Learning Theory

COMP9417 Machine Learning and Data Mining

Term 2, 2019

Acknowledgements

Material derived from slides for the book
"Elements of Statistical Learning (2nd Ed.)" by T. Hastie,
R. Tibshirani & J. Friedman. Springer (2009)
http://statweb.stanford.edu/~tibs/ElemStatLearn/

Material derived from slides for the book
"Machine Learning: A Probabilistic Perspective" by P. Murphy
MIT Press (2012)
http://www.cs.ubc.ca/~murphyk/MLbook

Material derived from slides for the book
"Machine Learning" by P. Flach
Cambridge University Press (2012)
http://cs.bris.ac.uk/~flach/mlbook

Material derived from slides for the book
"Bayesian Reasoning and Machine Learning" by D. Barber
Cambridge University Press (2012)
http://www.cs.ucl.ac.uk/staff/d.barber/brml

Material derived from figures for the book
"Python Data Science Handbook" by J. VanderPlas
O'Reilly Media (2017)
http://shop.oreilly.com/product/0636920034919.do

Material derived from slides for the course
"Machine Learning" by A. Srinivasan
BITS Pilani, Goa, India (2016)

Aims

This lecture will introduce you to some foundational results that apply in machine learning irrespective of any particular algorithm, and will enable you to define and reproduce some of the fundamental approaches and results from the computational and statistical theory. Following it you should be able to:

- describe a basic theoretical framework for sample complexity of learning
- describe the Probably Approximately Correct (PAC) learning framework
- describe the Vapnik-Chervonenkis (VC) dimension framework
- describe the Mistake Bounds framework and apply the WINNOW algorithm within this framework
- outline the "No Free Lunch" Theorem

Introduction

Are there general laws that apply to inductive learning?

From **computational learning theory** and **statistical learning theory**:

- in both cases, theoretical results have been obtained that apply in very general settings
- provide elegant frameworks leading to results on what can or cannot be learned algorithmically
- however, theoretical results are not always easy to obtain for practically useful machine learning methods and applications
  - need to make (sometimes unrealistic) assumptions
  - results may be overly pessimistic, e.g., worst-case bounds
- nonetheless, both areas have contributed results which are important for understanding some key issues in machine learning
- have also led to important advances in practical algorithms, such as boosting and support vector machines

Key Idea

Leaning theory aims at a body of theory that captures all important aspects of the fundamentals of the learning process and any algorithm or class of algorithms designed to do learning — i.e., we desire theory to capture the *algorithm-independent aspects of machine learning*.

BUT: we're not quite there yet . . .

Computational Learning Theory

We seek theory to relate:

- Probability of successful learning
- Number of training examples
- Complexity of hypothesis space
- Time complexity of learning algorithm
- Accuracy to which target concept is approximated
- Manner in which training examples presented

Computational Learning Theory

Some questions to ask, without focusing on any particular algorithm:

- Sample complexity
  - How many training examples required for learner to converge (with high probability) to a *successful* hypothesis ?
- Computational complexity
  - How much computational effort required for learner to converge (with high probability) to a successful hypothesis ?
- Hypothesis complexity
  - How do we measure the complexity of a hypothesis ?
  - How large is a hypothesis space ?
- Mistake bounds
  - How many training examples will the learner *misclassify* before converging to a successful hypothesis ?

Computational Learning Theory

What do we consider to be a *successful* hypothesis:

- identical to target concept ?
- mostly agrees with target concept . . . ?
- . . . does this most of the time ?

Computational Learning Theory

Instead of focusing on particular algorithms, learning theory aims to characterise *classes* of algorithms.

The framework of Probably Approximately Correct (PAC) learning can be used to address questions such as:

- How many training examples ?
- How much computational effort required ?
- How complex a hypothesis class needed ?
- How to quantify hypothesis complexity ?
- How many mistakes will be made ?

We start to look at PAC learning using Concept Learning.

Prototypical Concept Learning Task

Given:

Instances X: Possible days, each described by the attributes
Sky, AirTemp, Humidity, Wind, Water, Forecast

Target function c: $EnjoySport : X \rightarrow \{0, 1\}$

Hypotheses H: Conjunctions of literals. E.g.
$\langle ?, Cold, High, ?, ?, ? \rangle$

Training examples D: Positive and negative examples of target function
$\langle x_1, c(x_1) \rangle, \ldots \langle x_m, c(x_m) \rangle$

Determine:

A hypothesis h in H such that $h(x) = c(x)$ for all x in D?

A hypothesis h in H such that $h(x) = c(x)$ for all x in X?

Sample Complexity

Given: set of instances X

set of hypotheses H

set of possible target concepts C

training instances generated by a fixed, unknown probability distribution $\mathcal{D}$ over X

Learner observes a sequence D of training examples of form $\langle x, c(x)\rangle$, for some target concept $c \in C$

instances x are drawn from distribution $\mathcal{D}$

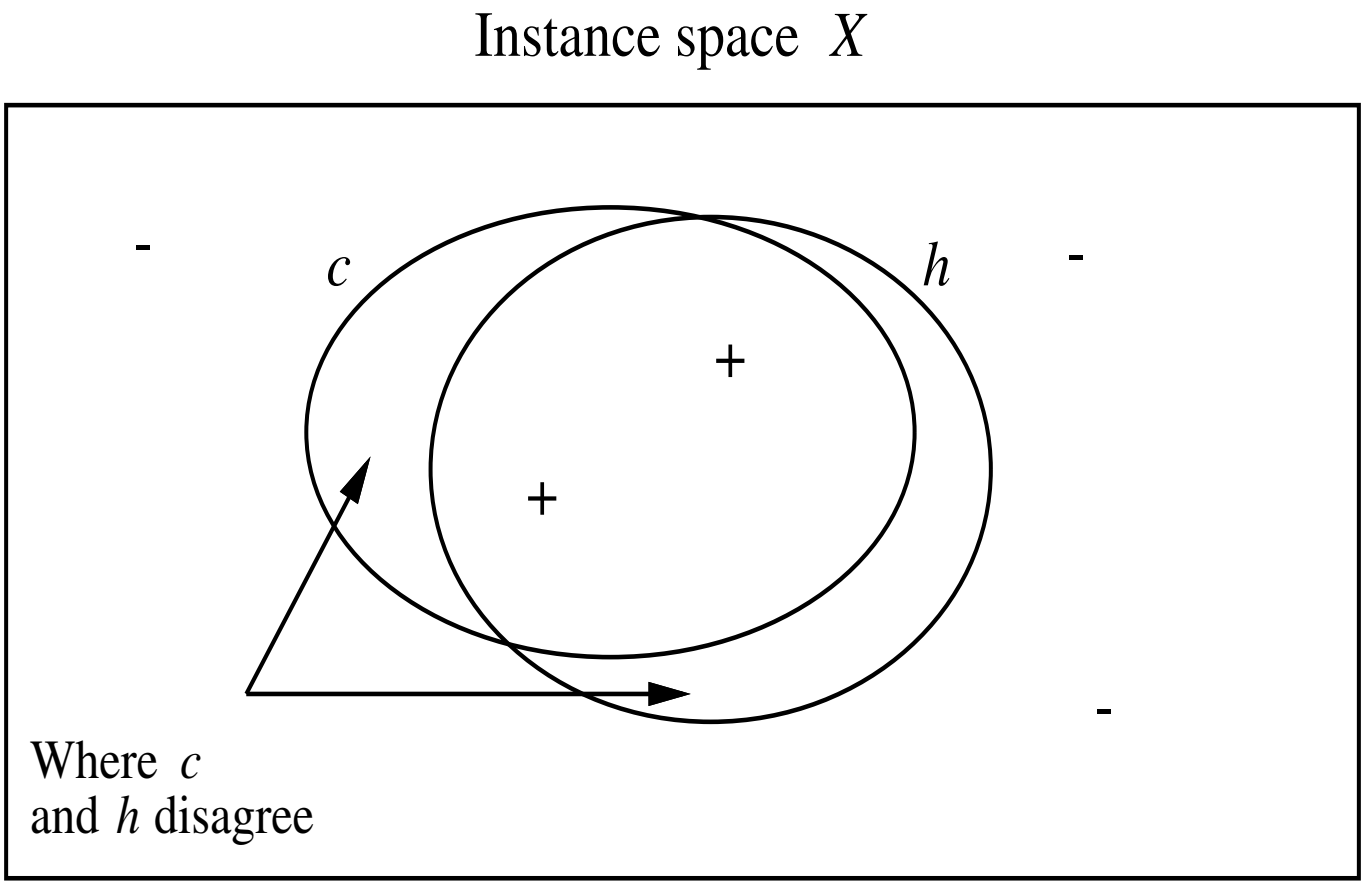
teacher provides target value $c(x)$ for each

