Algorithm-Independent Aspects of Machine Learning

COMP9417 Machine Learning and Data Mining

May 9, 2017

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
- outline the "No Free Lunch" and "Ugly Duckling" Theorems

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 (next lecture) and support vector machines (earlier lecture)

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

Characterise *classes* of algorithms using questions such as:

- 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 ?

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 the 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 $\mathcal{D}$

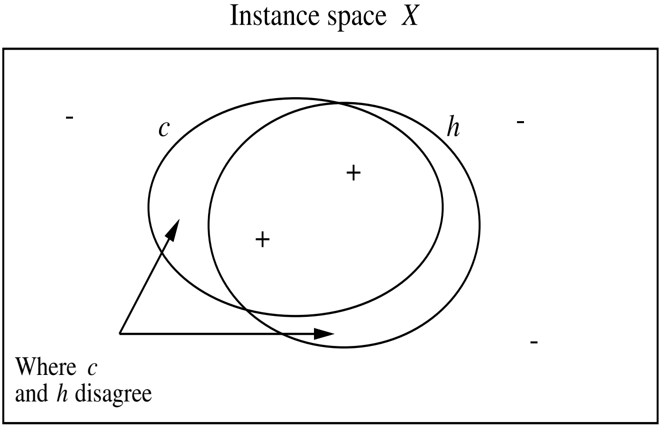
teacher provides target value $c(x)$ for each

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

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

Concept Learning as Search

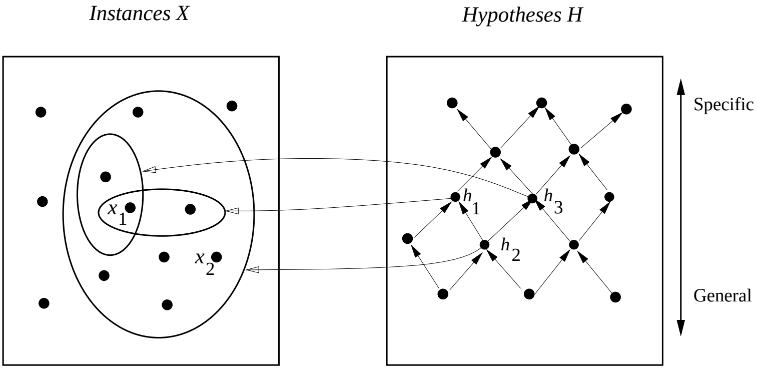
Hypothesis space

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

* any hypothesis with an $\emptyset$ constraint covers no instances, hence all are semantically equivalent.

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

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, ?*>

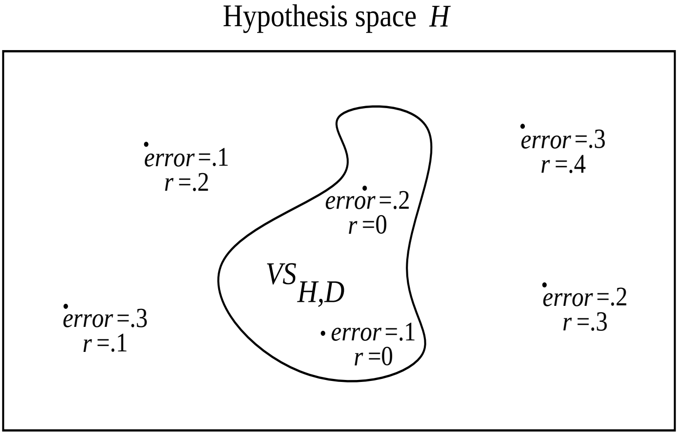
A generality order on hypotheses

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.

Exhausting the Version Space



Exhausting the Version Space

Note: in the diagram

$(r =$ training error, $error =$ 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

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

Learning Conjunctions of Boolean Literals

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

$$m \geq \frac{1}{.1}(\ln 973 + \ln(1/.05))$$

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

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

$$m \geq 98.8$$

C 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 *(Valiant, 1984)*.

Agnostic Learning

So far, assumed $c \in H$ — *consistent* learners

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 $|X| = 2^n$.

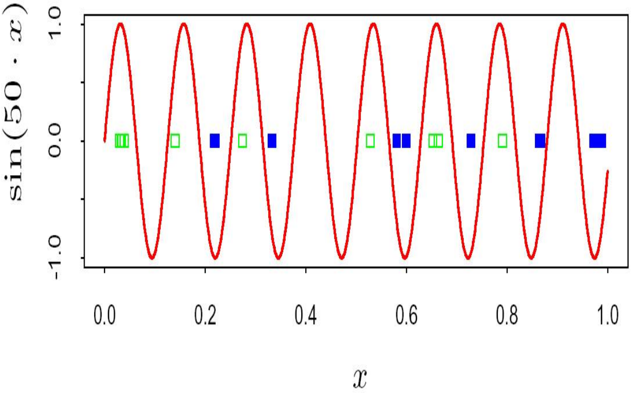
$$|C| = 2^{2^n}$$

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.

