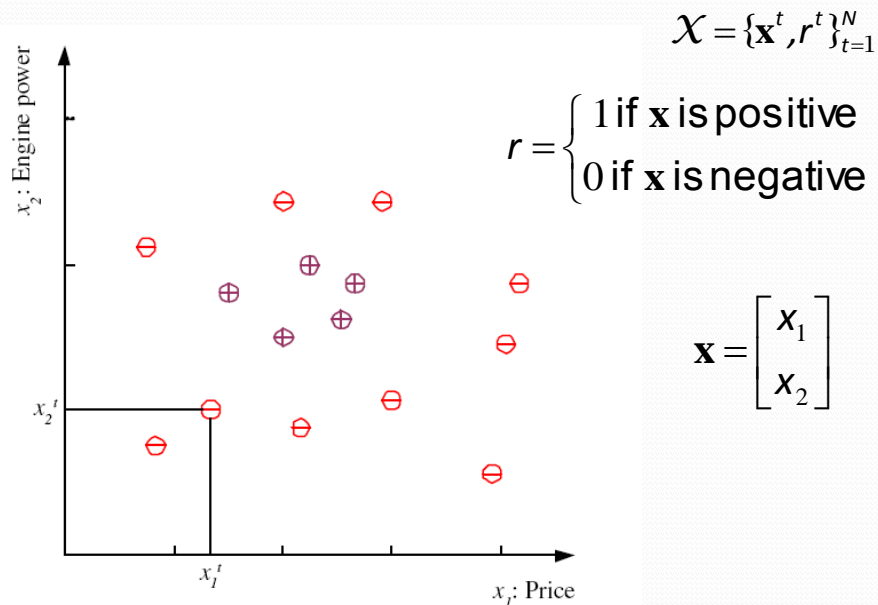


Alpaydin Chapter 2, Mitchell Chapter 7

- Alpaydin slides are in turquoise.
 - Ethem Alpaydin, copyright: The MIT Press, 2010.
 - alpaydin@boun.edu.tr
 - <http://www.cmpe.boun.edu.tr/~ethem/i2ml2e>
- All other slides are based on Mitchell.

1

Training set \mathcal{X}



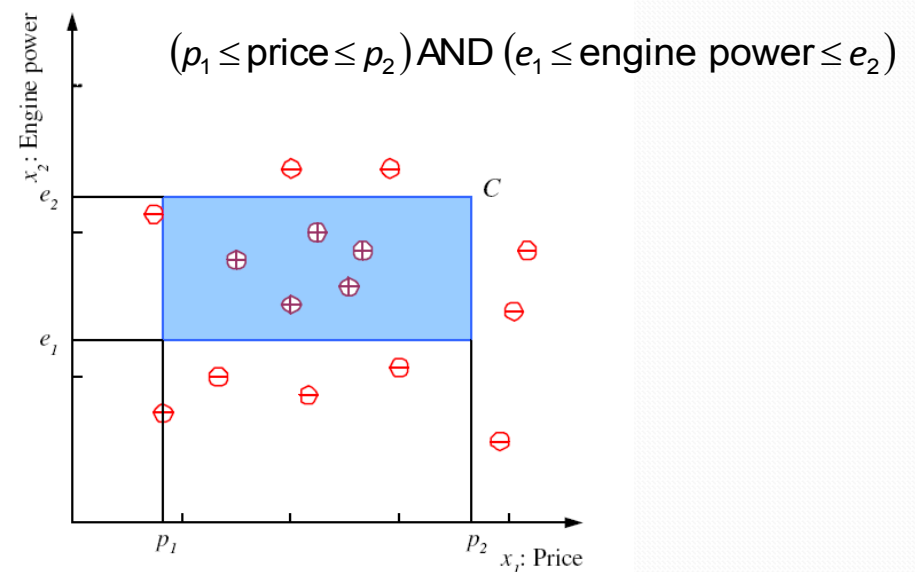
4

Learning a Class from Examples

- Class C of a “family car”
 - Prediction: Is car x a family car?
 - Knowledge extraction: What do people expect from a family car?
- Output:
 - Positive (+) and negative (–) examples
- Input representation:
 - x_1 : price, x_2 : engine power