Learner must output a hypothesis h estimating c

h is evaluated by its performance on subsequent instances drawn according to $\mathcal{D}$

Note: randomly drawn instances, noise-free classifications

True Error of a Hypothesis



True Error of a Hypothesis

Definition: *The* **true error** *(denoted* $error_{\mathcal{D}}(h)$*) 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* $\mathcal{D}$*.*

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

Two Notions of Error

Training error of hypothesis h with respect to target concept c

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

True error of hypothesis h with respect to c

- How often $h(x) \neq c(x)$ over future random instances

Our concern:

- Can we bound the true error of h given the training error of h?
- First consider when training error of h is zero (i.e., $h \in VS_{H,D}$)

Concept Learning as Search

Question: What can be learned ?
Answer: (only) what is in the *hypothesis space*

How big is the hypothesis space for *EnjoySport* ?

Instance space

$$\begin{aligned} \textit{Sky} \times \textit{AirTemp} \times \ldots \times \textit{Forecast} &= 3 \times 2 \times 2 \times 2 \times 2 \times 2 \\ &= 96 \end{aligned}$$

Concept Learning as Search

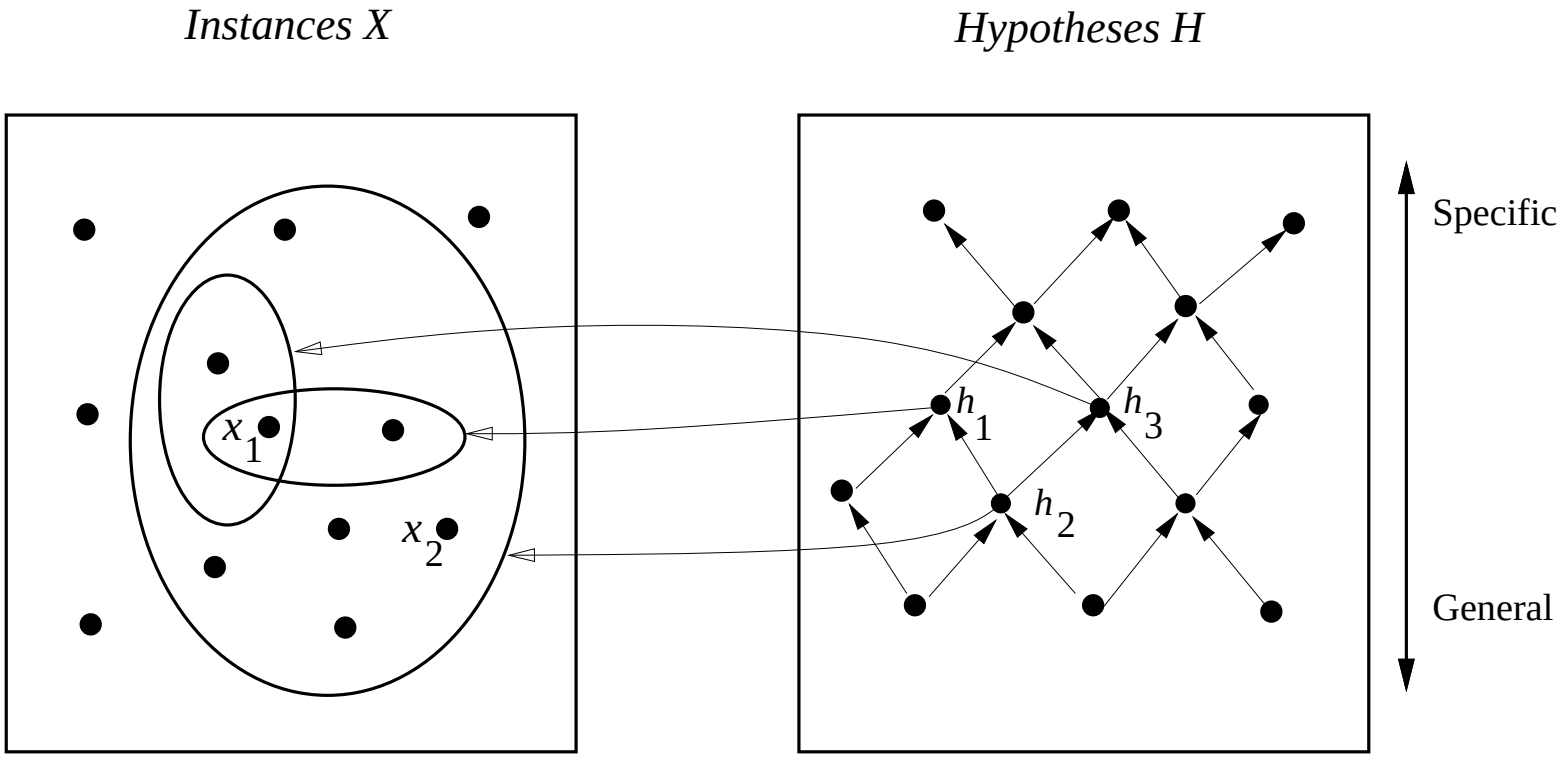
Hypothesis space

$$
\begin{aligned}
\textit{Sky} \times \textit{AirTemp} \times \ldots \times \textit{Forecast} &= 5 \times 4 \times 4 \times 4 \times 4 \times 4 \\
&= 5120 \\
\text{(semantically distinct}^{1}\text{ only)} &= 1 + (4 \times 3 \times 3 \times 3 \times 3 \times 3) \\
&= 973
\end{aligned}
$$

The learning problem $\equiv$ searching a hypothesis space. How ?

[1] Any hypothesis with an $\emptyset$ constraint covers no instances, hence all are semantically equivalent.

Instances, Hypotheses, and More-General-Than



x_1 = <*Sunny, Warm, High, Strong, Cool, Same*>

x_2 = <*Sunny, Warm, High, Light, Warm, Same*>

h_1 = <*Sunny, ?, ?, Strong, ?, ?*>

h_2 = <*Sunny, ?, ?, ?, ?, ?*>

h_3 = <*Sunny, ?, ?, ?, Cool, ?*>

A generality order on hypotheses

Definition: Let h_j and h_k be Boolean-valued functions defined over instances X. Then h_j is **more_general_than_or_equal_to** h_k (written $h_j \geq_g h_k$) if and only if

$$(\forall x \in X)[(h_k(x) = 1) \rightarrow (h_j(x) = 1)]$$

Intuitively, h_j is **more_general_than_or_equal_to** h_k if any instance satisfying h_k also satisfies h_j.

h_j is (strictly) *more_general_than* h_k (written $h_j >_g h_k$) if and only if $(h_j \geq_g h_k) \wedge (h_k \not\geq_g h_j)$.

h_j is *more_specific_than* h_k when h_k is *more_general_than* h_j.