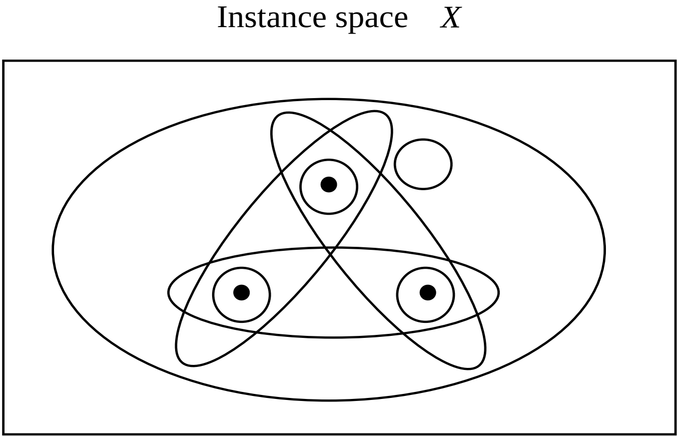
Classes separated based on $\sin(\alpha x)$, for frequency α, a *single* parameter.

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



Shattering a set of instances

Consider the following instances:

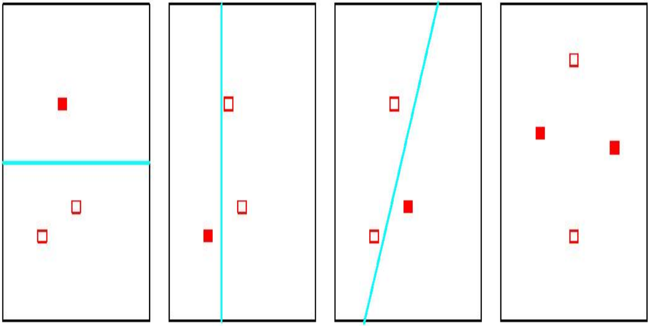
$$
\begin{aligned}
m &= \text{ManyTeeth} \wedge \neg\text{Gills} \wedge \neg\text{Short} \wedge \neg\text{Beak} \\
g &= \neg\text{ManyTeeth} \wedge \text{Gills} \wedge \neg\text{Short} \wedge \neg\text{Beak} \\
s &= \neg\text{ManyTeeth} \wedge \neg\text{Gills} \wedge \text{Short} \wedge \neg\text{Beak} \\
b &= \neg\text{ManyTeeth} \wedge \neg\text{Gills} \wedge \neg\text{Short} \wedge \text{Beak}
\end{aligned}
$$

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 ¬Gills ∧ ¬Beak, $\{g, s, b\}$ is represented by ¬ManyTeeth, $\{s\}$ is represented by ¬ManyTeeth ∧ ¬Gills ∧ ¬Beak, and so on. We say that this set of four instances is *shattered* by the hypothesis language of conjunctive concepts.

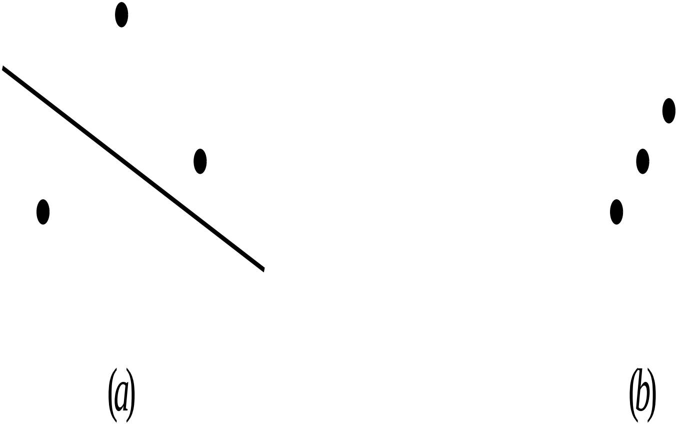
The Vapnik-Chervonenkis Dimension

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

VC Dim. of Linear Decision Surfaces



VC Dim. of Linear Decision Surfaces



Sample Complexity from VC Dimension

How many randomly drawn examples suffice to ϵ-exhaust $VS_{H,D}$ with probability at least $(1-\delta)$?

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

Mistake Bounds

So far: how many examples needed to learn?

What about: how many mistakes before convergence?

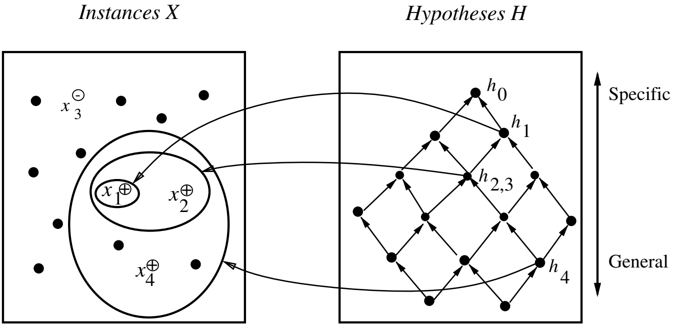
Let's consider similar setting to PAC learning:

- 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?