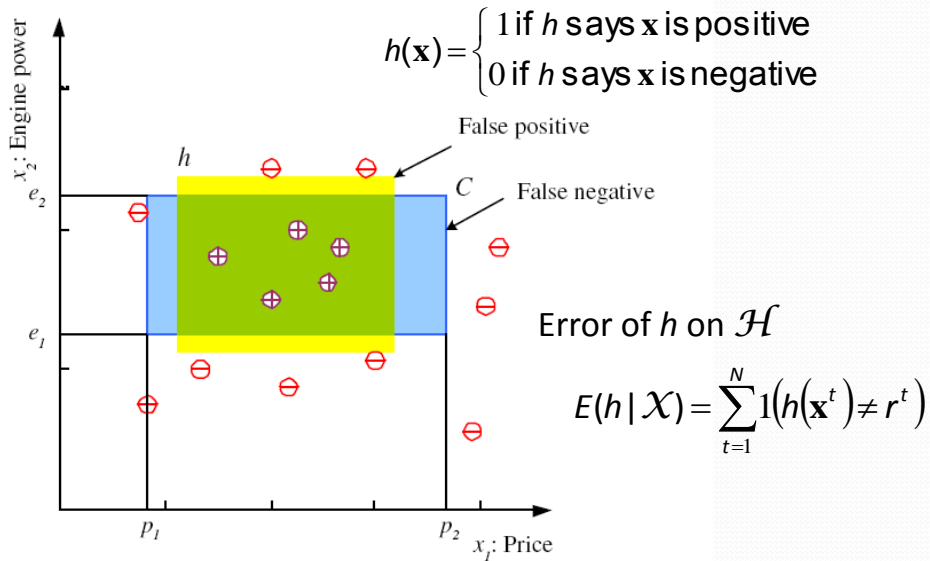
3

Class C

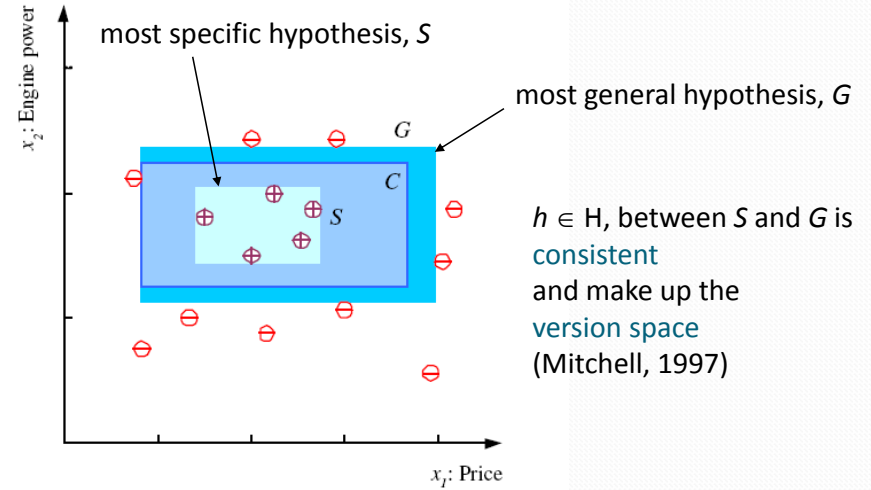


5

Hypothesis class \mathcal{H}



S, G, and the Version Space



Computational Learning Theory (from Mitchell Chapter 7)

- Theoretical characterization of the **difficulties** and **capabilities** of learning algorithms.
- Questions:
 - Conditions for successful/unsuccessful learning
 - Conditions of success for particular algorithms
- Two frameworks:
 - Probably Approximately Correct (PAC) framework: classes of hypotheses that can be learned; complexity of hypothesis space and bound on training set size.
 - Mistake bound framework: number of training errors made before correct hypothesis is determined.

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

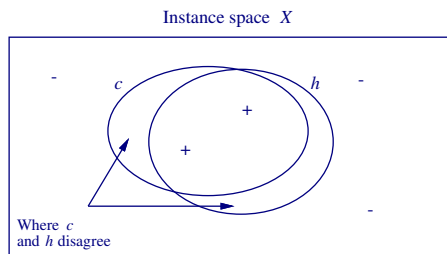
Specific Questions

- Sample complexity: How many training examples are needed for a learner to converge?
- Computational complexity: How much computational effort is needed for a learner to converge?
- Mistake bound: How many training examples will the learner misclassify before converging?

Issues: When to say it was successful? How are inputs acquired?

4

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} .

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

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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 $c(x)$

5

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

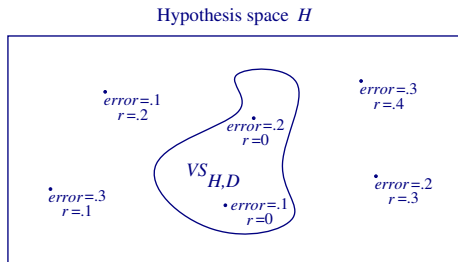
- How often $h(x) \neq c(x)$ over future random instances

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., $h \in VS_{H,D}$)

7

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} .

