee M_k) \wedge \cdots$
  - $\ln(|H|)=O(n^k)$

Therefore, all of these classes have polynomial sample complexity given a fixed value of k.

Basic Combinatorics Counting

	dups allowed	dups not allowed
order relevant	samples	permutations
order irrelevant	selections	combinations

Pick 2 from {a,b}

samples	permutations	selections	combinations
aa	ab	aa	ab
ab	ba	ab	
ba		bb	
bb			

k - samples: n^k

k - permutations: $\dfrac{n!}{(n-k)!}$

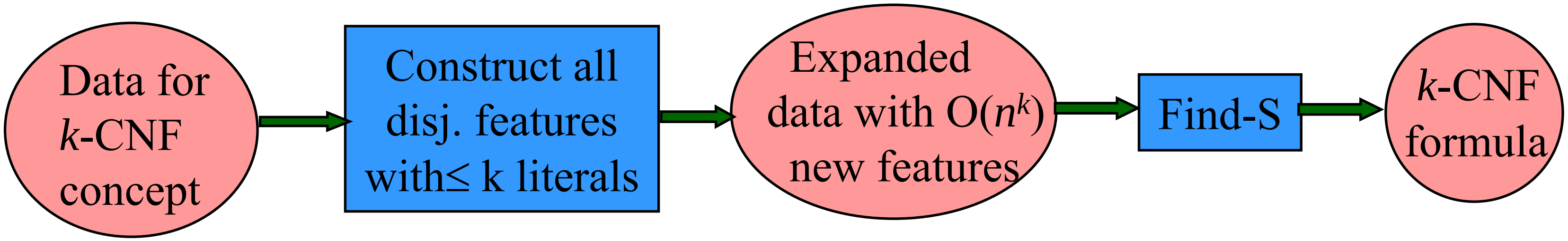
k - selections: $\binom{n+k-1}{k} = \dfrac{(n+k-1)!}{k!(n-1)!}$

k - combinations: $\binom{n}{k} = \dfrac{n!}{k!(n-k)!}$

All O(n^k)

Computational Complexity of Learning

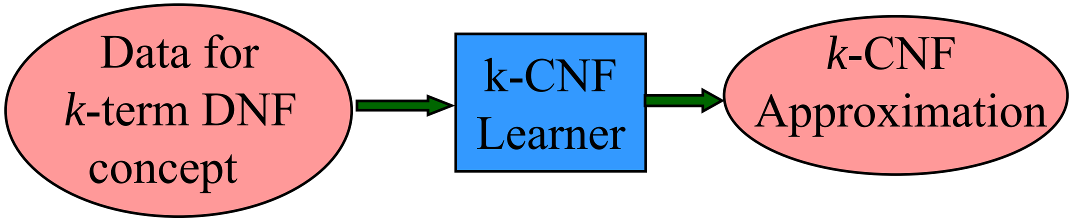
- However, determining whether or not there exists a *k*-term DNF or *k*-clause CNF formula consistent with a given training set is NP-hard. Therefore, these classes are not PAC-learnable due to computational complexity.
- There are polynomial time algorithms for learning *k*-CNF and *k*-DNF. Construct all possible disjunctive clauses (conjunctive terms) of at most *k* literals (there are $O(n^k)$ of these), add each as a new constructed feature, and then use FIND-S (FIND-G) to find a purely conjunctive (disjunctive) concept in terms of these complex features.



Sample complexity of learning *k*-DNF and *k*-CNF are $O(n^k)$
Training on $O(n^k)$ examples with $O(n^k)$ features takes $O(n^{2k})$ time

Enlarging the Hypothesis Space to Make Training Computation Tractable

- However, the language *k*-CNF is a superset of the language *k*-term-DNF since any *k*-term-DNF formula can be rewritten as a *k*-CNF formula by distributing AND over OR.
- Therefore, *C* = *k*-term DNF can be learned using *H* = *k*-CNF as the hypothesis space, but it is intractable to learn the concept in the form of a *k*-term DNF formula (also the *k*-CNF algorithm might learn a close approximation in *k*-CNF that is not actually expressible in *k*-term DNF).
  - Can gain an exponential decrease in computational complexity with only a polynomial increase in sample complexity.



- Dual result holds for learning *k*-clause CNF using *k*-DNF as the hypothesis space.

