Computational Learning Theory

Goals of Learning Theory

- Hypothesis Space and Inductive Bias
- Concepts
  - What kinds of tasks are learnable?
  - What kind of data is required for learnability?
  - What are the (space, time) requirements of the learning algorithms?
- Models
  - Develop algorithms that provably meet desired criteria
  - Prove guaranties for success full algorithms

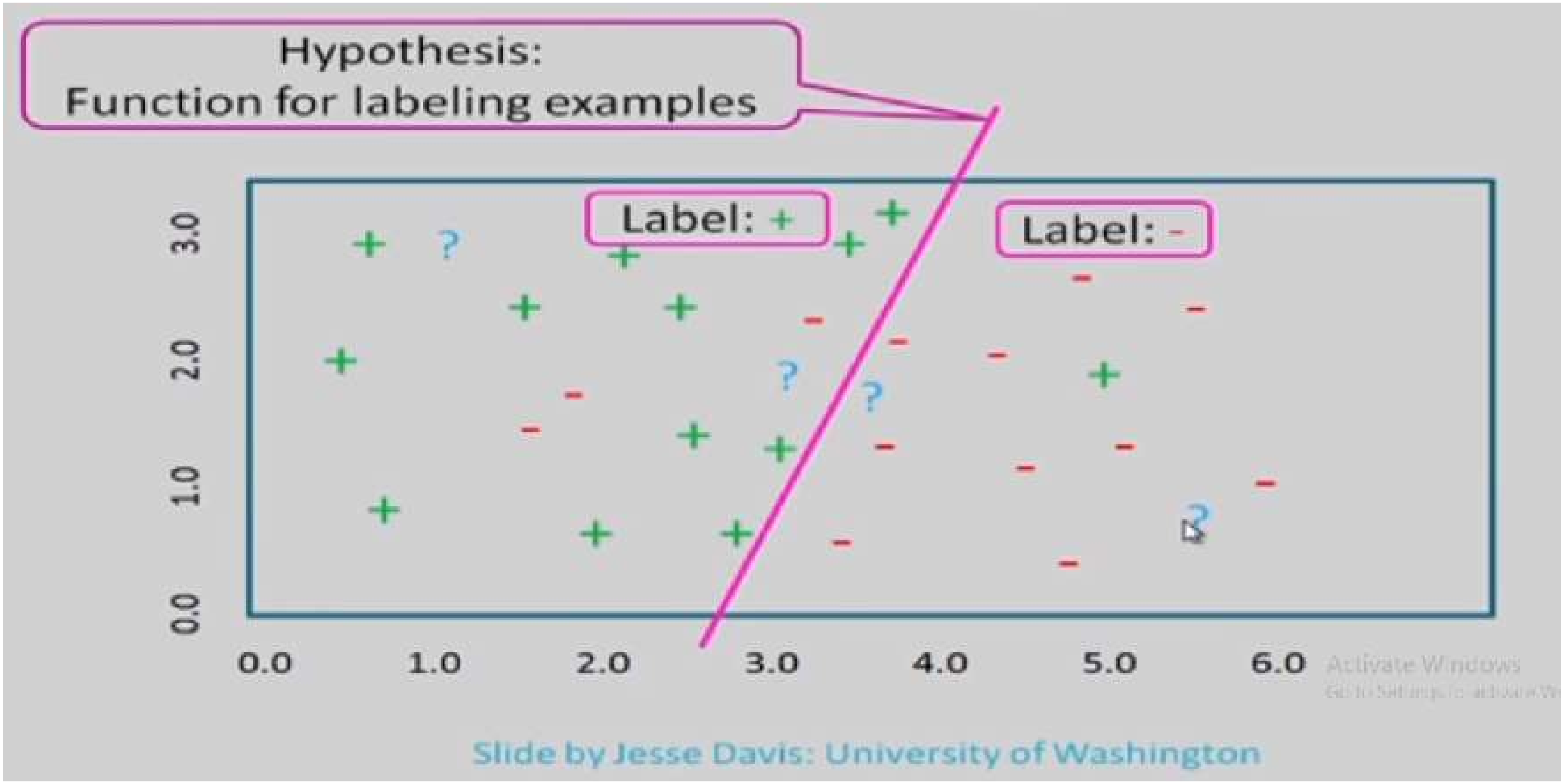
Inductive Learning

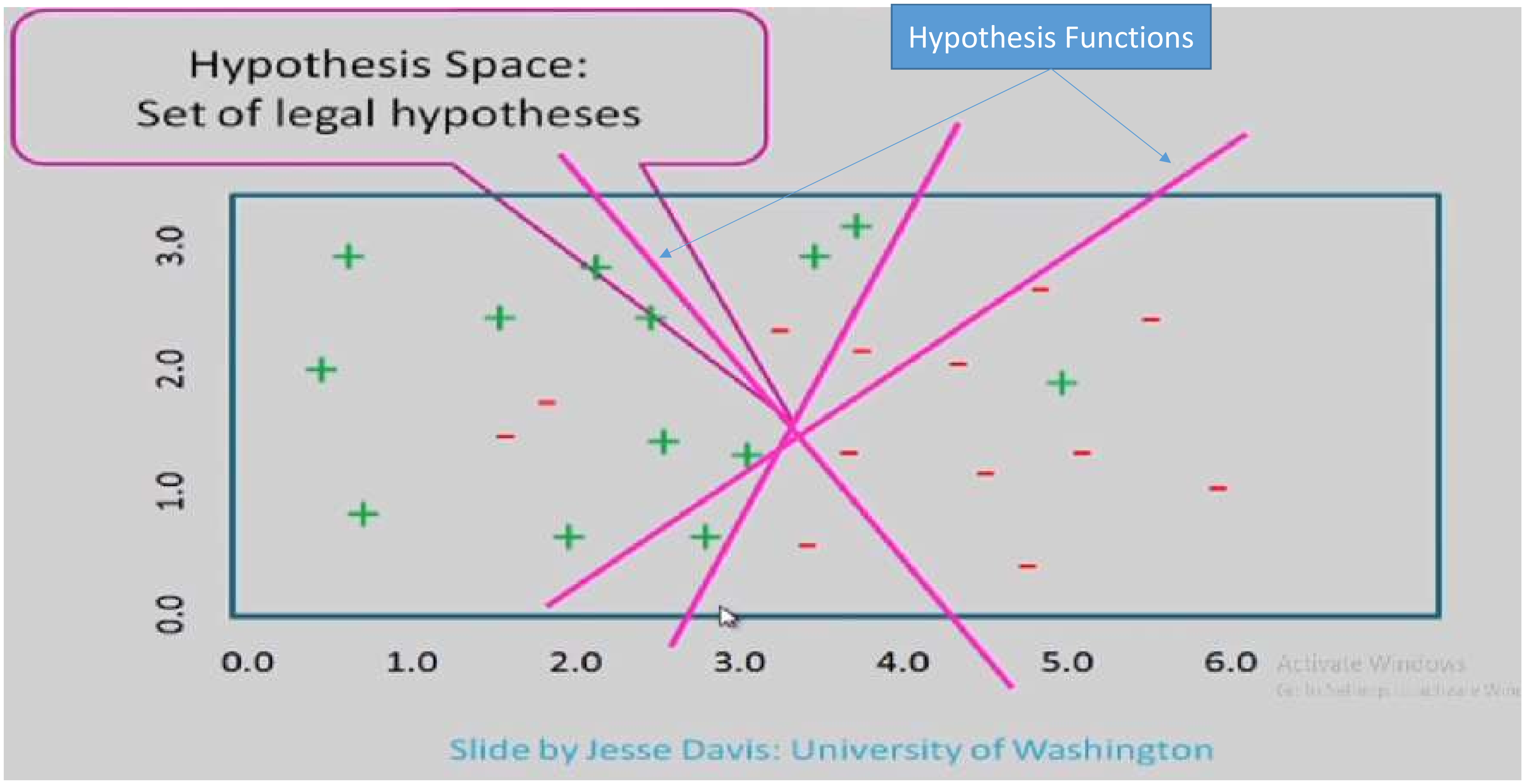
- We are given some data, and we are trying to do induction to try to identify a function (f) which can explain the data ($\hat{x}$).
- $y = f(\hat{x})$
- Examples: $(\hat{x}, y)$ or $(\hat{x}, f(\hat{x}))$
- So induction as opposed to deduction.
- Unless we can see all the instances, all the possible data paints or we make some restrictive assumptions about the language in which the hypothesis is expressed or some bias, this problem is not well defined. So that is why it is called an Inductive Problem.

Features

- Classification: $f(\hat{x})$ is discrete
- Regression: $f(\hat{x})$ is continuous
- Probability estimation: probability of the $\hat{x}$.