Version Space

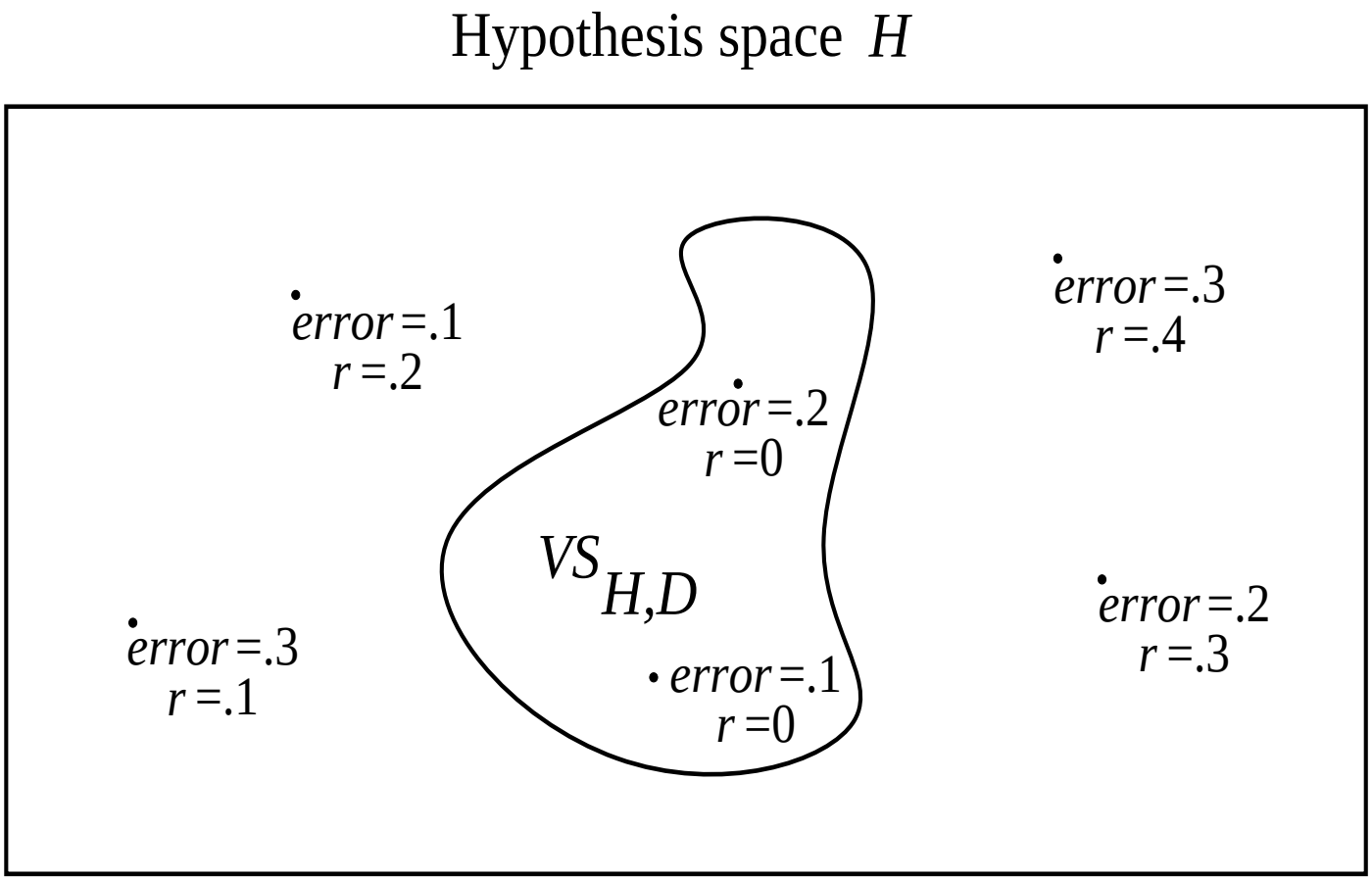
A hypothesis h is **consistent** *with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $\langle x, c(x)\rangle$ in D.*

$$Consistent(h, D) \equiv (\forall \langle x, c(x)\rangle \in D)\ h(x) = c(x)$$

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

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

Exhausting the Version Space



Exhausting the Version Space

Note: in the diagram

true error 就是test error

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

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

$$(\forall h \in VS_{H,D})\ error_{\mathcal{D}}(h) < \epsilon$$

So $VS_{H,D}$ is *not* ϵ-exhausted if it contains at least one h with $error_{\mathcal{D}}(h) \geq \epsilon$.

How many examples will ϵ-exhaust the VS?

Theorem:

[Haussler, 1988].

If the hypothesis space H is finite, and D is a sequence of $m \geq 1$ independent random examples of some target concept c, then for any $0 \leq \epsilon \leq 1$, the probability that the version space with respect to H and D is not ϵ-exhausted (with respect to c) is less than

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

Interesting! This bounds the probability that any consistent learner will output a hypothesis h with $error(h) \geq \epsilon$

How many examples will ϵ-exhaust the VS?

If we want this probability to be below δ

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

then

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

How many examples will ϵ-exhaust the VS?

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

Use our theorem:

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

Learning Conjunctions of Boolean Literals

Suppose H contains conjunctions of constraints on up to n Boolean attributes (i.e., n Boolean literals – any h can contain a literal, or its negation, or neither). Then $|H| = 3^n$, and

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

or

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

How About $EnjoySport$?

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

If H is as given in $EnjoySport$ then $|H| = 973$, and

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

How About $EnjoySport$?

... if want to assure that with probability 95%, VS contains only hypotheses with $error_{\mathcal{D}}(h) \leq .1$, then it is sufficient to have m examples, where

$$m \geq \frac{1}{0.1}(\ln 973 + \ln(1/0.05))$$

$$m \geq 10(\ln 973 + \ln 20)$$

$$m \geq 10(6.88 + 3.00)$$

$$m \geq 98.8$$

PAC Learning

Consider a class C of possible target concepts defined over a set of instances X of length n, and a learner L using hypothesis space H.

> Definition: C *is* **PAC-learnable** *by* L *using* H *if for all* $c \in C$, *distributions* $\mathcal{D}$ *over* X, ϵ *such that* $0 < \epsilon < 1/2$, *and* δ *such that* $0 < \delta < 1/2$, *learner* L *will with probability at least* $(1 - \delta)$ *output a hypothesis* $h \in H$ *such that* $error_{\mathcal{D}}(h) \leq \epsilon$, *in time that is polynomial in* $1/\epsilon$, $1/\delta$, n *and* $size(c)$.

Probably **A**pproximately **C**orrect Learning

L. Valiant, (1984; 2013).

Agnostic PAC Learning

So far, assumed $c \in H$ — *consistent* learners (noise-free)

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?

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

derived from Hoeffding bounds:

$$Pr[error_{\mathcal{D}}(h) > error_D(h) + \epsilon] \leq e^{-2m\epsilon^2}$$

Unbiased Learners

Unbiased concept class C contains all target concepts definable on instance space X.

$$|C| = 2^{|X|}$$

Say X is defined using n Boolean features, then $|X| = 2^n$.

