Computational learning and discovery

CSI 873 / MATH 689

Instructor: I. Griva

Wednesday 7:20 - 10 pm

Computational Learning Theory

What general laws constrain inductive learning?

We seek theory to relate:

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

Computational Learning Theory

answers such questions as

- **How many training examples are needed to converge with high probability to a successful learner? (Sample complexity).**

- **How much computational effort are needed for a learner to converge to a successful hypothesis? (Computational complexity).**

- **How many training example will the learner misclassify before converging to a successful hypothesis? (Mistake bounds).**

Sample complexity

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

1. If learner proposes instances, as queries to teacher
   - Learner proposes instance x, teacher provides $c(x)$
2. If teacher (who knows c) provides training examples
   - teacher provides sequence of examples of form $\langle x, c(x) \rangle$
3. If some random process (e.g., nature) proposes instances
   - instance x generated randomly, teacher provides $c(x)$

Sample complexity: Candidate elimination algorithm

Learner proposes instance x, teacher provides $c(x)$ (assume c is in learner's hypothesis space H)

Optimal query strategy: play 20 questions

- pick instance x such that half of hypotheses in VS classify x positive, half classify x negative
- When this is possible, need $\log_2 |H|$ queries to learn c
- when not possible, need even more

General notations

X is a set of instances over which the concept is defined

D is is the probability distribution that defines the probability of encountering each instance in X

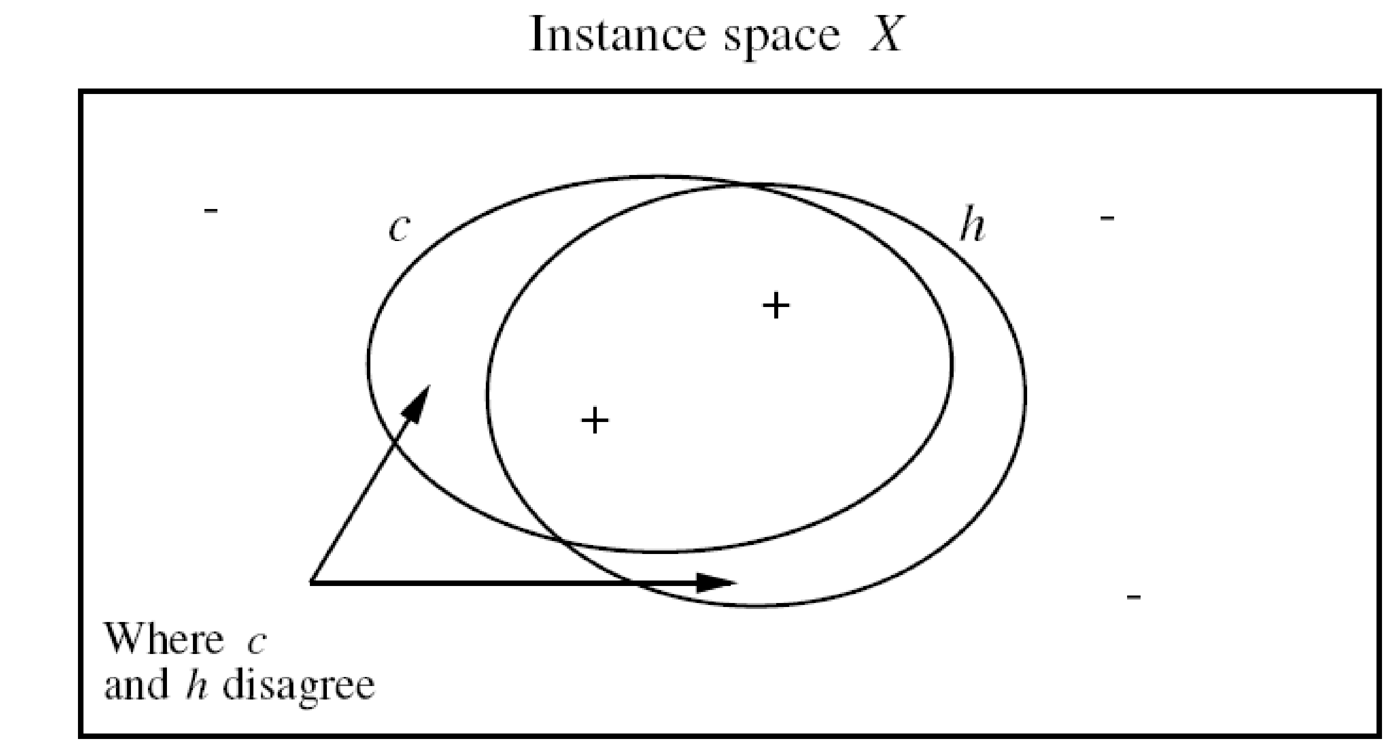
c is a target concept, $c: X \rightarrow \{0, 1\}$