- Features are properties that describe each instances. Each instances can be described in quantitative manner by the features
- Multiple feature: feature vector


Hypothesis:
Function for labeling examples
Label: +
Label: -
0.0
1.0
2.0
3.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
Activate Windows
Slide by Jesse Davis: University of Washington


Hypothesis Space:
Set of legal hypotheses
Hypothesis Functions
0.0
1.0
2.0
3.0
4.0
5.0
6.0
Slide by Jesse Davis: University of Washington

Language of Function

Hypothesis Space

- Hypothesis Space:
  - The space of all hypothesis that can in principle be output by a learning algorithm.
  - We can think about a supervised learning machine as a devise that explore a hypothesis space.
    - Each setting of the parameters in the machine is a different hypothesis about the function that maps the input vectors to output vectors.

$$\underbrace{h}_{\text{o/p of learning algo.}} \in \underbrace{\mathcal{H}}_{\text{Hypothesis Space}}$$

Terminology:

- Example $(\hat{x}, y)$: instance x with label y=f(x)
- Training data S: Collection of training data observed by learning algorithm
- Instance (feature) Space X: Set of all possible objects described by features
- Concept C: Subset of objects from X: $C \subseteq \mathsf{X}$ (C is unknown)
- Target function f: maps each instance $x \in$ X to the target label $y \in$ Y

Classifier

- Hypothesis h : Find function $h \in \mathcal{H}$ to approximate f.
- Hypothesis Space $\mathcal{H}$: set of functions we allow for approximating f
- The set of hypothesis that can be produced, can be restricted further by specifying a language bias
    - Constraints
    - Preferences
- Input: Training set $S \subseteq X$
- Output: $h \in \mathcal{H}$

Hypothesis Space: Example

- If there are N (let N=4) input features, there are 2^{16} ($2^{2^4} = 2^{2^N}$) possible Boolean functions.
- We can’t figure out which one is correct unless we see every possible i/p-o/p pair 2^4 (2^N)
- So for 4 input features (N=4), possible instances = 2^4 (2^N).
- Functions will classify some of the points as +ve and some of the points are –ve, out of 16 points.
- So the no. of functions are no. of possible subsets of these 2^4 =16 instances. Since binary classification, it is $2^{2^4} = 2^{16}$
- So, it seems hypothesis space is very large.

Inductive Bias

- Since, hypothesis space may be very large, we can select a hypothesis language
- May be un-restricted or restricted
- In case of restriction, a hypothesis language reflects an inductive bias of the learner.

Inductive Bias

- Need to make assumption
  - Experience alone does not allow us to make conclusions about unseen data instances
- Two types of bias(s)
  - Restriction Bias: Limit the hypothesis space
  - Preference Bias: Impose ordering on hypothesis space

Inductive Learning

- Inductive learning: Inducing a general function for training examples.
  - Construct hypothesis h to agree with (Concepts) c on the training examples
  - A hypothesis is consistent if it agrees with all training examples
  - A hypothesis is said to generalize well if it correctly predicts the values of Y for novel examples.
- Inductive learning is an ill-posed problem
  - Unless we see all possible examples the data is not sufficient for an inductive learning algorithm to find an unique solution.
  - Any hypothesis h found to approximate the target function C well over a sufficiently large set of training examples D will also approximate the target function well over unobserved examples.

Learning as Referencing the Hypothesis Space

- Concept learning is task of searching an hypothesis space of possible representations looking for the representation (S) that best fits the data points, given the bias.

- The tendency to prefer the hypothesis over another is called a bias (Preference bias).

- Given representation, data and a bias the problem of learning can be reduced to one of the SEARCH problems.

Occam’s Razor

- A classical example of inductive bias
  - The simplest consistent hypothesis about the target function is actually the best.
- Some other types of inductive bias
  - Minimum description length: when forming a hypothesis, attempt to minimize the length of the description of the hypothesis.
  - Maximum Margin: when drawing boundary between two classes, attempt to maximize the width of the boundary (Example: SVM)

Some Important Issues of Machine Learning

- What are the good hypothesis space?
- Algorithm that works with the hypothesis space.
- How to optimize the accuracy over the future data points (handling overfitting)?
- How can we have confidence in the results? (How much training data?)
- Are some training problems computationally intractable?

Goals of Learning Theory

- Hypothesis Space and Inductive Bias
- To understand
  - What kinds of tasks are learnable?
  - What kind of data is required for learnability?
  - What are the (space, time) requirements of the learning algorithms?
- To develop and analyze model
  - Develop algorithms that provably meet desired criteria
  - Prove guaranties for success full algorithms

Learning Theory

- What is the task ? (e.g. spam filtering)
- What types of data?
- Resource requirements
- Develop algorithms (under certain constraints) are provable?
- Confidence of the algorithm

Learning algorithms

- Design algorithms
  - In machine learning, we design algorithms that optimizes certain criteria
- Confidence of the algorithms
  - Generalization ability of the algorithm
    - How well this an algorithm works on testing data (future data)

PAC (Probably approximately correct) Models

C is the class, we wish to learn, h is the hypothesis class, h may not fully cover c, so there are some error region,

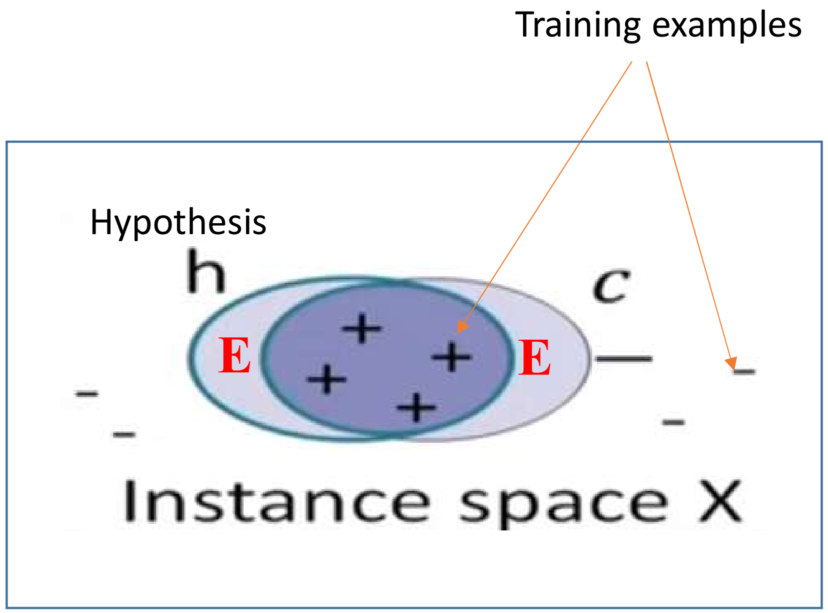
E = C xor H

We want the probability of this error region to be small i.e.

$$P(C \text{ xor } H) \leq \varepsilon$$

So, the hypothesis should be approximately correct and the error tolerance

$$0 \leq \varepsilon \leq \frac{1}{2}$$

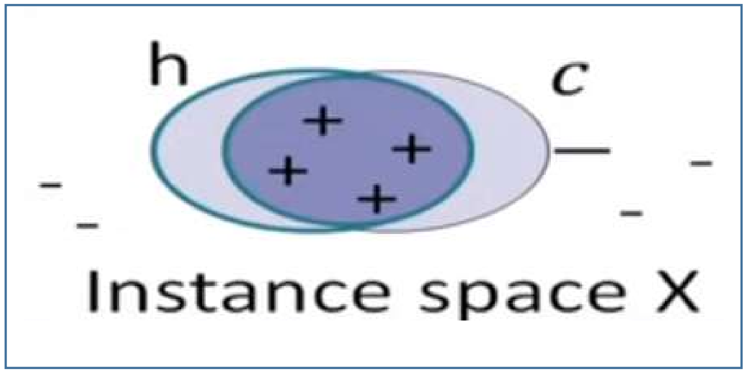


PAC (Probably approximately correct) Models

- Now hypothesis function is not always fully correct
- So the probability that the learning algorithm gives us the approximately correct hypothesis

$P(P(C \text{ xor } H) \leq \varepsilon) \geq (1-\delta)$ where δ the confidence parameter and $0 \leq \delta \leq \frac{1}{2}$

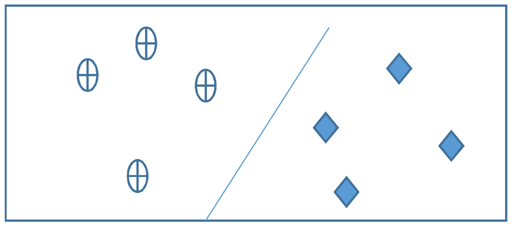
Prototypical Concept Learning Task



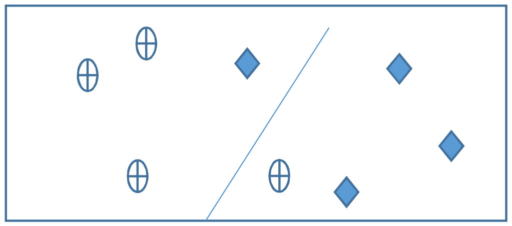
- Given
  - Instances X (e.g., X=R^d or X= $\{0,1\}^d$)
  - Distribution $\mathcal{D}$ over X
  - Target function C
  - Hypothesis space $\mathcal{H}$
  - Training Examples S ={($x_i, c(x_i)$) i.i.d from $\mathcal{D}$
- Determine
  - A hypothesis $h \epsilon \mathcal{H}$ s.t. h(x)=c(x) for all x in S?
  - A hypothesis $h \epsilon \mathcal{H}$ s.t. h(x)=c(x) for all x in X?
- An algorithm does optimization over S, find hypothesis h
- Goal: Find h which has small error over $\mathcal{D}$

Consistent Hypothesis

- Given the training samples, find the hypothesis h such that it agrees with the training examples, is called consistent hypothesis.



- For certain cases, we can't look for consistent hypothesis, so allow the inconsistent hypothesis.