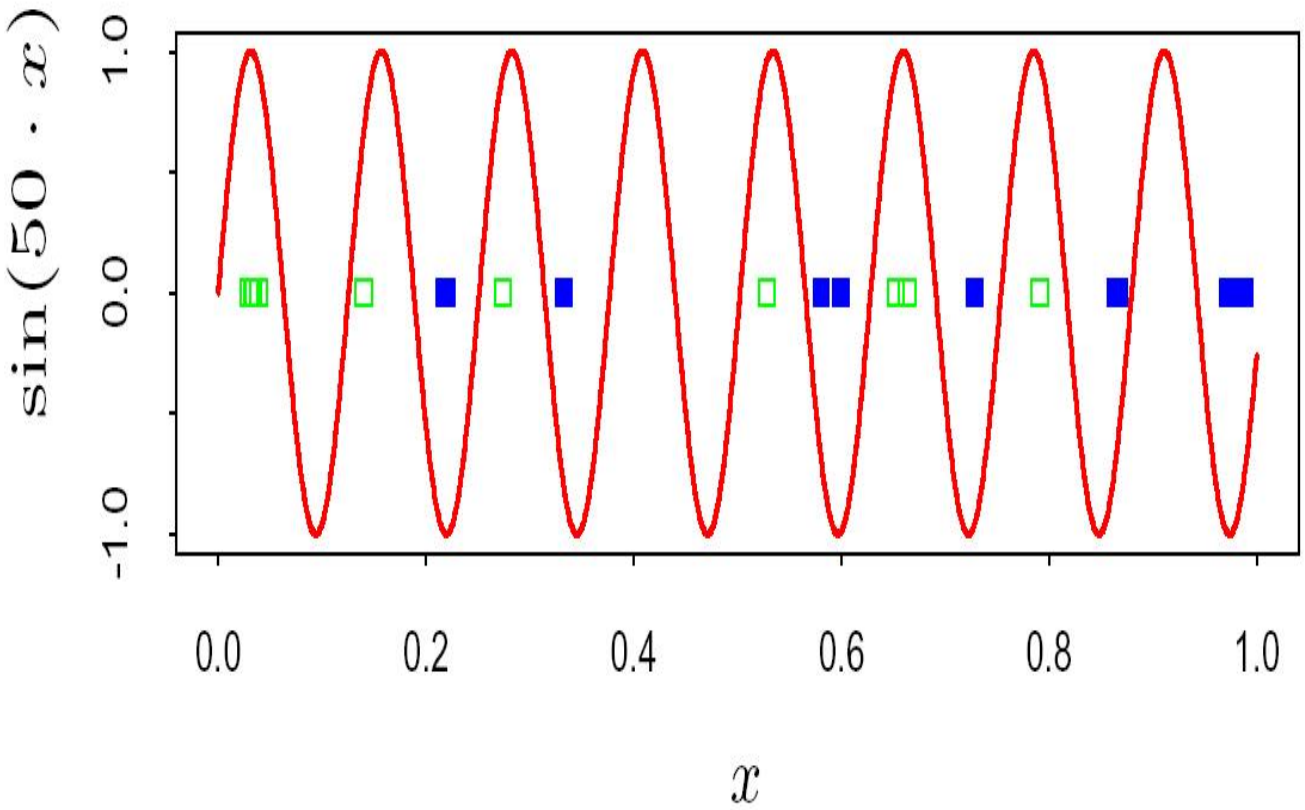
$$|C| = 2^{2^n}$$

An unbiased learner has a hypothesis space able to represent *all* possible target concepts, i.e., $H = C$.

$$m \geq \frac{1}{\epsilon}(2^n \ln 2 + \ln(1/\delta))$$

i.e., exponential (in the number of features) sample complexity !

How *Complex* is a Hypothesis ?



How *Complex* is a Hypothesis ?

The solid curve is the function $\sin(50x)$ for $x \in [0, 1]$.

The blue (solid) and green (hollow) points illustrate how the associated indicator function $I(\sin(\alpha\, x) > 0)$ can shatter (separate) an arbitrarily large number of points by choosing an appropriately high frequency α.

Classes separated based on $\sin(\alpha\, x)$, for frequency α, a *single* parameter.

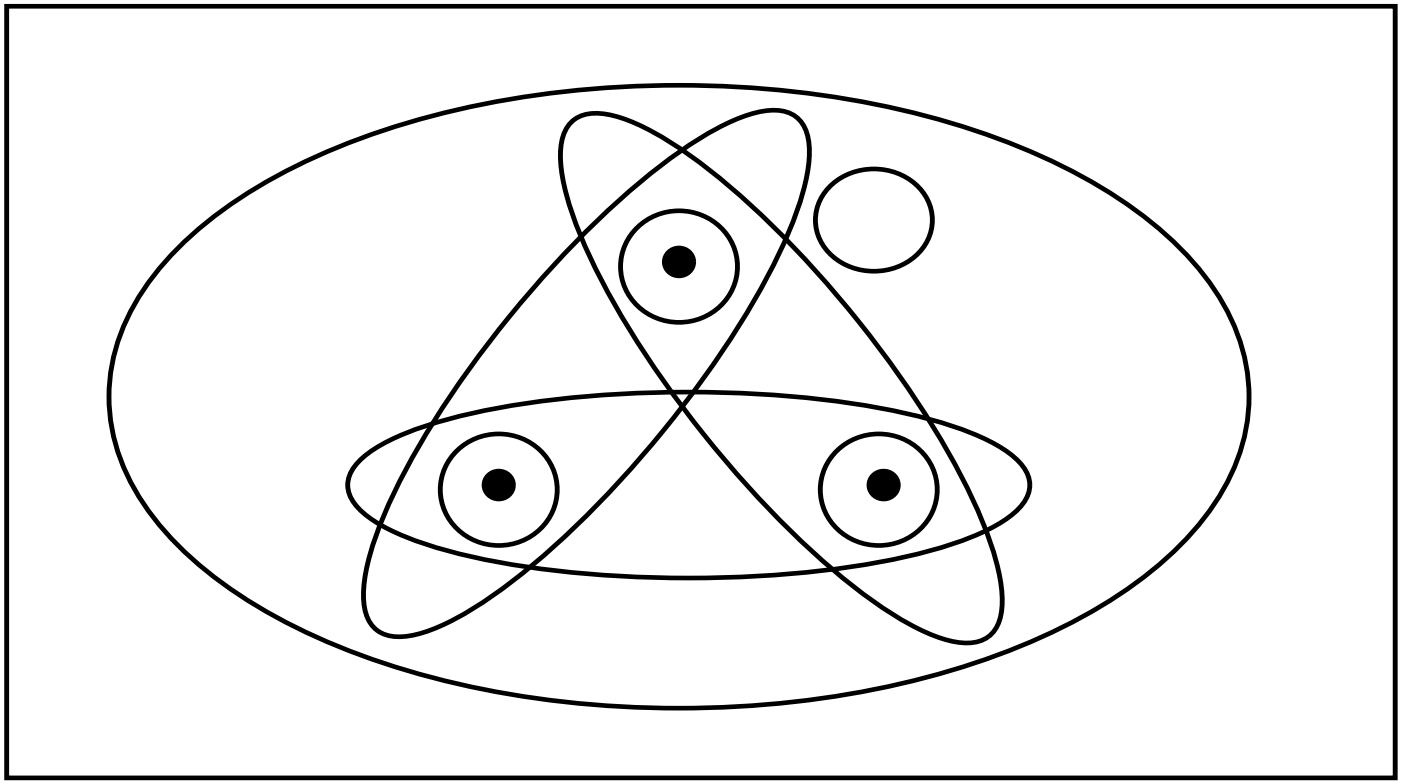
Shattering a Set of Instances

Definition: *a* **dichotomy** *of a set S is a partition of S into two disjoint subsets.*