Probabilistic Algorithms

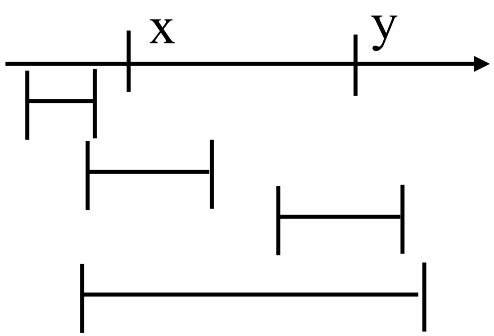
- Since PAC learnability only requires an approximate answer with ***high probability***, a probabilistic algorithm that only halts and returns a consistent hypothesis in polynomial time with a high-probability is sufficient.
- However, it is generally assumed that NP complete problems cannot be solved even with high probability by a probabilistic polynomial-time algorithm, i.e. RP $\neq$ NP.
- Therefore, given this assumption, classes like *k*-term DNF and *k*-clause CNF are not PAC learnable in that form.

Infinite Hypothesis Spaces

- The preceding analysis was restricted to finite hypothesis spaces.
- Some infinite hypothesis spaces (such as those including real-valued thresholds or parameters) are more expressive than others.
  - Compare a rule allowing one threshold on a continuous feature (length<3cm) vs one allowing two thresholds (1cm<length<3cm).
- Need some measure of the expressiveness of infinite hypothesis spaces.
- The ***Vapnik-Chervonenkis*** (***VC***) ***dimension*** provides just such a measure, denoted VC(*H*).
- Analagous to ln|*H*|, there are bounds for sample complexity using VC(*H*).

Shattering Instances

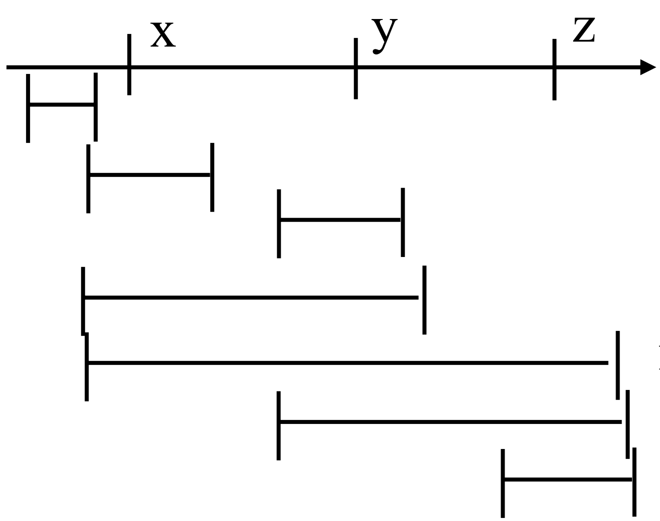
- A hypothesis space is said to shatter a set of instances iff for every partition of the instances into positive and negative, there is a hypothesis that produces that partition.
- For example, consider 2 instances described using a single real-valued feature being shattered by intervals.



+	–
	x,y
x	y
y	x
x,y	

Shattering Instances (cont)

- But 3 instances cannot be shattered by a single interval.



+	–
	x,y,z
x	y,z
y	x,z
x,y	z
x,y,z	
y,z	x
z	x,y
x,z	y

Cannot do (x,z | y)

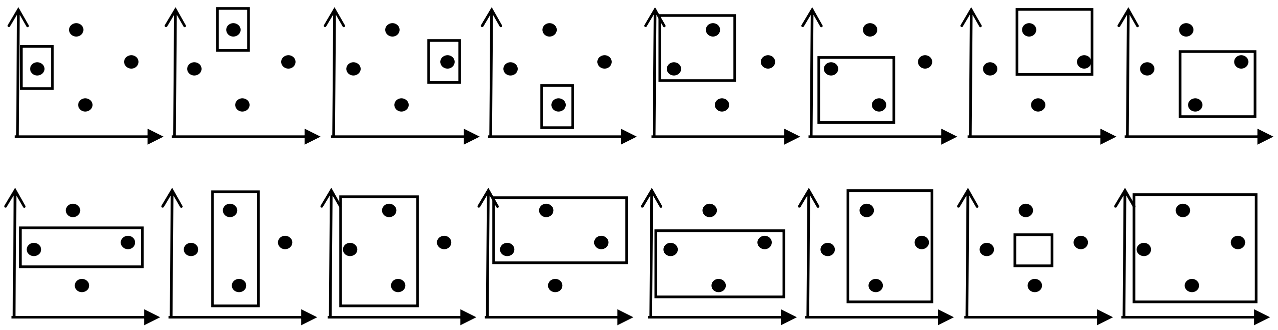
- Since there are 2^m partitions of m instances, in order for H to shatter instances: $|H| \geq 2^m$.