Restriction Bias:

- Can we be certain about how the learning algorithm generalizes?
- We would have to see all examples.
- Inductive inference
  - Generalize beyond the training data is impossible unless we add more assumptions (e.g. priors over $\mathcal{H}$).
    - We need a **bias**.
- Restriction Bias: We can put a bias on the form of hypothesis class to allow hypothesis of certain restricted types, what is called restriction bias.
- In other words, it restricts the hypothesis space to get simpler hypothesis.

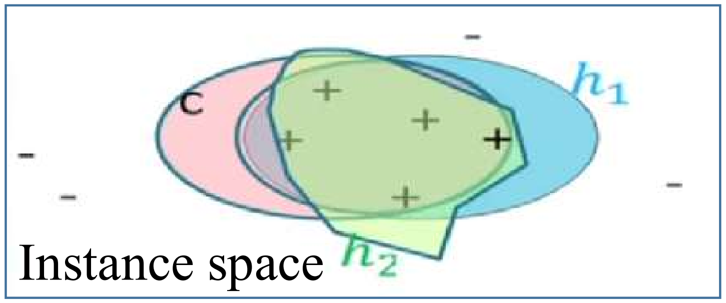
Preference Bias:

- Prefer some hypothesis over others. Small decision tree over large decision tree.

Function Approximation

- How many labelled examples are necessary in order to determine which of the 2^{2^N} hypothesis is the correct one?
- All 2^N instances are labelled.
- Inductive inference: Generalizing beyond the training data is impossible unless we add more assumption (e.g. bias)
- H = $\{h: X \rightarrow Y\}$ |H|= $2^{|X|=}2^{2^N}$
- N features, 2^N instances , so no. of possible partition of the instance space = 2^{2^N}

To find the one correct hypothesis, we have to check every 2^N instances.



Error of a hypothesis

- h measure the error (sample error) of h on sample S.
- The true error of the hypothesis h, with respect to the target concept c observation distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn according to the D

$$error_{\mathcal{D}}(h) = Pr_{x\sim\mathcal{D}}\,[c(x) \neq h(x)]$$

- In a perfect situation, we'd like the true error to be 0.
- Bias: Fix hypothesis space $\mathcal{H}$ such that $h\epsilon\mathcal{H}$
- C may not be in $\mathcal{H}$ → Find h close to c
- A hypothesis h is approximately correct if

$$error_{\mathcal{D}}(h) \leq \varepsilon$$

PAC Model

- Goal: h has small error over D.
- True error: $error_{\mathcal{D}}(h) = Pr_{x \sim \mathcal{D}}\,[h(x) \neq c^*(x)]$
- How often $h(x) \neq c^*(x)$ over future instances drawn at random from $\mathcal{D}$
- But, we can only measure:
- Training error : $error_s(h) = \frac{1}{m}\sum_i I(h(x_i) \neq c^*(x))$
- How often $h(x) \neq c^*(x)$ over training instances
- Sample complexity: how to bound $error_{\mathcal{D}}(h)$in terms of $error_S(h)$

PAC Learning

- PAC learning concerns efficient learning.

- We would like to prove that with high probability (P(1- δ)) an efficient (space and time complexity is in order of polynomial time) learning algorithm will find a hypothesis that is approximately identical (error$\leq \varepsilon$) to the hidden target concept.

- We specify two parameters, ε and δ and require that with probability at least (1-δ) a system learn a concept with error at most ε.

Sample complexity of the supervised learning

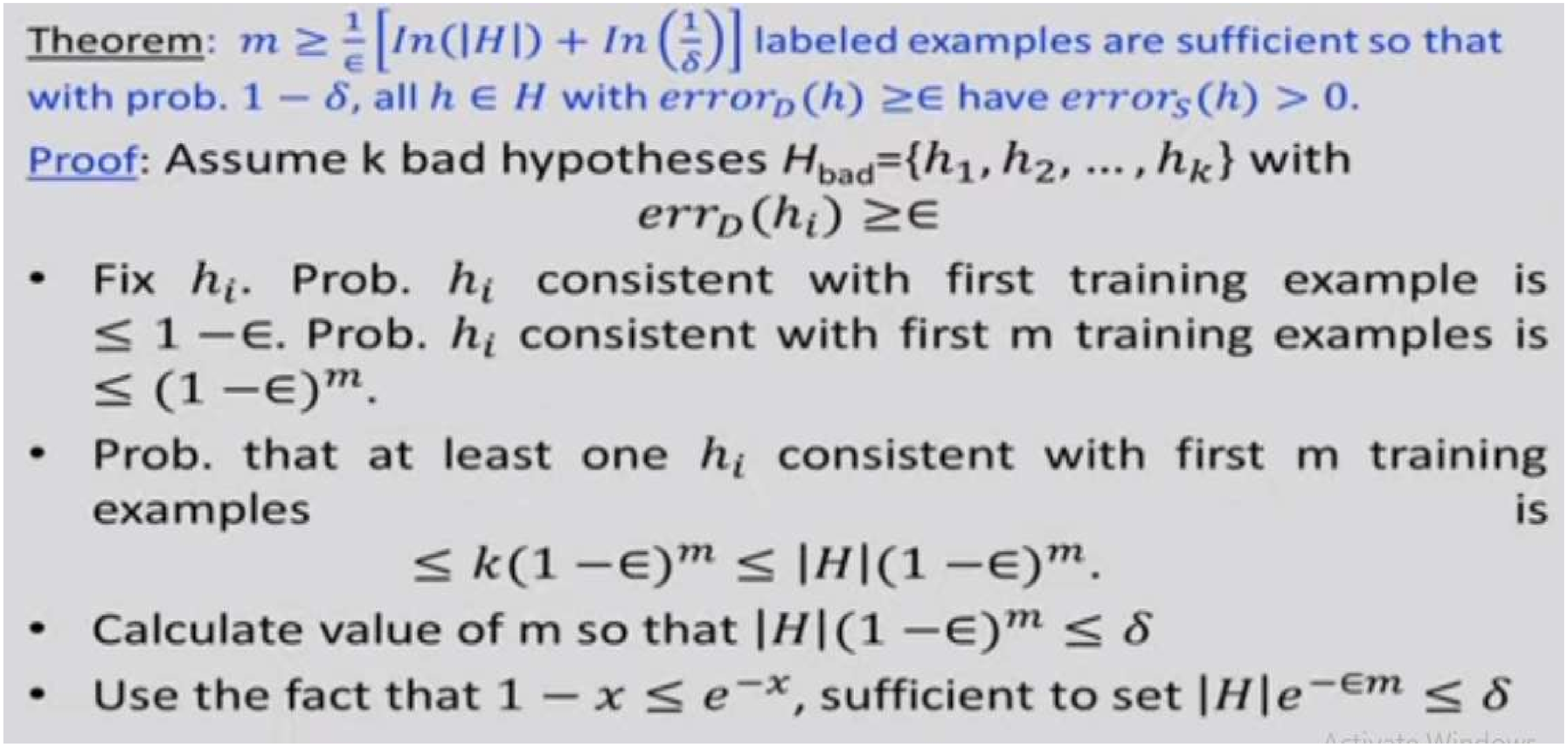
- Theorem: If the size of the training sample (m) is greater or equal to Z then it is sufficient to be able to PAC learner hypothesis where

$$Z = \frac{1}{\varepsilon}[ln(|\mathcal{H}|) + ln\left(\frac{1}{\delta}\right)] \qquad \text{i.e.} \qquad m \geq \frac{1}{\varepsilon}[ln(|H|) + ln\left(\frac{1}{\delta}\right)]$$

Labeled example are sufficient so that with probability 1-δ, all $h \epsilon \mathcal{H}$ with $error_D(h) \geq$ ε have $error_S(h)$ ≥0 [i.e. PAC]

- inversely linear in ε
- logarithmic to | $\mathcal{H}$|.
- ε error parameters: D might place low weight on certain parts of the space
- δ confidence parameters: there is a small chance the examples we get are not representative of the distribution.