Definition: *a set of instances S is* **shattered** *by hypothesis space H if and only if for every dichotomy of S there exists some hypothesis in H consistent with this dichotomy.*

Three Instances Shattered

Instance space X



Shattering a set of instances

Consider the following instances:

$m =$ ManyTeeth $\wedge$ $\neg$Gills $\wedge$ $\neg$Short $\wedge$ $\neg$Beak

$g =$ $\neg$ManyTeeth $\wedge$ Gills $\wedge$ $\neg$Short $\wedge$ $\neg$Beak

$s =$ $\neg$ManyTeeth $\wedge$ $\neg$Gills $\wedge$ Short $\wedge$ $\neg$Beak

$b =$ $\neg$ManyTeeth $\wedge$ $\neg$Gills $\wedge$ $\neg$Short $\wedge$ Beak

There are 16 different subsets of the set $\{m, g, s, b\}$. Can each of them be represented by its own conjunctive concept? The answer is yes: for every instance we want to exclude, we add the corresponding negated literal to the conjunction. Thus, $\{m, s\}$ is represented by $\neg$Gills $\wedge$ $\neg$Beak, $\{g, s, b\}$ is represented by $\neg$ManyTeeth, $\{s\}$ is represented by $\neg$ManyTeeth $\wedge$ $\neg$Gills $\wedge$ $\neg$Beak, and so on. We say that this set of four instances is *shattered* by the hypothesis language of conjunctive concepts.

Shattering a set of instances

Suppose we have a dataset described by d Boolean features, and a hypothesis space of conjunctions of up to d Boolean literals. Then the largest subset of instances that can be shattered is at least d.

To see this argument more clearly, suppose $d = 3$ and that the i-th instance is represented by having only the i-th Boolean literal set to true, simplified here to the corresponding bitstring:

instance$_1$: 100

instance$_2$: 010

instance$_3$: 001

Now any dichotomy can be constructed by a conjunctive hypothesis that excludes any instance simply by adding the appropriate literal. For example, the hypothesis including only instance$_2$ is $\neg l_1 \wedge \neg l_3$. In fact, it can be shown that the largest subset of instances that can be shattered in this setting has size *exactly* d.

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* $VC(H) \equiv \infty$.

Note: the VC dimension can be defined for an infinite hypothesis space H since it depends only on the size of finite subsets of X.

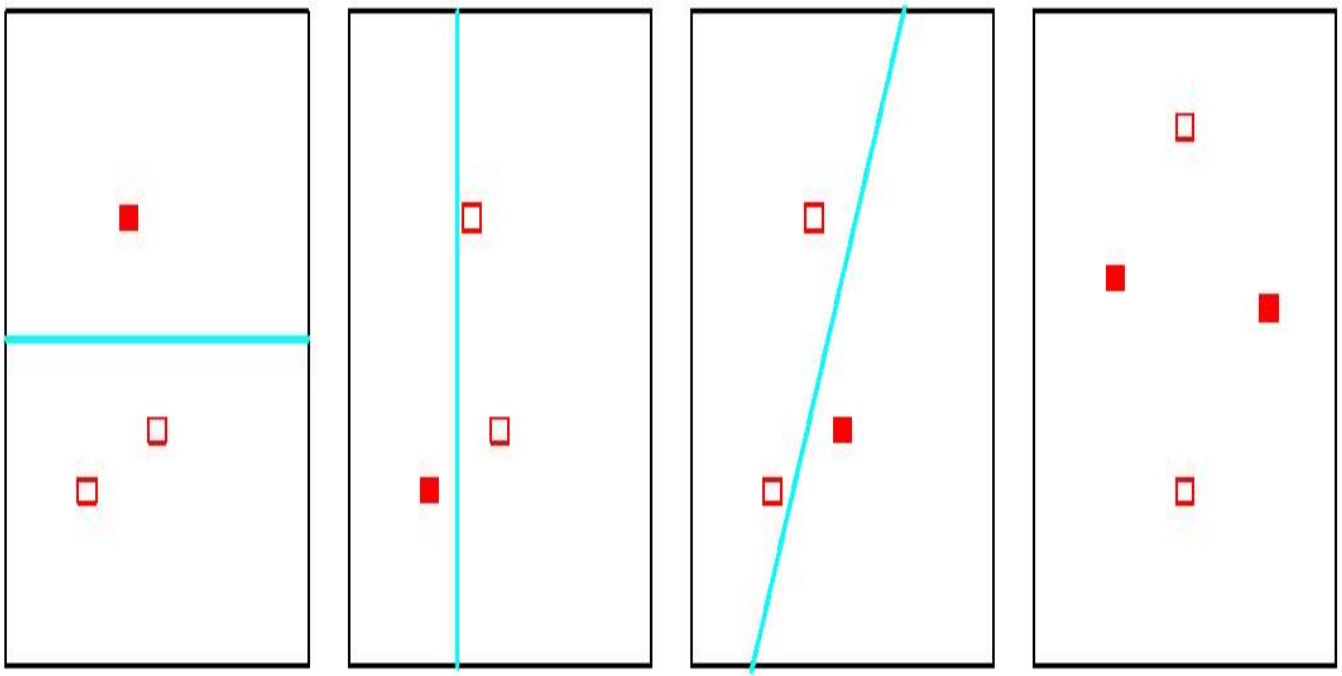
VC Dimension of Conjunctive Concepts

From the earlier slide on shattering a set of instances by a conjunctive hypothesis, if we have an instance space X where each instance is described by d Boolean features, and a hypothesis space H of conjunctions of up to d Boolean literals, then the VC Dimension $VC(H) = d$.

What about some other type of hypothesis space ?

Let's look at linear classifiers.

VC Dimension of Linear Decision Surfaces



From the left, shown are three dichotomies of the same three instances. Can a linear classifier be found for the other five dichotomies? On the right, this set of four instances clearly cannot be shattered by a hypothesis space of linear classifiers.

VC Dimension of Linear Decision Surfaces

Consider linear classifiers in two dimensions. What is the VC dimension of this class of hypotheses H?

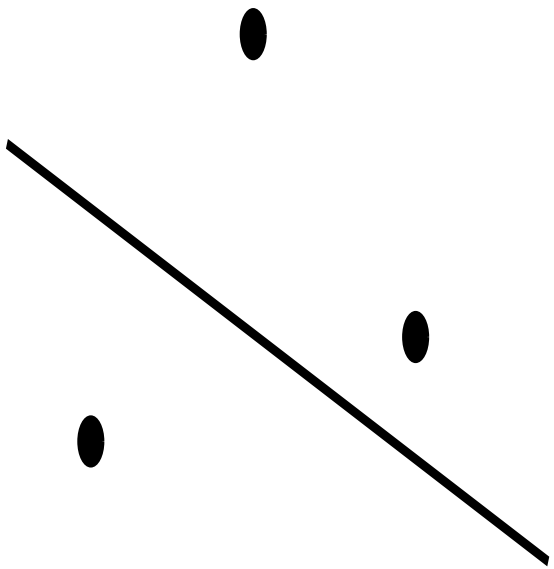
Clearly, for a subset of 2 instances we can find a linear classifier for all possible dichotomies. What about a subset of 3 instances ?

The same argument as for 2 instances applies (see first three examples on previous slide, and case (a) on next slide), as long as the instances are not collinear (case (b) on next slide). So the VC dimension is at least 3.