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

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Proof of ϵ -Exhausting Theorem

Theorem: Prob. of $VS_{H,D}$ not being ϵ -exhausted is $\leq |H|e^{-\epsilon m}$.

Proof:

- Let $h_i \in H$ ($i = 1..k$) be those that have true error greater than ϵ wrt c ($k \leq |H|$).
- We fail to ϵ -exhaust the VS iff at least one h_i is consistent with all m sample training instances (note: they have true error greater than ϵ).
- Prob. of a single hypothesis with error $> \epsilon$ is consistent for one random sample is at most $(1 - \epsilon)$.
- Prob. of that hypothesis being consistent with m samples is $(1 - \epsilon)^m$.
- Prob. of at least one of k hypotheses with error $> \epsilon$ is consistent with m samples is $k(1 - \epsilon)^m$.
- Since $k \leq |H|$, and for $0 \leq \epsilon \leq 1$, $(1 - \epsilon) \leq e^{-\epsilon}$:

$$k(1 - \epsilon)^m \leq |H|(1 - \epsilon)^m \leq |H|e^{-\epsilon m}$$

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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

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

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

If we want this probability to be below δ

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

then

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

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PAC Learning

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

Definition: \mathcal{C} is **PAC-learnable** by L using H if for all $c \in \mathcal{C}$, 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 $size(c)$.

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Agnostic Learning

So far, we assumed that $c \in H$. What if it is not the case?

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?

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

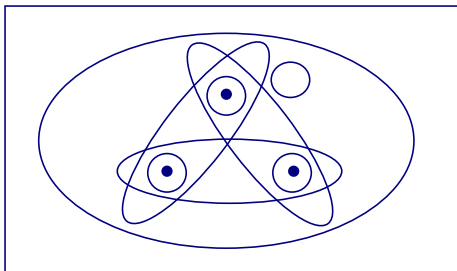
derived from Hoeffding bounds:

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

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Three Instances Shattered

Instance space X



Each closed contour indicates one dichotomy. What kind of hypothesis space H can shatter the instances?

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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.

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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 that $|H|$ can be infinite, while $VC(H)$ finite!

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VC Dim. of Linear Decision Surfaces



- When H is a set of lines, and S a set of points, $VC(H) = 3$.
- (a) can be shattered, but (b) cannot be. However, if at least one subset of size 3 can be shattered, that's fine.
- Set of size 4 cannot be shattered, for any combination of points (think about an XOR-like situation).

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Sample Complexity from VC Dimension

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

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

$VC(H)$ is directly related to the sample complexity:

- More expressive H needs more samples.
- More samples needed for H with more tunable parameters.

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VC Dimension: Another Example

$S = \{3.1, 5.7\}$, and hypothesis space includes intervals $a < x < b$.

- Dichotomies: both, none, 3.1, or 5.7.
- Are there intervals that cover all the above dichotomies?

What about $S = x_0, x_1, x_2$ for an arbitrary x_i ? (cf. collinear points).

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Mistake Bounds

So far: how many examples needed to learn?

What about: how many mistakes before convergence?

- This is an interesting question because some learning systems may need to start operating while still learning.

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?

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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 $M_A(C)$.

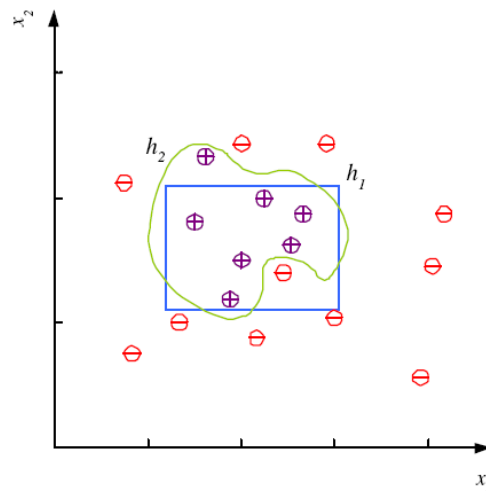
$$Opt(C) \equiv \min_{A \in \text{learning algorithms}} M_A(C)$$

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Noise and Model Complexity

Use the simpler one because

- Simpler to use (lower computational complexity)
- Easier to train (lower space complexity)
- Easier to explain (more interpretable)
- Generalizes better (lower variance - Occam's razor)