Sample Complexity of the Supervised Learning



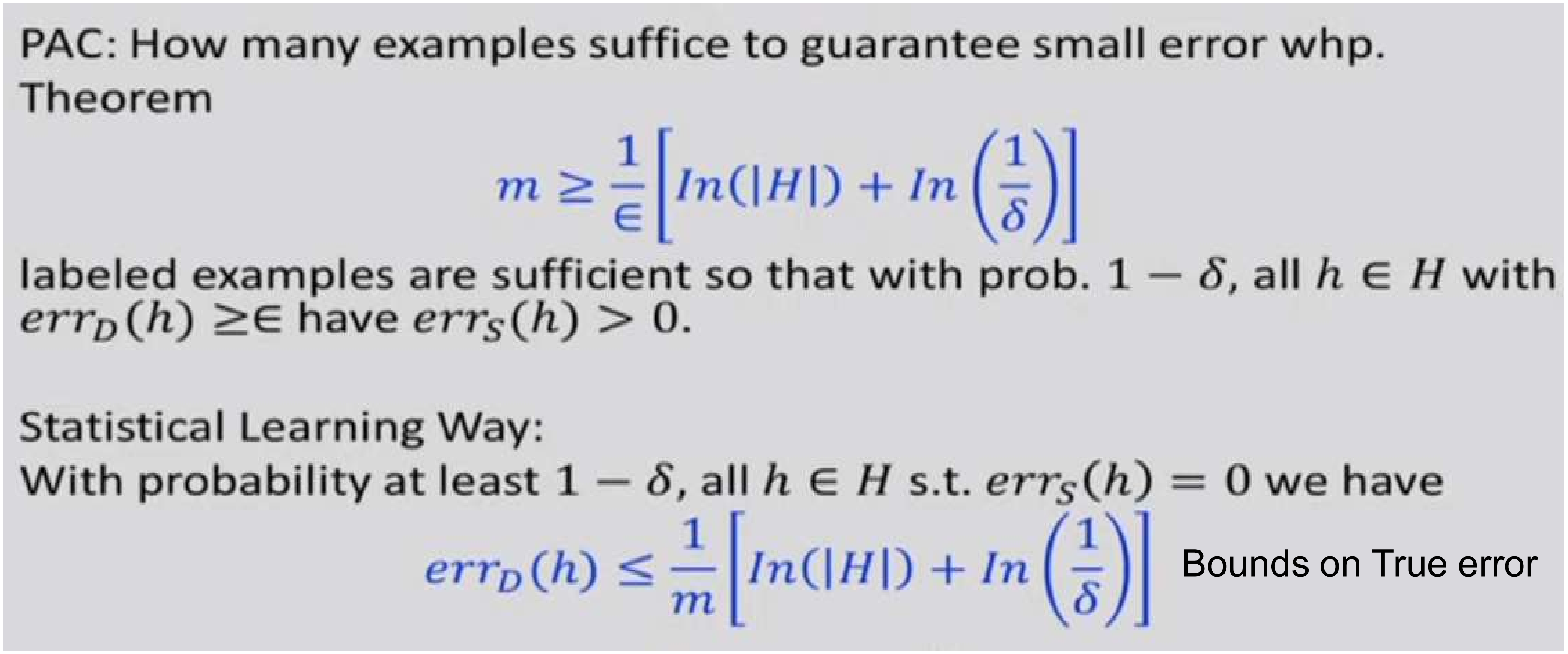
Theorem: $m \geq \frac{1}{\epsilon}\left[In(|H|) + In\left(\frac{1}{\delta}\right)\right]$ labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $error_D(h) \geq \epsilon$ have $error_S(h) > 0$.

Proof: Assume k bad hypotheses H_{bad}=$\{h_1, h_2, \ldots, h_k\}$ with

$$err_D(h_i) \geq \epsilon$$

- Fix h_i. Prob. h_i consistent with first training example is $\leq 1 - \epsilon$. Prob. h_i consistent with first m training examples is $\leq (1-\epsilon)^m$.
- Prob. that at least one h_i consistent with first m training examples is
$$\leq k(1-\epsilon)^m \leq |H|(1-\epsilon)^m.$$
- Calculate value of m so that $|H|(1-\epsilon)^m \leq \delta$
- Use the fact that $1 - x \leq e^{-x}$, sufficient to set $|H|e^{-\epsilon m} \leq \delta$

Finite Hypothesis Space Realizable Case



PAC: How many examples suffice to guarantee small error whp.

Theorem

$$m \geq \frac{1}{\epsilon}\left[In(|H|) + In\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \epsilon$ have $err_S(h) > 0$.

Statistical Learning Way:

With probability at least $1-\delta$, all $h \in H$ s.t. $err_S(h) = 0$ we have

$$err_D(h) \leq \frac{1}{m}\left[In(|H|) + In\left(\frac{1}{\delta}\right)\right]$$

Bounds on True error

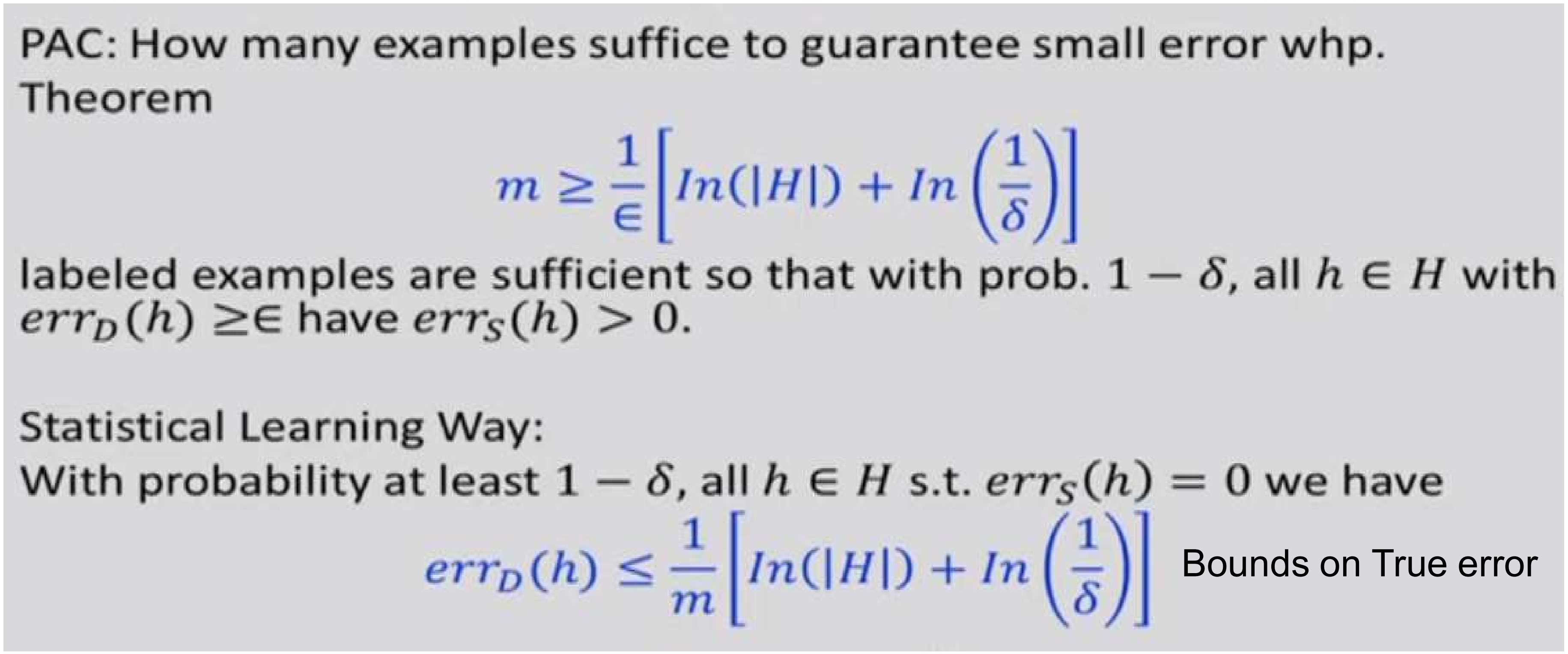
Summary

- We have looked at the case where the learner looks at m training examples, outputs a consistent hypothesis.
- We derived bounds on how many examples the learner has to see so that the consistent hypothesis is a PAC hypothesis.
- In other words, we have seen, how many examples are needed to be seen in order to guarantee that consistent hypothesis has error$\leq \varepsilon$ and we want to do this with the confidence ($\geq$1-δ).
- But there are scenarios where we can't get consistent hypothesis but the hypothesis that the learner outputs is inconsistent that is it has error in the training sets.

Finite Hypothesis Space: Inconsistent hypothesis

- The hypothesis output by the learner has non zero errors in the training sets.

Finite Hypothesis Space Realizable Case



PAC: How many examples suffice to guarantee small error whp.

Theorem

$$m \geq \frac{1}{\in}\left[In(|H|) + In\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1 - \delta$, all $h \in H$ with $err_D(h) \geq \in$ have $err_S(h) > 0$.

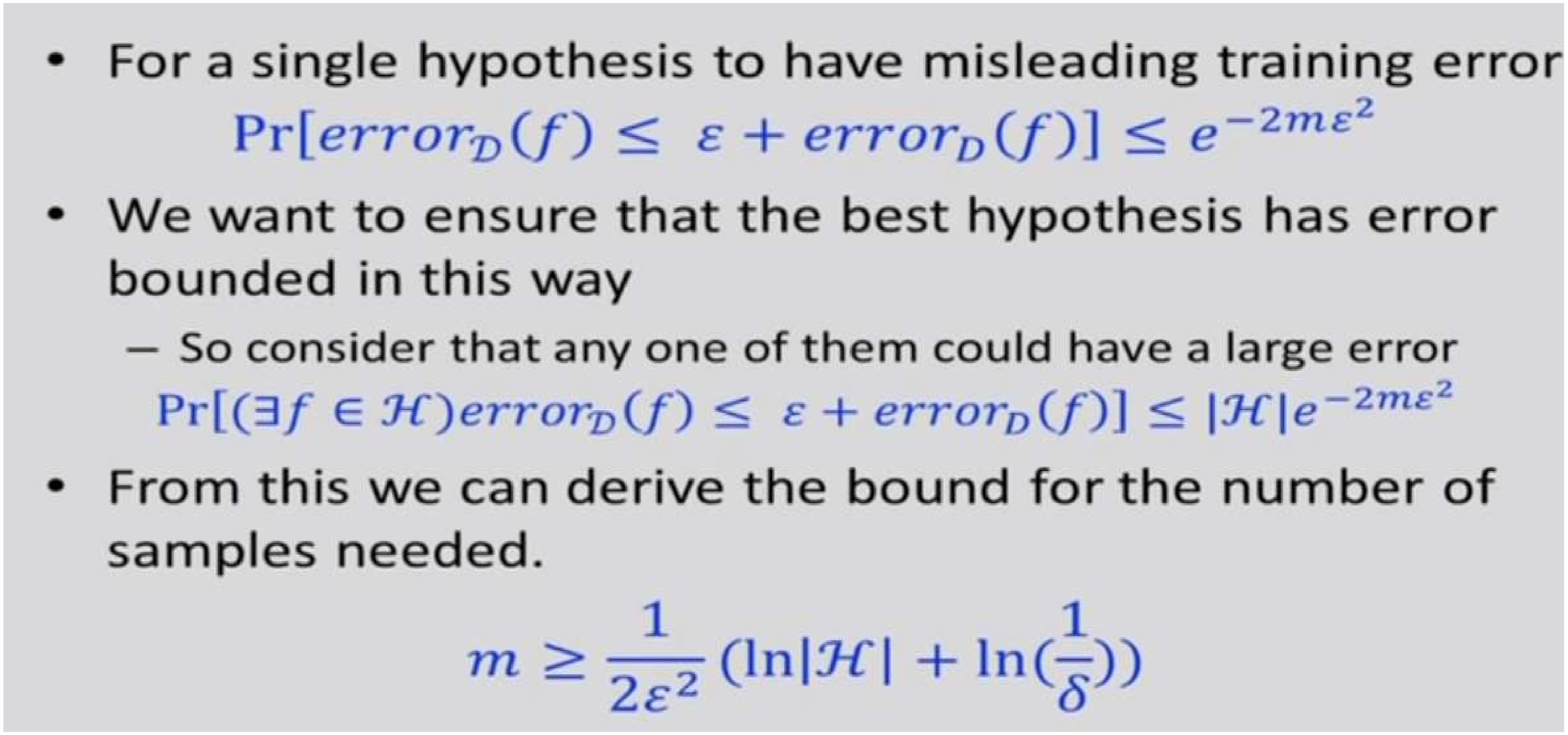
Statistical Learning Way:

With probability at least $1 - \delta$, all $h \in H$ s.t. $err_S(h) = 0$ we have

$$err_D(h) \leq \frac{1}{m}\left[In(|H|) + In\left(\frac{1}{\delta}\right)\right]$$

Bounds on True error

Sample Complexity: inconsistent finite | $\mathcal{H}$ |



- For a single hypothesis to have misleading training error

$$\Pr[error_{\mathcal{D}}(f) \leq \ \varepsilon + error_{D}(f)] \leq e^{-2m\varepsilon^2}$$

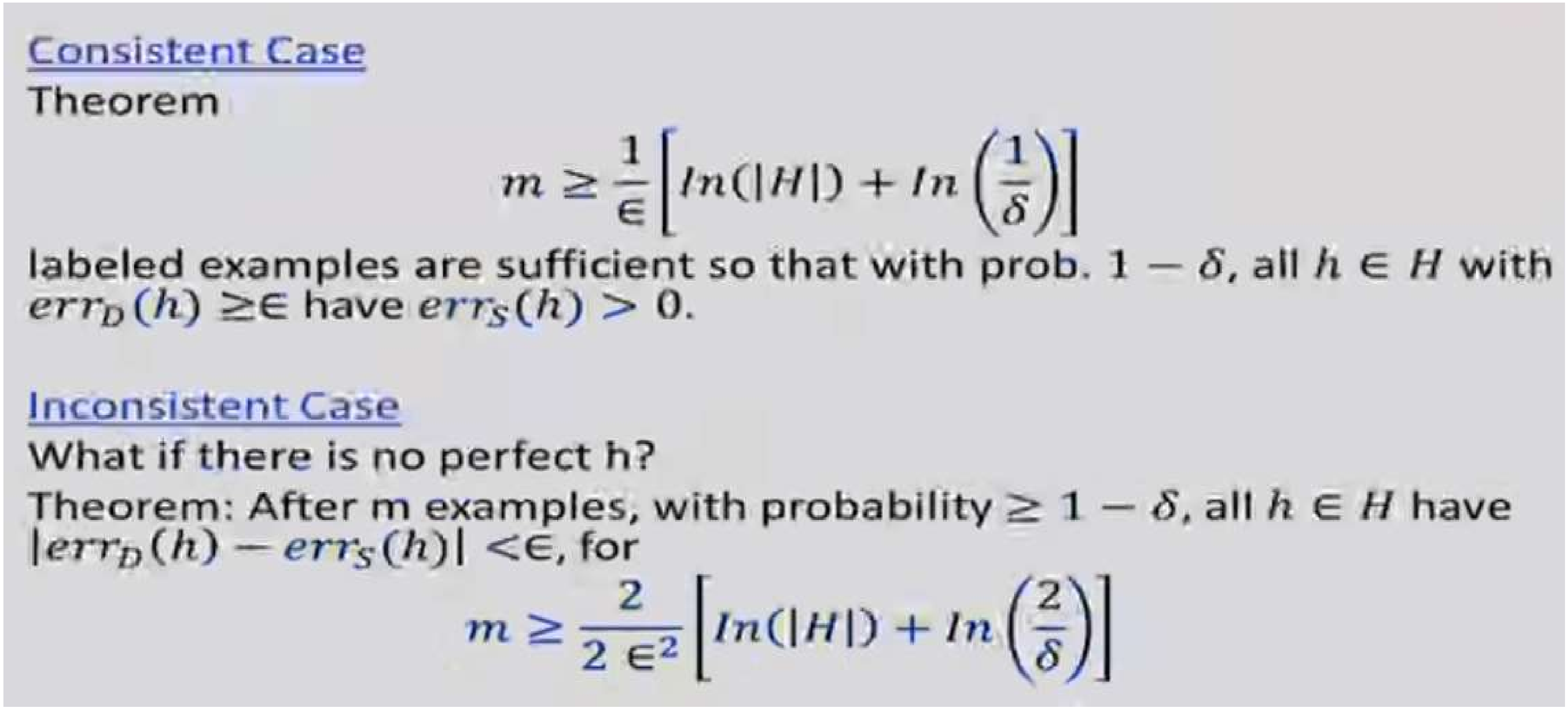
- We want to ensure that the best hypothesis has error bounded in this way
  - So consider that any one of them could have a large error

$$\Pr[(\exists f \in \mathcal{H}) error_{\mathcal{D}}(f) \leq \ \varepsilon + error_{D}(f)] \leq |\mathcal{H}| e^{-2m\varepsilon^2}$$

- From this we can derive the bound for the number of samples needed.

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

Sample Complexity: Finite Hypothesis Space



Consistent Case

Theorem

$$m \geq \frac{1}{\epsilon}\left[ln(|H|) + ln\left(\frac{1}{\delta}\right)\right]$$

labeled examples are sufficient so that with prob. $1-\delta$, all $h \in H$ with $err_D(h) \geq \epsilon$ have $err_S(h) > 0$.

Inconsistent Case

What if there is no perfect h?

Theorem: After m examples, with probability $\geq 1-\delta$, all $h \in H$ have $|err_D(h) - err_S(h)| < \epsilon$, for

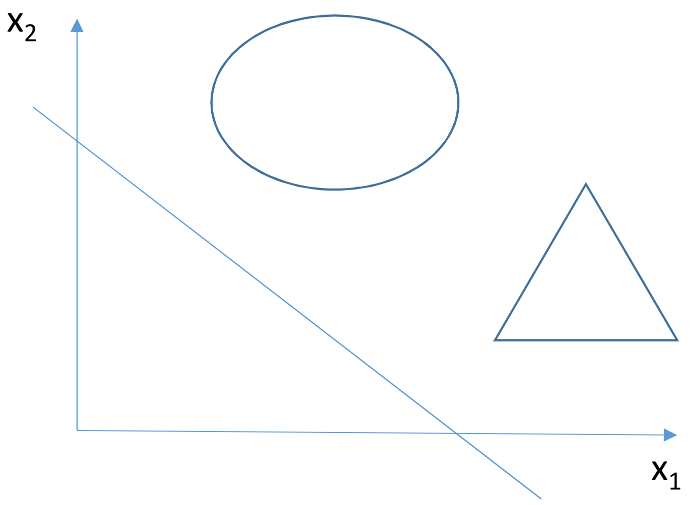
$$m \geq \frac{2}{2\,\epsilon^2}\left[ln(|H|) + ln\left(\frac{2}{\delta}\right)\right]$$

VC Dimension

Sample Complexity: Infinite Hypothesis Space

- Hypothesis Space is infinite.
- Need some measure of expressiveness of infinite hypothesis spaces.
- The Vapnik-Chervonenkis (VC) dimension provides such measures, denoted VC(H).
- Analogous to $ln(|\mathcal{H}|)$, there are bounds for sample complexity using VC(H)