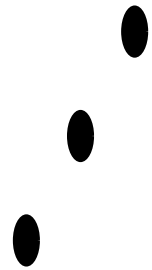
However, in this setting, there is no set of 4 points that can be shattered.

In general, for linear classifiers in d dimensions the VC dimension is $d + 1$.

VC Dimension of Linear Decision Surfaces



(a)



(b)

Sample Complexity from VC Dimension

We can now generalise the PAC-learning result obtained earlier to answer the question: how many randomly drawn examples suffice to ϵ-exhaust $VS_{H,D}$ with probability at least $(1-\delta)$?

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$

So we see that the concept of the VC dimension of a hypothesis class gives us a general framework for characterising the complexity or *capacity* of hypotheses in terms of their ability to express all possible target concepts in a particular learning setting.

For example, the argument developed for the VC dimension of linear classifiers can be extended to multi-layer perceptrons to obtain sample complexity bounds in the PAC-learning framework.

Mistake Bounds

So far: how many examples needed to learn ?

What about: how many mistakes before convergence ?

Let's consider similar setting to PAC learning:

- Instances drawn at random from X according to distribution $\mathcal{D}$
- Learner must classify each instance before receiving correct classification from teacher
- Can we bound the number of mistakes learner makes before converging?

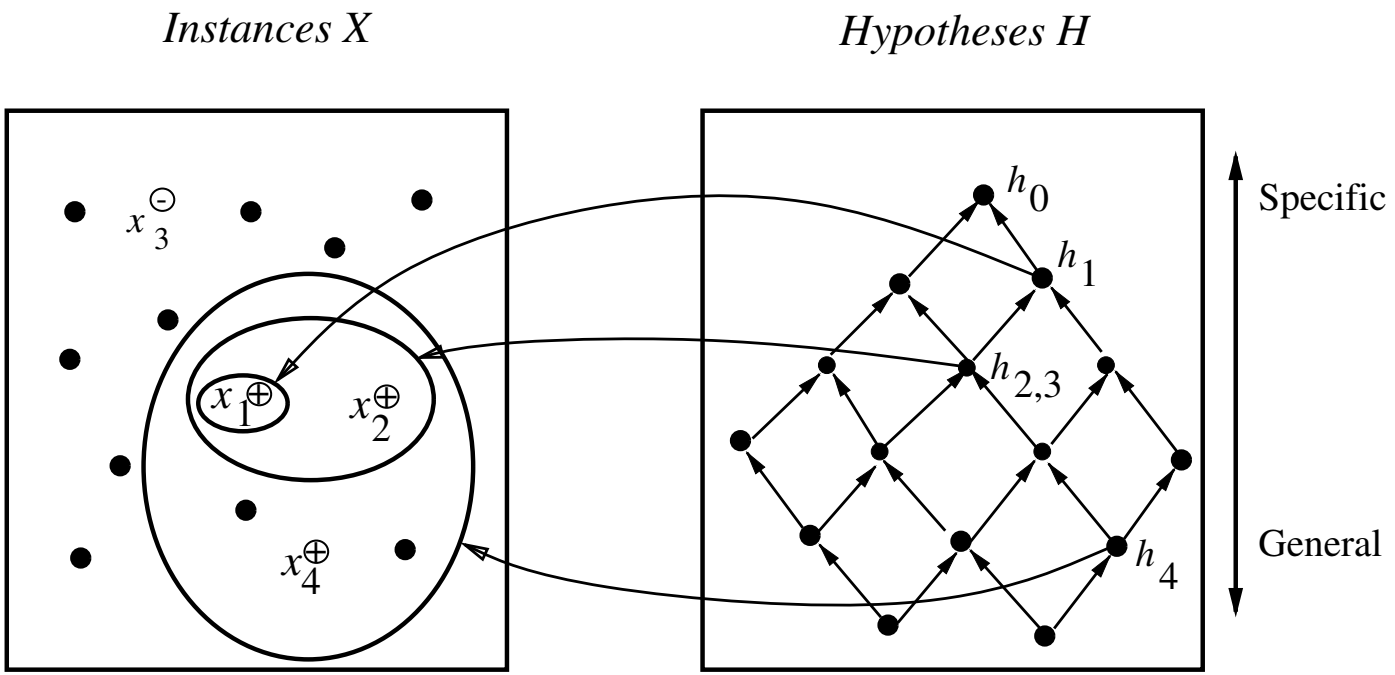
Again, we start by analysing concept learning.

The FIND-S Algorithm

An online, specific-to-general, concept learning algorithm:

- Initialize h to the most specific hypothesis in H
- For each positive training instance x
  - For each attribute constraint a_i in h
    - If the constraint a_i in h is satisfied by x
    - Then do nothing
    - Else replace a_i in h by the next more general constraint satisfied by x

Hypothesis Space Search by FIND-S



x_1 = <*Sunny Warm Normal Strong Warm Same*>, +

x_2 = <*Sunny Warm High Strong Warm Same*>, +

x_3 = <*Rainy Cold High Strong Warm Change*>, -

x_4 = <*Sunny Warm High Strong Cool Change*>, +

h_0 = <∅, ∅, ∅, ∅, ∅, ∅>

h_1 = <*Sunny Warm Normal Strong Warm Same*>

h_2 = <*Sunny Warm ? Strong Warm Same*>

h_3 = <*Sunny Warm ? Strong Warm Same*>

h_4 = <*Sunny Warm ? Strong ? ?* >

FIND-S - does it work ?

Assume: a hypothesis $h_c \in H$ describes target function c, and training data is error-free.

By definition, h_c is consistent with all positive training examples so can never cover a negative example.

For each h generated by FIND-S h_c is **more_general_than_or_equal_to** h.

So h can never cover a negative example.

Complaints about FIND-S

- Can't tell whether it has learned concept
  - learned hypothesis is an element of the VS
  - but may not be the only consistent hypothesis
- Can't tell when training data inconsistent
  - cannot handle noisy data
- Picks a maximally specific h (why?)
  - might require maximally general h

Mistake Bounds: FIND-S

Consider FIND-S when H = conjunction of Boolean literals

FIND-S:

- *Initialize h to the most specific hypothesis* $l_1 \wedge \neg l_1 \wedge l_2 \wedge \neg l_2 \ldots l_n \wedge \neg l_n$
- *For each positive training instance x*
  - *Remove from h any literal that is not satisfied by x*
- *Output hypothesis h.*

How many mistakes before converging to correct h?

Mistake Bounds: FIND-S

FIND-S will converge to error-free hypothesis in the limit if

- $C \subseteq H$
- data are noise-free

How many mistakes before converging to correct h?

Mistake Bounds: FIND-S

- FIND-S initially classifies all instances as negative
- will generalize for positive examples by dropping unsatisfied literals
- since $c \in H$, will never classify a negative instance as positive (if it did:
  - would exist a hypothesis h' such that $c \geq_g h'$
  - would exist an instance x such that $h'(x) = 1$ and $c(x) \neq 1$
  - which contradicts definition of generality ordering $\geq_g$)
- mistake bound from number of positives classified as negatives

How many mistakes before converging to correct h?

Mistake Bounds: FIND-S

- $2n$ terms in initial hypothesis
- first mistake, remove half of these terms, leaving n
- each further mistake, remove at least 1 term
- in worst case, will have to remove all n remaining terms
  - would be most general concept - everything is positive
- worst case number of mistakes would be $n + 1$
- worst case sequence of learning steps, removing only one literal per step

Mistake Bounds: Halving Algorithm

Find-S returns the single most-specific consistent hypothesis.

An extension of the Find-S concept learning algorithm is the Candidate-Elimination algorithm which returns *all* consistent hypotheses, i.e., it finds the Version Space.