The Find-S 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 that is 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 and can never cover a negative example.

For each h generated by $\mathrm{Find\text{-}S}$, 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 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

Winnow

Mistake bounds following Littlestone (1987) who developed Winnow,

- an 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

Winnow2

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

WINNOW

- user-supplied threshold θ
    - class is 1 if $\sum w_i a_i > \theta$
- note similarity to perceptron training rule
    - WINNOW uses multiplicative weight updates
    - $\alpha > 1$
- will do better than perceptron with many irrelevant attributes
    - an *attribute-efficient* learner

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 $c(x) \neq 1$
    - 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

Consider the Halving Algorithm:

- Learn concept using version space CANDIDATE-ELIMINATION algorithm
- Classify new instances by majority vote of version space members

How many mistakes before converging to correct h?

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

Mistake Bounds: Halving Algorithm

Consider the Halving Algorithm:

- Learn concept using version space CANDIDATE-ELIMINATION algorithm
- Classify new instances by majority vote of version space members

How many mistakes 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 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

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

- generalisation of HALVING ALGORITHM
- predicts by *weighted vote* of set of prediction algorithms
- learns by altering weights for prediction algorithms
- a *prediction algorithm* simply predicts value of target concept given instance
    - elements of hypothesis space H
    - different learning algorithms
- inconsistency between prediction algorithm and training example
    - reduce weight of prediction algorithm
- bound no. of mistakes of ensemble by no. of mistakes made by *best* prediction algorithm

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 constant β, $0 \leq \beta \leq 1$.

Equivalent to Halving Algorithm when $\beta = 0$. Otherwise, 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

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

No Free Lunch Theorem

- uniformly averaged over all target functions, the expected off-training-set error for all learning algorithms is the same
- even for a fixed training set, averaged over all target functions no learning algorithm yields an off-training-set error that is superior to any other

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

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:

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

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

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

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

No Free Lunch example

BUT

if we have *no prior knowledge* about which F we are trying to learn, neither algorithm is superior to the other

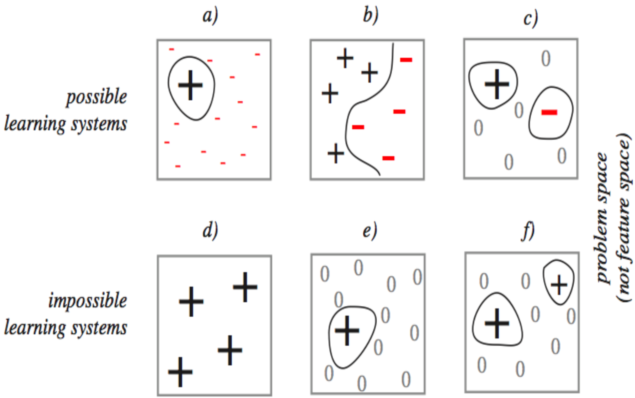
both fit the training data correctly, but there are 2^5 target functions consistent with $\mathcal{D}$
and for each there is exactly one other function whose output is inverted with respect to each of the off-training set patterns
so the performance of algorithms 1 and 2 will be inverted
thus ensuring 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

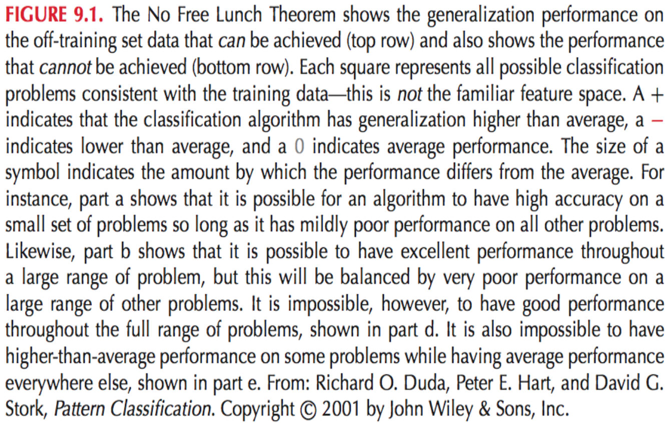


FIGURE 9.1. The No Free Lunch Theorem shows the generalization performance on the off-training set data that *can* be achieved (top row) and also shows the performance that *cannot* be achieved (bottom row). Each square represents all possible classification problems consistent with the training data—this 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:

- Even popular, theoretically 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 that are relevant.
- Experience with a *broad range of techniques* is the best insurance for solving arbitrary new classification problems.

from: 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*.

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
- Bias-variance decomposition
  - Ensemble learning methods