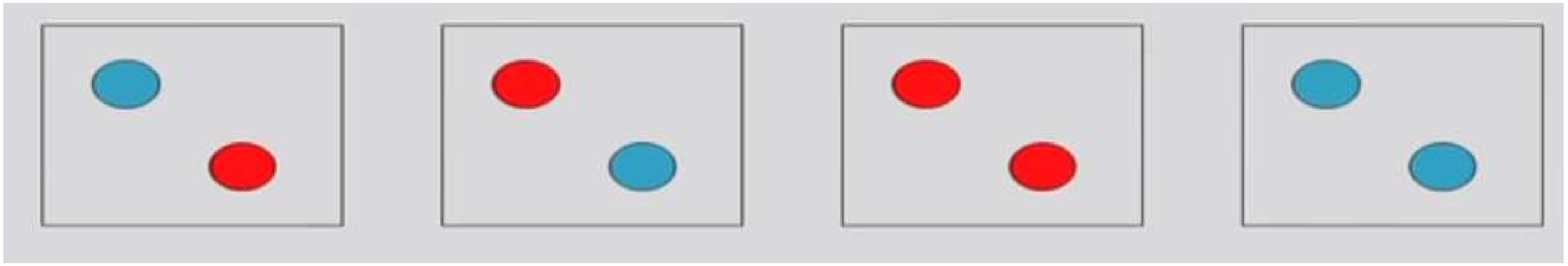
Examples of Infinite Hypothesis Space



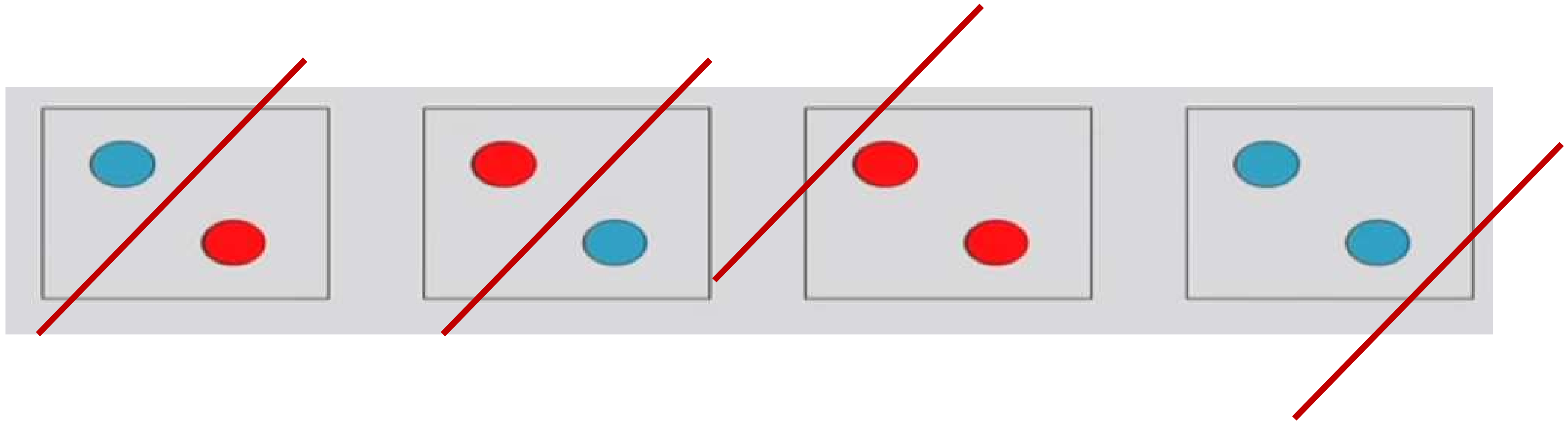
X_1 and x_2 are real valued attributes, then the number of linear functions can be infinite.

Shattering

- Consider a hypothesis for the 2 class problem.
- A set of N points (instances)can be labeled as + and – in 2^N ways.
- If for every such labelling, a function can be found in $\mathcal{H}$ consistent with this labelling, we said that set of instances is shattered by $\mathcal{H}$.



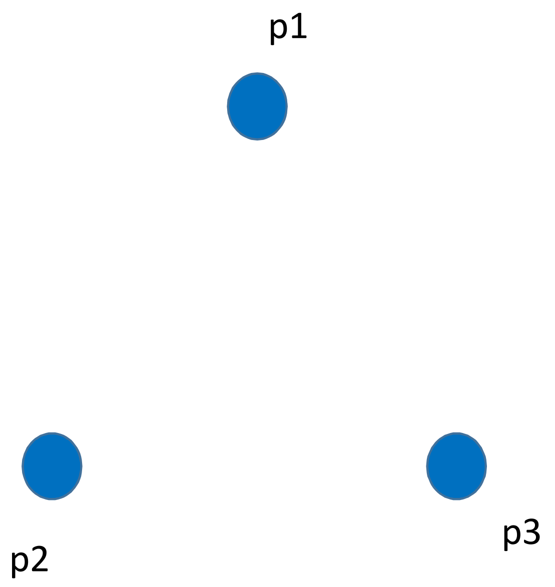
Shattering



So all possible labeling of these two points, we can find a hypothesis from the hypothesis space which is consistent with the labeling.

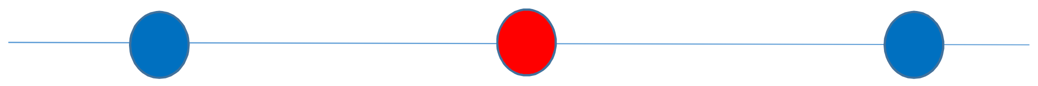
For binary classification, how many possible ways we can partition this space? It is $2^3=8$.

And for every possible such labeling, we can find a linear separator those points.



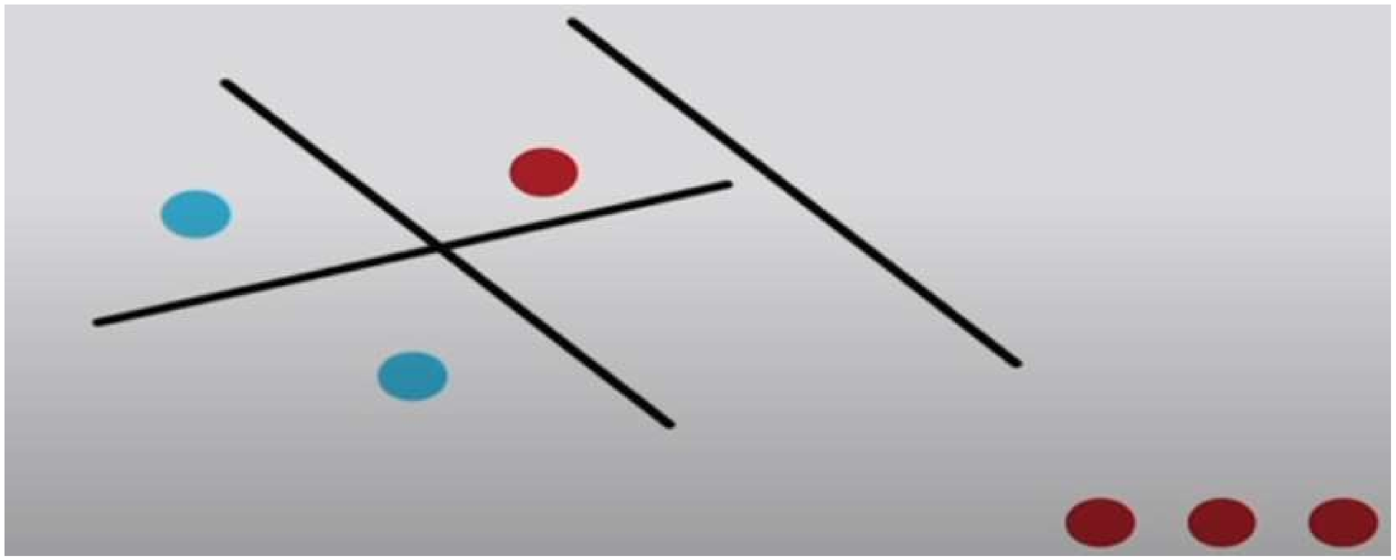
Can a linear separator partition following setting?

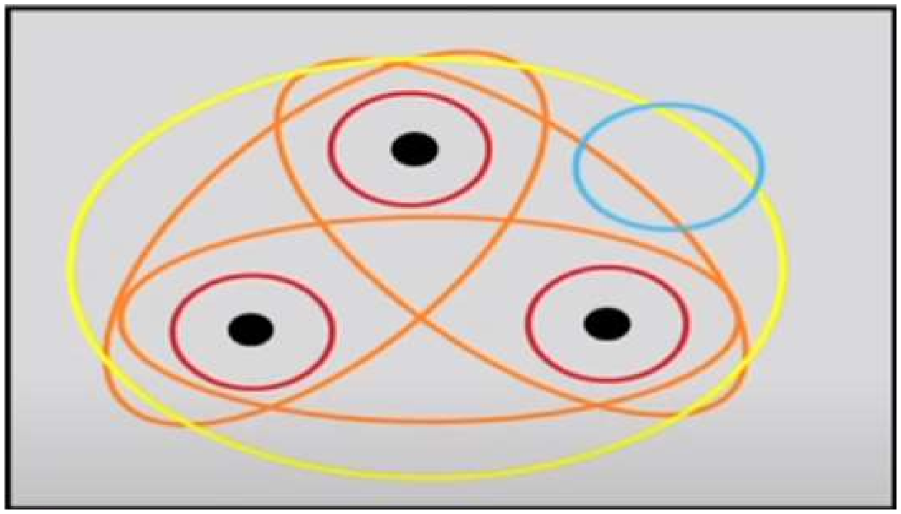
So, this particular setting of three points can not be shattered by a hypothesis space comprises of straight lines.