Now consider the Halving Algorithm:

- Learns concept using Candidate-Elimination algorithm
- Classifies new instances by majority vote of Version Space hypotheses

How many mistakes will the Halving Algorithm make before converging to correct h?

- ... in worst case?
- ... in best case?

Mistake Bounds: Halving Algorithm

Halving Algorithm learns exactly when the version space contains only one consistent hypothesis which corresponds to the target concept

- at each step, remove all hypotheses whose vote was incorrect
- mistake when majority vote classification is incorrect
- mistake bound in converging to correct h ?

Mistake Bounds: Halving Algorithm

- how many mistakes worst case ?
  - on every step, mistake because majority vote is incorrect
  - each mistake, number of hypotheses reduced by at least half
  - hypothesis space size $|H|$, worst-case mistake bound $\lfloor \log_2 |H| \rfloor$
- how many mistakes best case ?
  - on every step, no mistake because majority vote is correct
  - still remove all incorrect hypotheses, up to half
  - best case, no mistakes in converging to correct h

WINNOW

Mistake bounds are based on the work of Nick Littlestone[2] who developed the WINNOW family of algorithms.

- online, mistake-driven algorithm
  - similar to perceptron
  - learns linear threshold function
- designed to learn in the presence of many irrelevant features
  - number of mistakes grows only *logarithmically* with number of irrelevant features
- Next slide shows the algorithm known as WINNOW2
  - in WINNOW1 attribute *elimination* not demotion

[2] N. Littlestone. "Learning Quickly When Irrelevant Attributes Abound: A New Linear-threshold Algorithm". Machine Learning 2(4): 285-318 (1987)

Winnow2

While some instances are misclassified
  For each instance x
    classify x using current weights w
    If predicted class is *incorrect*
      If x has class 1
        For each $x_i = 1$, $w_i \leftarrow \alpha w_i$ # Promotion
        (if $x_i = 0$, leave w_i unchanged)
      Otherwise
        For each $x_i = 1$, $w_i \leftarrow \frac{w_i}{\alpha}$ # Demotion
        (if $x_i = 0$, leave w_i unchanged)

Here x and w are vectors of features and weights, respectively.

WINNOW2

- user-supplied threshold θ
  - class is 1 if $\sum w_i a_i > \theta$
- note similarity to perceptron training rule
  - WINNOW2 uses multiplicative weight updates
  - $\alpha > 1$
- will do *much better* than perceptron with many irrelevant attributes
  - an *attribute-efficient* learner
- what are irrelevant attributes ?
  - assume that the target concept can be expressed using a *finite* subset r of attributes or features
  - if there are n attributes in total, $n - r$ are irrelevant
  - mistake-bounds for WINNOW-type algorithms are *logarithmic* in the number of irrelevant attributes
  - typically, the worst-case mistake-bound is something like $\mathcal{O}(r \log n)$

Optimal Mistake Bounds

Let $M_A(C)$ be the max number of mistakes made by algorithm A to learn concepts in C. (maximum over all possible $c \in C$, and all possible training sequences)

$$M_A(C) \equiv \max_{c \in C} M_A(c)$$

Definition: Let C be an arbitrary non-empty concept class. The **optimal mistake bound** for C, denoted $Opt(C)$, is the minimum over all possible learning algorithms A of $M_A(C)$.

$$Opt(C) \equiv \min_{A \in learning\ algorithms} M_A(C)$$

$$VC(C) \leq Opt(C) \leq M_{Halving}(C) \leq log_2(|C|).$$

Weighted Majority

Based on[3]:

- a generalisation of Halving Algorithm
- predicts by *weighted vote* of set of prediction algorithms
- learns by altering weights for prediction algorithms
- any *prediction algorithm* simply predicts value of target concept given an instance; they can be
  - elements of hypothesis space H, or even
  - different learning algorithms
- if there is inconsistency between prediction algorithm and training example
  - then reduce weight of prediction algorithm
- bound number of mistakes of ensemble by number of mistakes made by *best* prediction algorithm

[3] N. Littlestone, M. Warmuth. "The Weighted Majority Algorithm". Inf. Comput. 108(2): 212-261 (1994)

Weighted Majority

a_i is the i-th prediction algorithm
w_i is the weight associated with a_i

For all i, initialize $w_i \leftarrow 1$
For each training example $\langle x, c(x) \rangle$

  Initialize q_0 and q_1 to 0
  For each prediction algorithm a_i

    If $a_i(x) = 0$ then $q_0 \leftarrow q_0 + w_i$
    If $a_i(x) = 1$ then $q_1 \leftarrow q_1 + w_i$

  If $q_1 > q_0$ then predict $c(x) = 1$
  If $q_0 > q_1$ then predict $c(x) = 0$
  If $q_0 = q_1$ then predict 0 or 1 at random for $c(x)$
  For each prediction algorithm a_i

    If $a_i(x) \neq c(x)$ then $w_i \leftarrow \beta w_i$

Weighted Majority

Weighted Majority algorithm begins by assigning weight of 1 to each prediction algorithm.

On misclassification by a prediction algorithm its weight is reduced by multiplication by a constant β, $0 \leq \beta \leq 1$.

Equivalent to Halving Algorithm when $\beta = 0$. Otherwise, this just down-weights contribution of algorithms which make errors.

Key result: number of mistakes made by Weighted Majority algorithm will never be greater than a constant factor times the number of mistakes made by the best member of the pool, plus a term that grows only logarithmically in the number of prediction algorithms in the pool.

Some questions about Machine Learning

1. Are there reasons to prefer one learning algorithm over another ?
2. Can we expect any method to be superior overall ?
3. Can we even find an algorithm that is overall superior to random guessing ?

Some questions about Machine Learning

- Perhaps surprisingly, the answer to each of these questions is *no*!
- Unless one has some prior knowledge on, or can make some assumptions about, the distribution of target functions.
- This is a consequence of a number of results collectively known as the "No Free Lunch" Theorem
- Since these results specifically address the issue of generalising from a training-set to minimize *off training-set error* they are also referred to as "Conservation Laws of Generalization".

No Free Lunch Theorem

统一的平均所有的目标函数,对于其off–train–set error 所有的算法都是一样的

Two main results are:

- Uniformly averaged over all target functions, the expected off-training-set error for all learning algorithms is the same.
- Assuming that the training set $\mathcal{D}$ can be learned correctly by all algorithms, averaged over all target functions no learning algorithm gives an off-training set error superior to any other:

假设有set D 能够完全正确的被所有算法学习到,平均所有目标函数,没有任何学习算法所产生的

$$\Sigma_F[\mathbb{E}_1(E|F,\mathcal{D}) - \mathbb{E}_2(E|F,\mathcal{D})] = 0$$

off–training–error 大于任何一种算法(都是一样的)

where F is the set of possible target functions, E is the off-training set error, and $\mathbb{E}_1$, $\mathbb{E}_2$ are expectations for two learning algorithms.

No Free Lunch Theorem

- There are also related results for cases where the distribution on target functions is not uniform.
- Therefore, all statements of the form "learning algorithm 1 is better than algorithm 2" are ultimately statements about the relevant target functions.

No Free Lunch example

- Consider a data set with three Boolean features, labelled by a target function F
- Suppose we have two different (deterministic) algorithms that generate two different hypotheses, both of which fit the training data $\mathcal{D}$ exactly
- The first algorithm assumes all instances x are in the target function F, unless labelled otherwise in training set $\mathcal{D}$, and the second algorithm assumes the opposite
- For *this particular target function* F the first algorithm is clearly superior in terms of off-training-set error
- But this cannot be determined from the performance on training data $\mathcal{D}$ alone !