VC Dimension

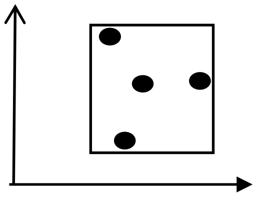
- An unbiased hypothesis space shatters the entire instance space.
- The larger the subset of X that can be shattered, the more expressive the hypothesis space is, i.e. the less biased.
- The Vapnik-Chervonenkis dimension, VC(H). of hypothesis space H defined over instance space X is the size of the largest finite subset of X shattered by H. If arbitrarily large finite subsets of X can be shattered then $VC(H) = \infty$
- If there exists at least one subset of X of size d that can be shattered then $VC(H) \geq d$. If no subset of size d can be shattered, then $VC(H) < d$.
- For a single intervals on the real line, all sets of 2 instances can be shattered, but no set of 3 instances can, so $VC(H) = 2$.
- Since $|H| \geq 2^m$, to shatter m instances, $VC(H) \leq \log_2|H|$

VC Dimension Example

- Consider axis-parallel rectangles in the real-plane, i.e. conjunctions of intervals on two real-valued features. Some 4 instances can be shattered.

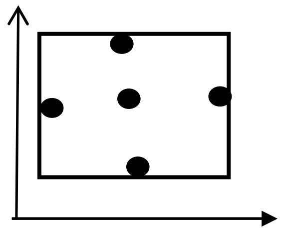


Some 4 instances cannot be shattered:



VC Dimension Example (cont)

- No five instances can be shattered since there can be at most 4 distinct extreme points (min and max on each of the 2 dimensions) and these 4 cannot be included without including any possible 5th point.



- Therefore VC(*H*) = 4
- Generalizes to axis-parallel hyper-rectangles (conjunctions of intervals in *n* dimensions): VC(*H*)=2*n*.

Upper Bound on Sample Complexity with VC

- Using VC dimension as a measure of expressiveness, the following number of examples have been shown to be sufficient for PAC Learning (Blumer *et al*., 1989).

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

- Compared to the previous result using $\ln|H|$, this bound has some extra constants and an extra $\log_2(1/\varepsilon)$ factor. Since $VC(H) \leq \log_2|H|$, this can provide a tighter upper bound on the number of examples needed for PAC learning.

Conjunctive Learning with Continuous Features

- Consider learning axis-parallel hyper-rectangles, conjunctions on intervals on n continuous features.
  - $1.2 \leq \text{length} \leq 10.5 \wedge 2.4 \leq \text{weight} \leq 5.7$
- Since VC(H)=2n sample complexity is

$$\frac{1}{\varepsilon}\left(4\log_2\left(\frac{2}{\delta}\right)+16n\log_2\left(\frac{13}{\varepsilon}\right)\right)$$

- Since the most-specific conjunctive algorithm can easily find the tightest interval along each dimension that covers all of the positive instances ($f_{min} \leq f \leq f_{max}$) and runs in linear time, O(|D|n), axis-parallel hyper-rectangles are PAC learnable.

Sample Complexity Lower Bound with VC

- There is also a general lower bound on the minimum number of examples necessary for PAC learning (Ehrenfeucht, *et al.*, 1989):

  Consider any concept class *C* such that VC(*H*)≥2 any learner *L* and any 0<ε<1/8, 0<δ<1/100. Then there exists a distribution *D* and target concept in *C* such that if *L* observes fewer than:

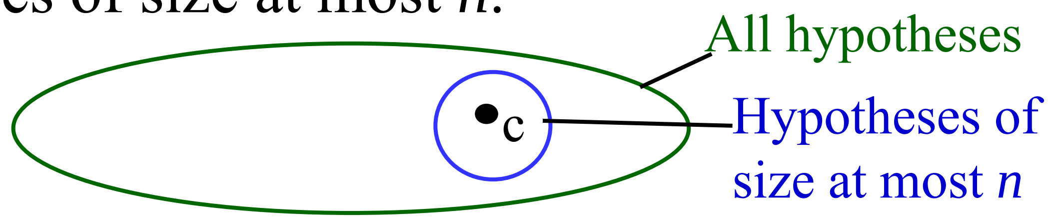
$$\max\left(\frac{1}{\varepsilon}\log_2\left(\frac{1}{\delta}\right), \frac{VC(C)-1}{32\varepsilon}\right)$$

  examples, then with probability at least δ, *L* outputs a hypothesis having error greater than ε.