Three points in R^2

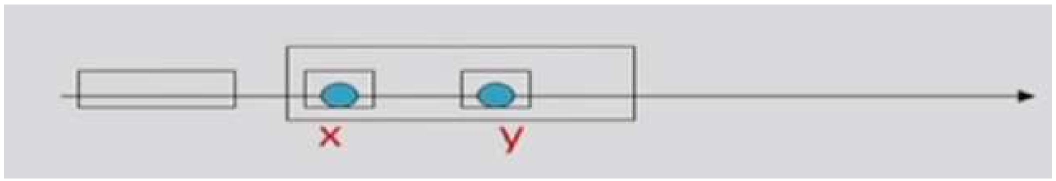
- It is enough to find one set of three points that can be shattered.
- It is not necessary to be able to shutter every possible set of three points in 2 dimension.





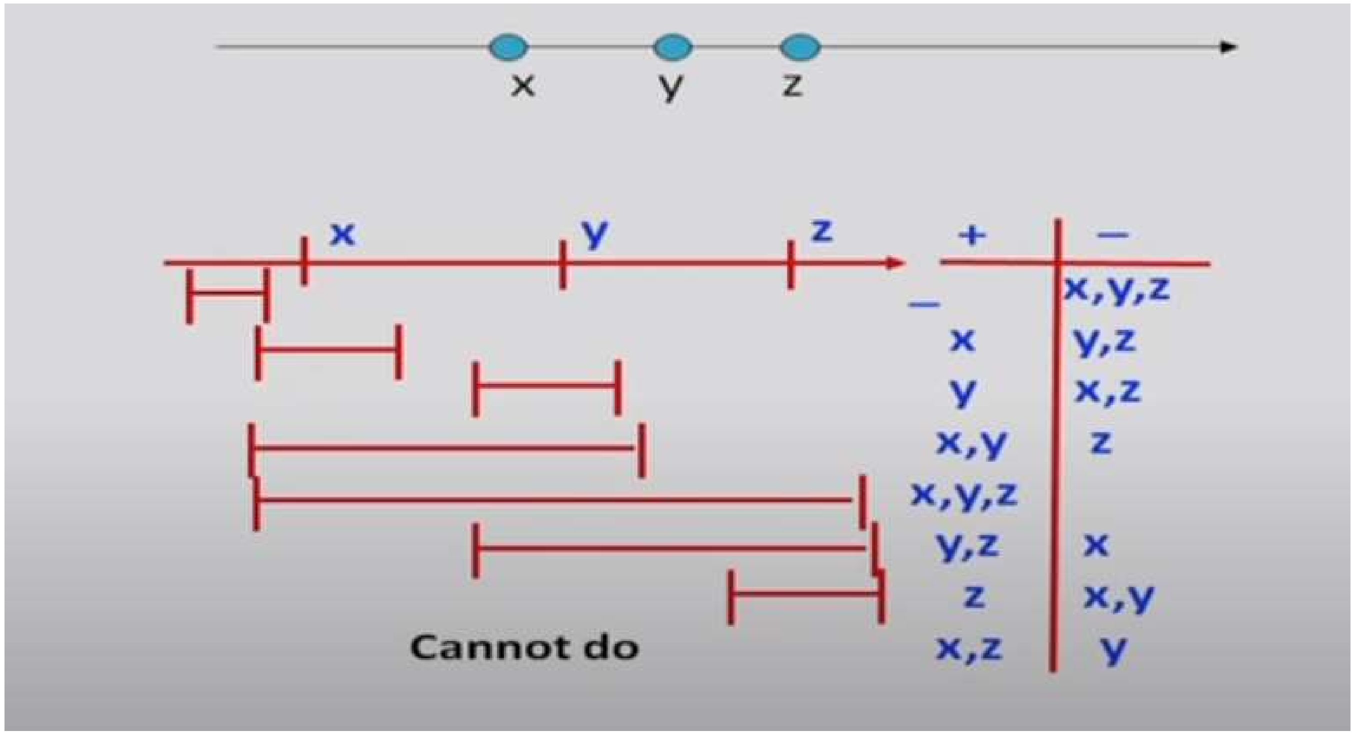
Shattering Instances

- Consider 2 instances described using a single real valued feature being shattered by a single interval.



Shattering Instances

But three instances can not be shattered by a single interval.



+	−
−	x,y,z
x	y,z
y	x,z
x,y	z
x,y,z	
y,z	x
z	x,y
x,z	y

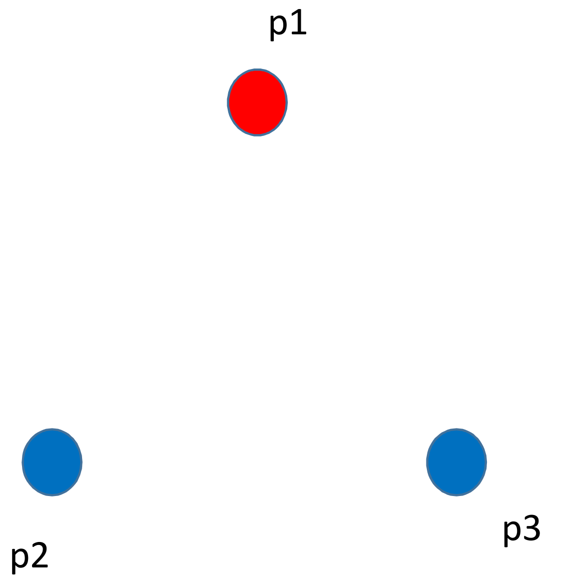
VC Dimension

- The Vapnin-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 subset of X can be shuttered then VC(H)=α.
- If there exist at least of subset of X of size d that can be shattered by H then VC(H)≥d.
- If no subset can be shattered by H, then VC(H)<d.
- For a single intervals on the real line, all sets of 2 instances can be shattered, no set of three instances can, VC (H)=2.

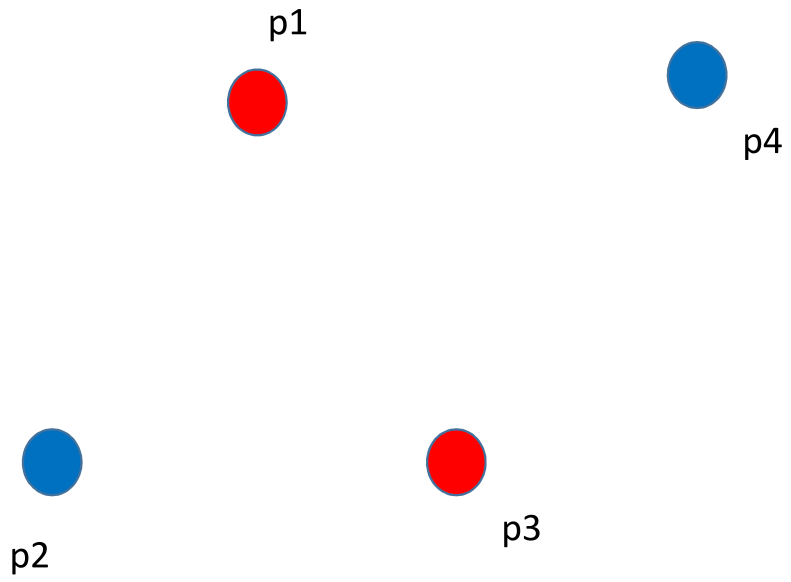
VC Dimension

- An unbiased hypothesis space shatters the entire instance space.
- The larger the subset of X that can be shattered, the more expressive (and less biased) the hypothesis space is.
- The VC dimension of the set of oriented lines in 2-D is three.
- Since there are 2^m partitions of m instances, in order for H to shatter instances: $|H| \geq 2^m$.
- Since $|H| \geq 2^m$, to shatter m instances, $VC(H) \leq \log_2 |H|$

For Binary Classification



Can be shuttered

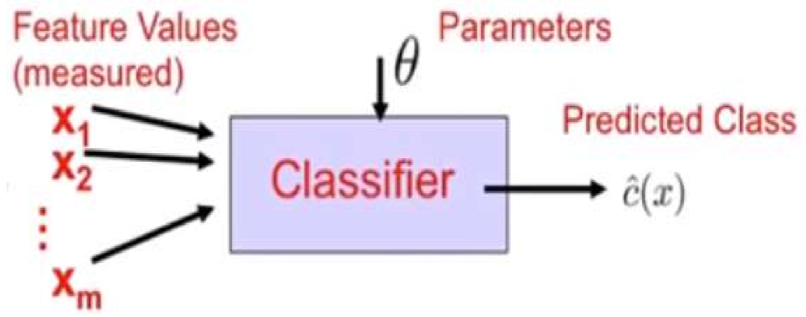


Can't be shuttered

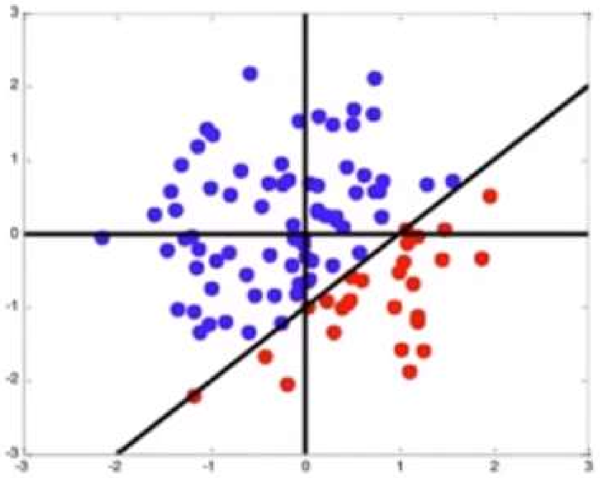
So, the VC dimension of the set of oriented lines in 2-D is three.