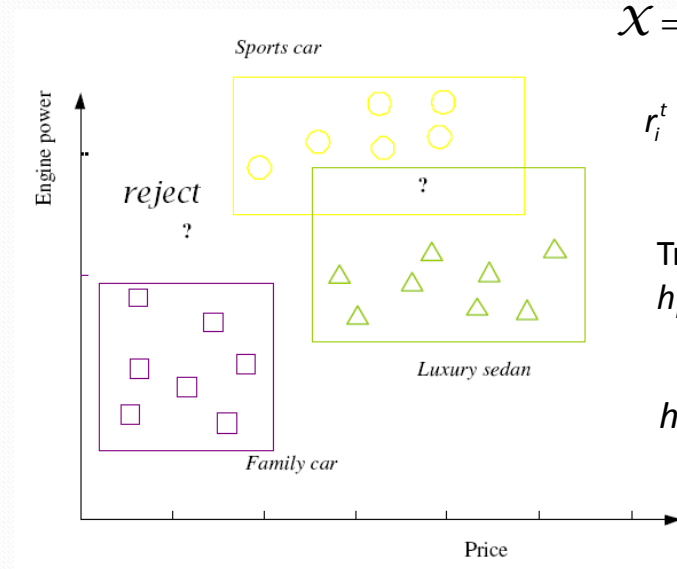
Mistake Bounds and VC Dimension

Littlestone (1987) showed:

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

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Multiple Classes, C_i $i=1, \dots, K$



$$\mathcal{X} = \{\mathbf{x}^t, r^t\}_{t=1}^N$$

$$r_i^t = \begin{cases} 1 & \text{if } \mathbf{x}^t \in C_i \\ 0 & \text{if } \mathbf{x}^t \in C_j, j \neq i \end{cases}$$

Train hypotheses $h_i(\mathbf{x}), i=1, \dots, K:$

$$h_i(\mathbf{x}^t) = \begin{cases} 1 & \text{if } \mathbf{x}^t \in C_i \\ 0 & \text{if } \mathbf{x}^t \in C_j, j \neq i \end{cases}$$

Regression

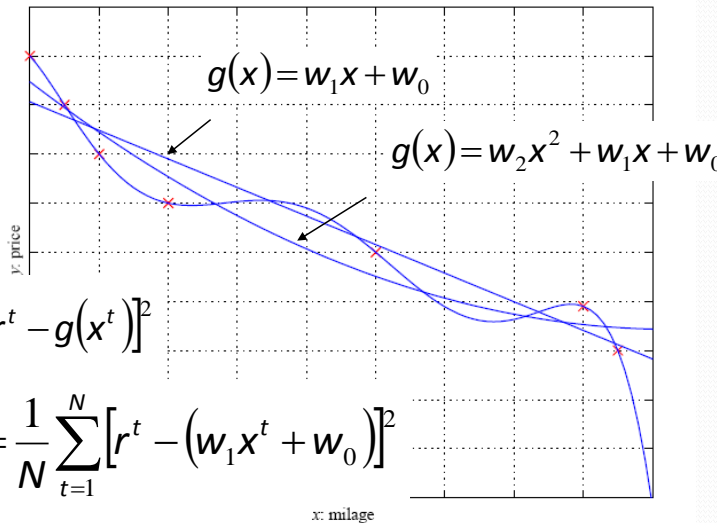
$$\mathcal{X} = \{x^t, r^t\}_{t=1}^N$$

$$r^t \in \mathcal{R}$$

$$r^t = f(x^t) + \varepsilon$$

$$E(g | \mathcal{X}) = \frac{1}{N} \sum_{t=1}^N [r^t - g(x^t)]^2$$

$$E(w_1, w_0 | \mathcal{X}) = \frac{1}{N} \sum_{t=1}^N [r^t - (w_1 x^t + w_0)]^2$$



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Model Selection & Generalization

- Learning is an ill-posed problem, data is not sufficient to find a unique solution
- The need for inductive bias assumptions about \mathcal{H}
- Generalization: How well a model performs on new data
- Overfitting: \mathcal{H} more complex than C or f
- Underfitting: \mathcal{H} less complex than C or f

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Triple Trade-Off

- There is a trade-off between three factors (Dietterich, 2003):
 1. Complexity of \mathcal{H} , $c(\mathcal{H})$,
 2. Training set size, N ,
 3. Generalization error, E , on new data
- As $N \uparrow$, $E \downarrow$
- As $c(\mathcal{H}) \uparrow$, first $E \downarrow$ and then $E \uparrow$

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Cross-Validation

- To estimate generalization error, we need data unseen during training. We split the data as
 - Training set (50%)
 - Validation set (25%)
 - Test (publication) set (25%)
- Resampling when there is few data

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Dimensions of a Supervised Learner

1. Model: $g(\mathbf{x}|\theta)$

2. Loss function: $E(\theta|\mathcal{X}) = \sum_t L(r^t, g(\mathbf{x}^t|\theta))$

3. Optimization procedure:

$$\theta^* = \operatorname{argmin}_{\theta} E(\theta|\mathcal{X})$$