- Ignoring constant factors, this lower bound is the same as the upper bound except for the extra $\log_2(1/\varepsilon)$ factor in the upper bound.

Analyzing a Preference Bias

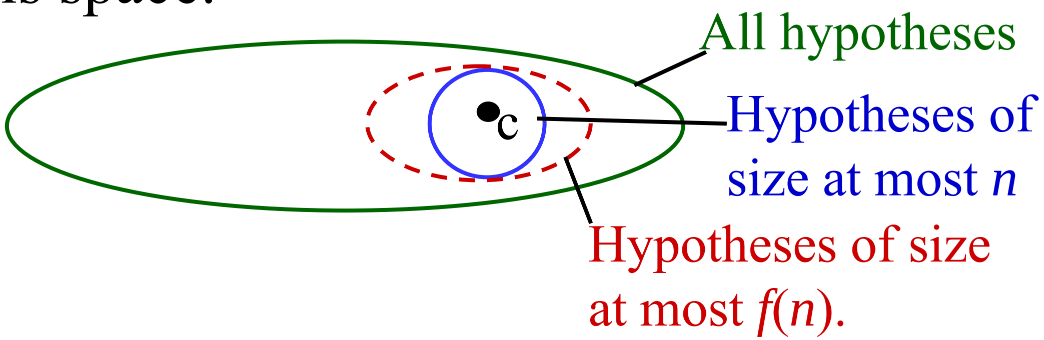
- Unclear how to apply previous results to an algorithm with a preference bias such as simplest decisions tree or simplest DNF.
- If the size of the correct concept is *n*, and the algorithm is guaranteed to return the minimum sized hypothesis consistent with the training data, then the algorithm will always return a hypothesis of size at most *n*, and the effective hypothesis space is all hypotheses of size at most *n*.



- Calculate $|H|$ or VC(H) of hypotheses of size at most n to determine sample complexity.

Computational Complexity and Preference Bias

- However, finding a minimum size hypothesis for most languages is computationally intractable.
- If one has an approximation algorithm that can bound the size of the constructed hypothesis to some polynomial function, $f(n)$, of the minimum size n, then can use this to define the effective hypothesis space.



- However, no worst case approximation bounds are known for practical learning algorithms (e.g. ID3).

"Occam's Razor" Result (Blumer *et al.*, 1987)

- Assume that a concept can be represented using at most n bits in some representation language.
- Given a training set, assume the learner returns the consistent hypothesis representable with the least number of bits in this language.
- Therefore the effective hypothesis space is all concepts representable with at most n bits.
- Since n bits can code for at most 2^n hypotheses, $|H|=2^n$, so sample complexity if bounded by:

$$\left(\ln\frac{1}{\delta}+\ln 2^n\right)/\varepsilon=\left(\ln\frac{1}{\delta}+n\ln 2\right)/\varepsilon$$

- This result can be extended to approximation algorithms that can bound the size of the constructed hypothesis to at most n^k for some fixed constant k (just replace n with n^k)

Interpretation of "Occam's Razor" Result

- Since the encoding is unconstrained it fails to provide any meaningful definition of "simplicity."
- Hypothesis space could be any sufficiently small space, such as "the 2^n most complex boolean functions, where the complexity of a function is the size of its smallest DNF representation"
- Assumes that the correct concept (or a close approximation) is actually in the hypothesis space, so assumes *a priori* that the concept is simple.
- Does not provide a theoretical justification of Occam's Razor as it is normally interpreted.

COLT Conclusions

- The PAC framework provides a theoretical framework for analyzing the effectiveness of learning algorithms.
- The sample complexity for any consistent learner using some hypothesis space, H, can be determined from a measure of its expressiveness $|H|$ or VC(H), quantifying bias and relating it to generalization.
- If sample complexity is tractable, then the computational complexity of finding a consistent hypothesis in H governs its PAC learnability.
- Constant factors are more important in sample complexity than in computational complexity, since our ability to gather data is generally not growing exponentially.
- Experimental results suggest that theoretical sample complexity bounds over-estimate the number of training instances needed in practice since they are worst-case upper bounds.