$(x, c(x))$ is a training example

H is the set of all possible hypotheses the learner considers to identify the target concept

The goal is to find a hypothesis h in H such that $h(x) = c(x)$ for all x in X

True error of the 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 $\mathcal{D}$.

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

True error vs training 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:

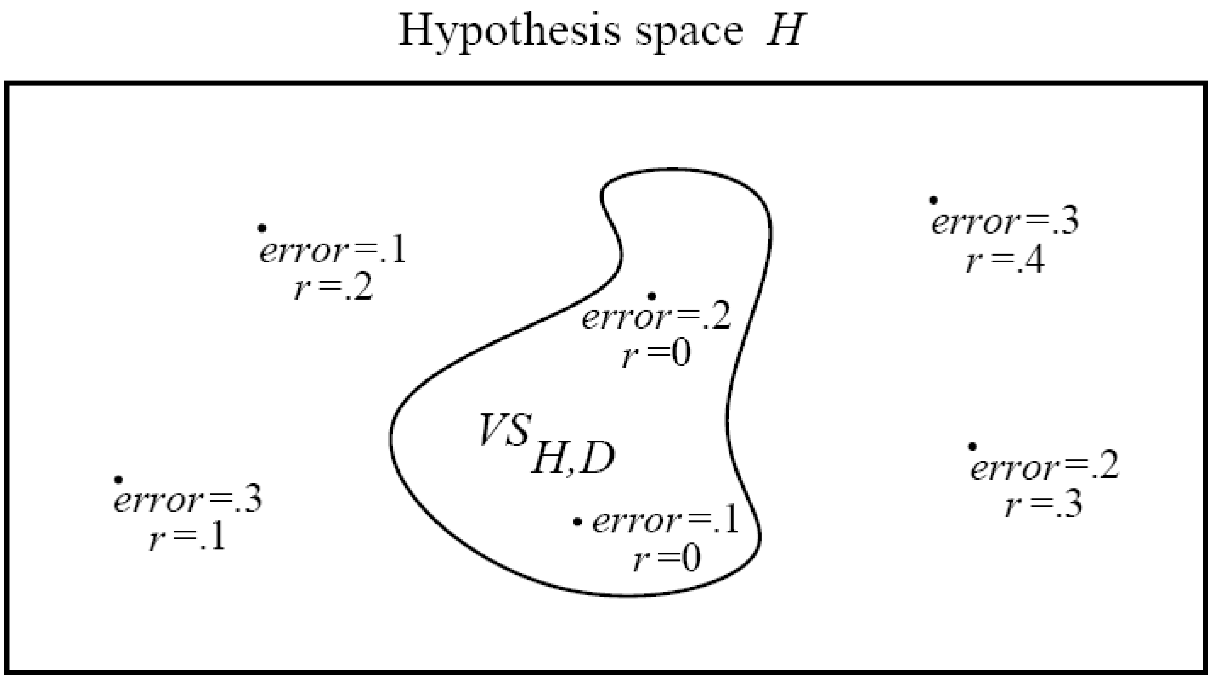
- Can we bound the true error of h given the training error of h?

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 $size(c)$.

Exhausting the version space



(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 $\mathcal{D}$.

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

Exhausting the version space

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

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

Exhausting the version space

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

If we want to this probability to be below δ

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

then

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

Learning conjunction 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:

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

Suppose H contains conjunctions of constraints on up to n boolean attributes (i.e., n boolean literals). Then $|H| = 3^n$, and

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

or

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

Learning *Enjoy Sport*

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

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

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

... 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

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

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

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

$$m \geq 98.8$$

Agnostic Learning

So far, assumed $c \in H$

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

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

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

derived from Hoeffding bounds:

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

Shattering 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.