No Free Lunch example

	x	F	h_1	h_2
$\mathcal{D}$	000	1	1	1
	001	-1	-1	-1
	010	1	1	1
	011	-1	1	-1
	100	1	1	-1
	101	-1	1	-1
	110	1	1	-1
	111	1	1	-1

$$\mathbb{E}_1(E|F,\mathcal{D}) = 0.4$$

$$\mathbb{E}_2(E|F,\mathcal{D}) = 0.6$$

No Free Lunch example

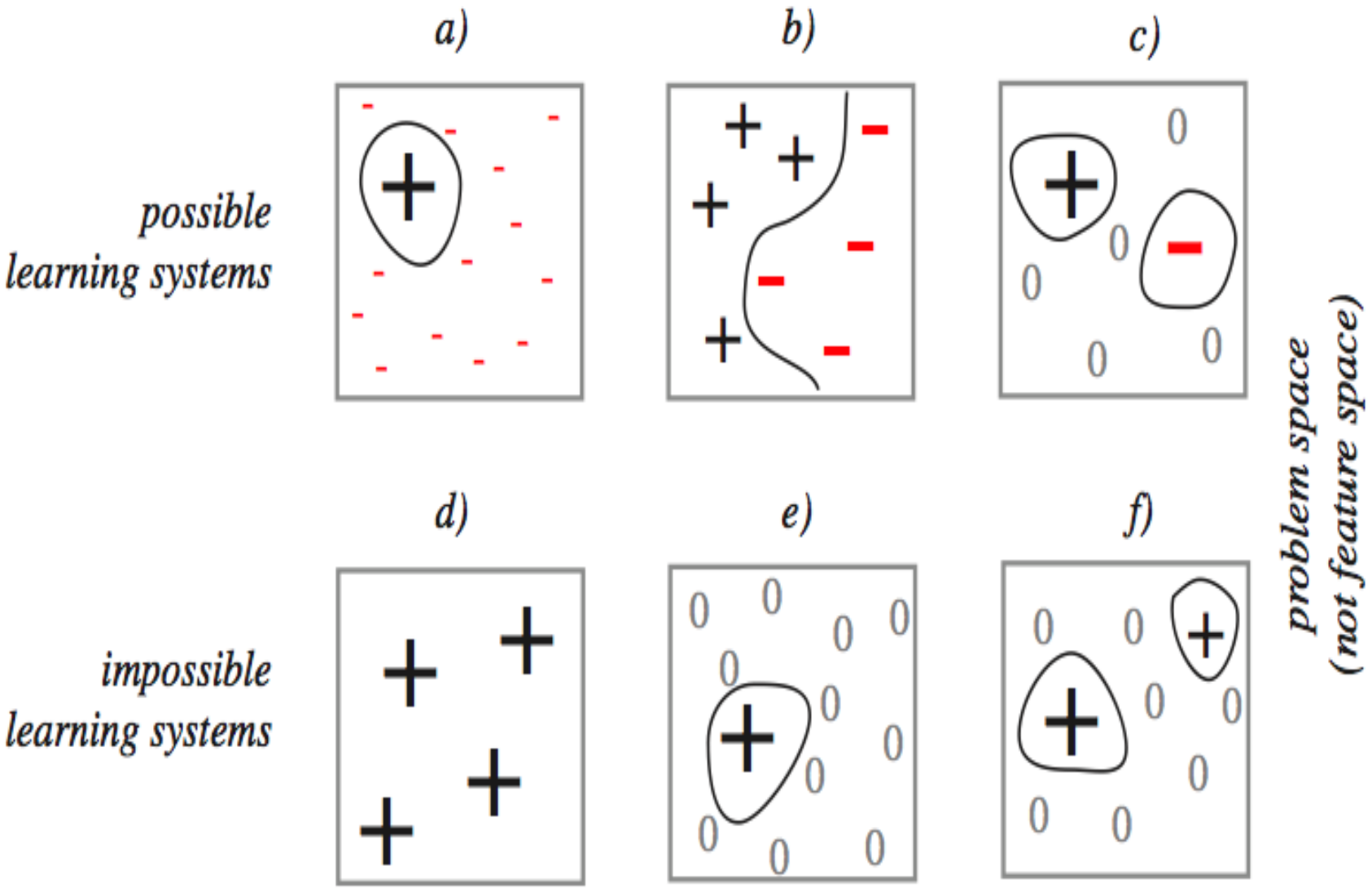
- But note that the algorithm designer does not *know* F here
- Furthermore, if we have *no prior knowledge* about which F we are trying to learn, neither algorithm is superior to the other
- Both fit the training data correctly, but there are a total of 2^5 target functions consistent with $\mathcal{D}$
- For each of these target functions there is exactly one other function whose output is inverted with respect to each of the off-training set instances
- So the performance of algorithms 1 and 2 will be inverted, and their off-training-set error differences cancel
- Thus ensuring expected (average) error difference of zero

A Conservation Theorem of Generalization Performance

For every possible learning algorithm for binary classification the sum of performance over all possible target functions is exactly zero !

- on some problems we get positive performance
- so there *must* be other problems for which we get an *equal and opposite amount* of negative performance

A Conservation Theorem of Generalization Performance



A Conservation Theorem of Generalization Performance

FIGURE 9.1. The No Free Lunch Theorem shows the generalization performance on the off-training set data that *can* be achieved (top row) and also shows the performance that *cannot* be achieved (bottom row). Each square represents all possible classification problems consistent with the training data—this is *not* the familiar feature space. A + indicates that the classification algorithm has generalization higher than average, a − indicates lower than average, and a 0 indicates average performance. The size of a symbol indicates the amount by which the performance differs from the average. For instance, part a shows that it is possible for an algorithm to have high accuracy on a small set of problems so long as it has mildly poor performance on all other problems. Likewise, part b shows that it is possible to have excellent performance throughout a large range of problem, but this will be balanced by very poor performance on a large range of other problems. It is impossible, however, to have good performance throughout the full range of problems, shown in part d. It is also impossible to have higher-than-average performance on some problems while having average performance everywhere else, shown in part e. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

A Conservation Theorem of Generalization Performance

Takeaways for machine learning practitioners:

- Even popular, theoretically well-founded algorithms will perform poorly on some domains, i.e., those where the learning algorithm is not a "good match" to the class of target functions.
- It is the *assumptions* about the learning domains, i.e., hidden target functions, that are relevant.
- Experience with a *broad range of techniques* is the best insurance for solving arbitrary new classification problems.

See: Duda, Hart & Stork (2001)

Ugly Duckling Theorem

In the absence of assumptions there is no privileged or "best" feature representation.

For n objects, the set of concepts is 2^n. The number of concepts of which any pair of objects is a member (has the same concept definition, or pattern) is 2^{n-1}

- using a finite number of predicates to distinguish any two patterns denoting sets of objects, the number of predicates shared by any two such patterns is constant and independent of those patterns.

Therefore, even the notion of similarity between patterns depends on assumptions, i.e., *inductive bias*.

See: Duda, Hart & Stork (2001)

Algorithm Independent Aspects of Machine Learning

- Algorithm independent analyses using techniques from computational complexity, pattern recognition, statistics, etc.
- Some results *over-conservative* from practical viewpoint, e.g., worst-case rather than average-case analyses
- Nonetheless, has led to many practically useful algorithms, e.g.,
- PAC
  - Boosting
- VC dimension
  - SVM
- Mistake Bounds
  - Winnow, Weighted Majority
- Bias-variance decomposition
  - Ensemble learning methods