Learners and Complexity

- We have seen many versions of underfit/overfit trade-off.
  - Complexity of the learner
  - Representational power



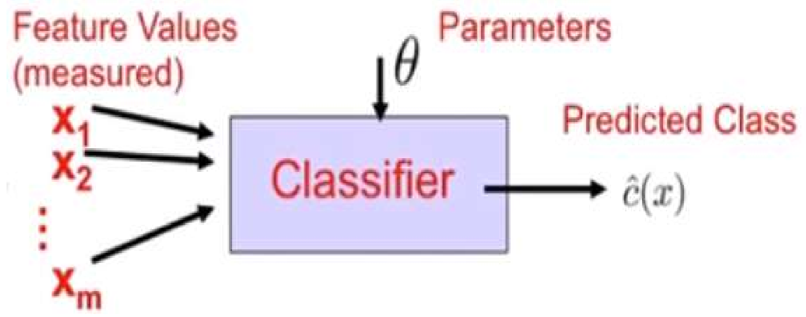
- Different learners have different power



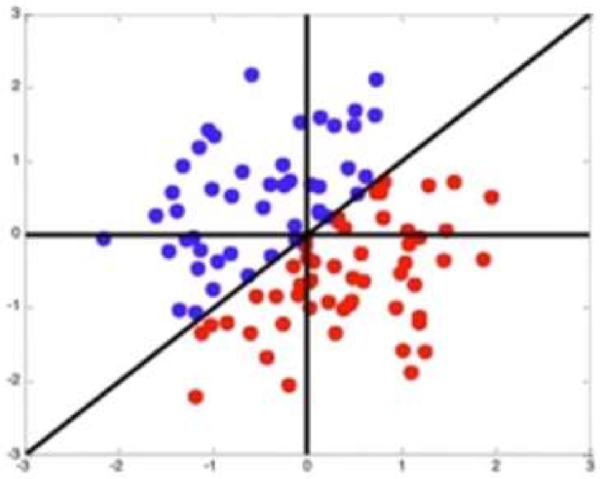
Example: $\hat{c}(x) = sign(\theta_1 x_1 + \theta_2 x_2 + \theta_0)$

Learners and Complexity

- We have seen many versions of underfit/overfit trade-off.
  - Complexity of the learner
  - Representational power



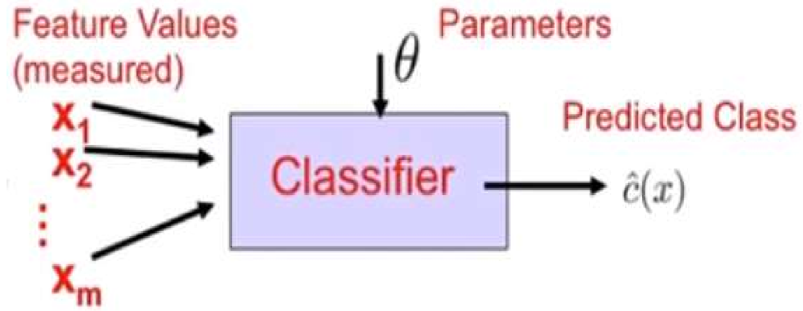
- Different learners have different power



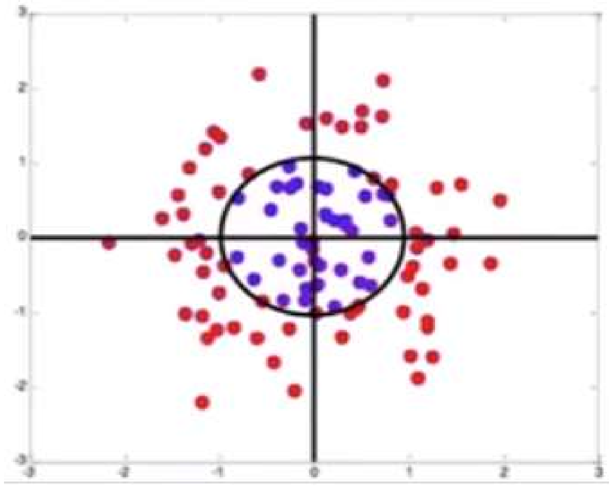
Example: $\hat{c}(x) = sign(\theta_1 x_1 + \theta_2 x_2)$

Learners and Complexity

- We have seen many versions of underfit/overfit trade-off.
  - Complexity of the learner
  - Representational power



- Different learners have different power



Example: $\hat{c}(x) = sign(x^T x - \theta_0)$

Learners and Complexity

- We have seen many versions of underfit/overfit trade-off.
  - Complexity of the learner
  - Representational power
- Different learners have different power
- Usual trade-off:
  - More power = represent more complex systems, might overfit
  - Less power = won’t overfit, but may not find best learner
- How can we quantify the representational power?
  - Not easily…
  - One solution is VC (Vapnik-Chervonenkis) dimension

Preliminaries

- Let's assume our training data are iid (independent and identically distributed) from some distribution p(x).
- Define "risk" and "empirical risk"
  - These are just "long term" test and observed training error

$$R(\theta) = TestError = E[\delta\big(c \neq \hat{c}(x;\theta)\big)]$$

$$R^{emp}(\theta) = TrainError = \frac{1}{m}(\textstyle\sum_i \delta(c^{(i)} \neq \hat{c}(x^{(i)};\theta)))$$

- How are these related? Depends on overfitting…
  - Under-fitting domain: pretty similar
  - Overfitting domain: test results might be lots wors!

VC Dimension and Risk

- Given some classifier, let H be its VC dimension
  - Represents the “representational power” of the classifier.

$$R(\theta) = TestError = E[\delta(c \neq \hat{c}(x;\theta))]$$

$$R^{emp}(\theta) = TrainError = \frac{1}{m}(\sum_i \delta(c^{(i)} \neq \hat{c}(x^{(i)};\theta)))$$

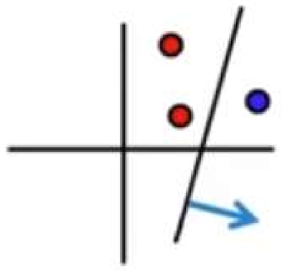
- With high probability (1-η), Vapnik showed

$$Test\ Error \leq Train\ Error + \sqrt{\frac{Hlog\left(\frac{2m}{H}\right) + H - \log(\frac{\eta}{4})}{m}}$$

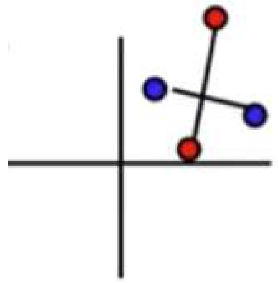
VC Dimension: Examples

- What is the VC dimension of the two dimensional line,

$$f(x;\theta) = sign(\theta_1 x_1 + \theta_2 x_2 + \theta_0)?$$



VC dimension is ≥ 3 YES



VC dimension is ≥ 4 : NO

It turns out, for a general linear classifier (perceptron) in d dimensional space with a constant term, the VC dimension is d+1

VC Dimension

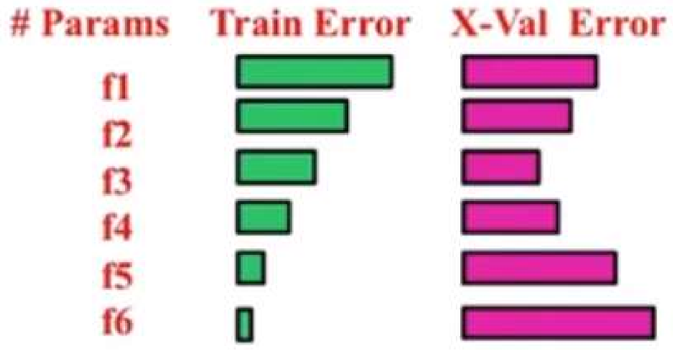
- VC dimension measures the power of the learner.
- Does **not** necessarily equal to the # of parameters.

- Number of parameters does not necessarily equal complexity
  - Can define a classifier with lot of parameters but not much power (how?)
  - Can define a classifier with one parameter but lots of power (how?)

- Lots of work to determine what the VC dimension of various learners is…

Using VC dimension

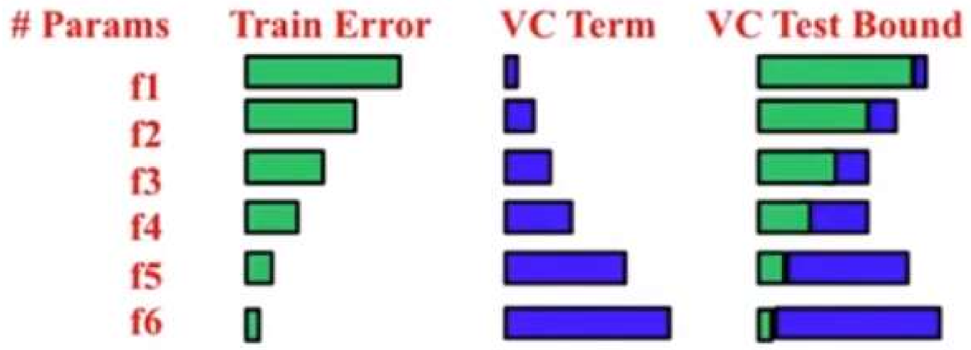
- Used validation/cross-validation to select complexity
  - Fundamental problem of model selection



Using VC dimension

- Used validation/cross-validation to select complexity
- Use VC dimension based bound on test error similarity

- Structural risk minimization (SRM)



to continue...