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 dimension of linear decision surface

(a) (b)

Sample complexity and VC dimension

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

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

Sufficient condition

Sample complexity and VC dimension

Theorem 7.3. Lower bound on sample complexity. Consider any concept class C such that $VC(C) \geq 2$, any learner L, and any $0 < \epsilon < \frac{1}{8}$, and $0 < \delta < \frac{1}{100}$. Then there exists a distribution $\mathcal{D}$ and target concept in C such that if L observes fewer examples than

$$\max\left[\frac{1}{\epsilon}\log(1/\delta), \frac{VC(C)-1}{32\epsilon}\right]$$

then with probability at least δ, L outputs a hypothesis h having $error_{\mathcal{D}}(h) > \epsilon$.

Necessary condition

VC dimension of neural network

Theorem 7.4. VC-dimension of directed acyclic layered networks. (See Kearns and Vazirani 1994.) Let G be a layered directed acyclic graph with n input nodes and $s \geq 2$ internal nodes, each having at most r inputs. Let C be a concept class over $\Re^r$ of VC dimension d, corresponding to the set of functions that can be described by each of the s internal nodes. Let C_G be the G-composition of C, corresponding to the set of functions that can be represented by G. Then $VC(C_G) \leq 2ds \log(es)$, where e is the base of the natural logarithm.

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?

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: *Candidate Elimination 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?

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 $M_A(C)$.

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

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

Relative Mistake Bound for Weighted Majority

Theorem 7.5. Relative mistake bound for WEIGHTED-MAJORITY. Let D be any sequence of training examples, let A be any set of n prediction algorithms, and let k be the minimum number of mistakes made by any algorithm in A for the training sequence D. Then the number of mistakes over D made by the WEIGHTED-MAJORITY algorithm using $\beta = \frac{1}{2}$ is at most

$$2.4(k + \log_2 n)$$

Summary

- The probably approximately correct (PAC) model considers algorithms that learn target concepts from some concept class C, using training examples drawn at random according to an unknown, but fixed, probability distribution. It requires that the learner probably (with probability at least $[1-\delta]$) learn a hypothesis that is approximately (within error ϵ) correct, given computational effort and training examples that grow only polynomially with $1/\epsilon$, $1/\delta$, the size of the instances, and the size of the target concept.
- Within the setting of the PAC learning model, any consistent learner using a finite hypothesis space H where $C \subseteq H$ will, with probability $(1-\delta)$, output a hypothesis within error ϵ of the target concept, after observing m randomly drawn training examples, as long as

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

  This gives a bound on the number of training examples sufficient for successful learning under the PAC model.

Summary (continued)

- One constraining assumption of the PAC learning model is that the learner knows in advance some restricted concept class C that contains the target concept to be learned. In contrast, the *agnostic learning* model considers the more general setting in which the learner makes no assumption about the class from which the target concept is drawn. Instead, the learner outputs the hypothesis from H that has the least error (possibly nonzero) over the training data. Under this less restrictive agnostic learning model, the learner is assured with probability $(1-\delta)$ to output a hypothesis within error ϵ of the best possible hypothesis in H, after observing m randomly drawn training examples, provided

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

- The number of training examples required for successful learning is strongly influenced by the complexity of the hypothesis space considered by the learner. One useful measure of the complexity of a hypothesis space H is its Vapnik-Chervonenkis dimension, $VC(H)$. $VC(H)$ is the size of the largest subset of instances that can be shattered (split in all possible ways) by H.

Summary (continued)

- An alternative upper bound on the number of training examples sufficient for successful learning under the PAC model, stated in terms of $VC(H)$ is

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

  A lower bound is

$$m \geq \max\left[\frac{1}{\epsilon}\log(1/\delta), \frac{VC(C)-1}{32\epsilon}\right]$$

- An alternative learning model, called the *mistake bound model*, is used to analyze the number of training examples a learner will misclassify before it exactly learns the target concept. For example, the HALVING algorithm will make at most $\lfloor \log_2 |H| \rfloor$ mistakes before exactly learning any target concept drawn from H. For an arbitrary concept class C, the best worst-case algorithm will make $Opt(C)$ mistakes, where

$$VC(C) \leq Opt(C) \leq \log_2(|C|)$$

- The WEIGHTED-MAJORITY algorithm combines the weighted votes of multiple prediction algorithms to classify new instances. It learns weights for each of these prediction algorithms based on errors made over a sequence of examples. Interestingly, the number of mistakes made by WEIGHTED-MAJORITY can be bounded in terms of the number of mistakes made by the best prediction algorithm in the pool.