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Computational Learning Theory

Machine Learning

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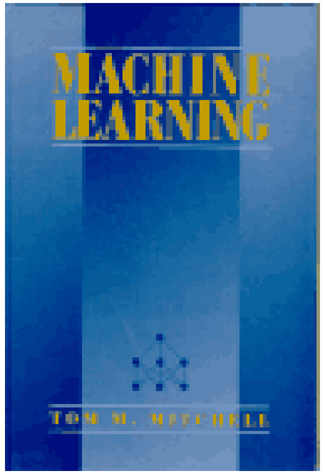
Outline and References

- Outline
  - Basics [ML 7.1,7.2]
  - PAC-Learning [ML 7.3]
  - VC Dimension [ML 7.4]

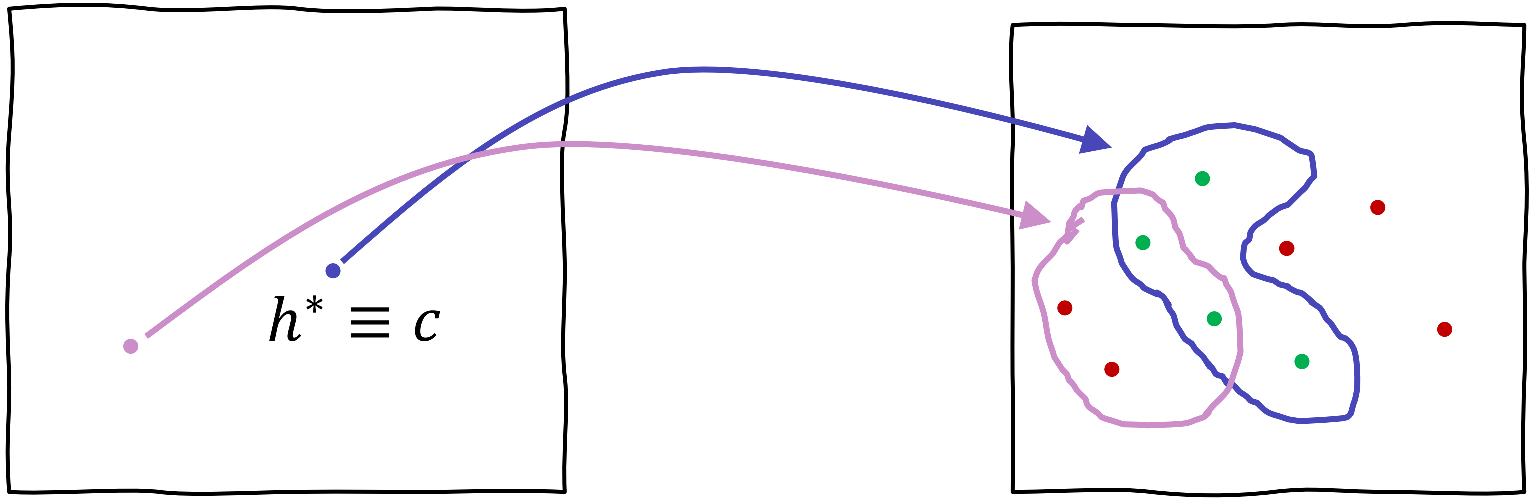
- References
  - Machine Learning, Mitchell [ML]



What is computational learning theory?

- It aims at studying the general laws of inductive learning, by modeling:
  - Complexity of hypothesis space
  - Bound on training samples
  - Bound on accuracy
  - Probability of succesfull learning
  - ...
- This allows to answer to questions like:
  - How many training samples do a learner need to **converge** (with some probability) to a **successful** (with some minimum accuracy) hypothesis?
  - How many training samples will be misclassified by the learner before converging to a succesful hypothesis?
  - ...

(Let’s Go Back to) The Big Picture



$H = \{h: x \rightarrow t\}$

Labelled X

- A learner (L) wants to learn a *concept* (c) that maps the data in the input space (X) to a target (t)
- Let assume that L found an hypothesis h^* with no errors on the training data
- How many training samples of X are necessary to be sure that L actually learned the true concept, i.e., $h^* \equiv c$?

«No Free Lunch» Theorems

- Let $ACC_G(L)$ be the **generalization accuracy** of learner L, i.e., the accuracy of L on samples that are **not** in the training set
- Let $\mathcal{F}$ be the set of all the possible concepts $y = f(\mathbf{x})$
- For any learner L and any possible training set:

$$\frac{1}{|\mathcal{F}|}\sum_{\mathcal{F}} Acc_G(L) = \frac{1}{2}$$

  - **Proof Sketch**: for every concept f where $ACC_G(L) = 0.5 + \delta$, exists a concept f' where $ACC_G(L) = 0.5 - \delta$: $\forall \mathbf{x} \in \mathcal{D}, f'(\mathbf{x}) = f(\mathbf{x}); \forall x \notin \mathcal{D}, f'(\mathbf{x}) \neq f(\mathbf{x})$

  - **Corollary:** for any two learners, L_1 and L_2, if $\exists f$ where $ACC_G(L_1) > ACC_G(L_2)$ then $\exists f'$ where $ACC_G(L_2) > ACC_G(L_1)$

«No Free Lunch» Theorems

- Let $ACC_G(L)$ be the **generalization accuracy** of learner L, i.e., the accuracy of L on samples that are **not** in the training set
- Let
- For

  - ...cept f'
  - **C**... (L_2) then $\exists f'$ where $ACC_G(L_2) > ACC_G(L_1)$

What does this mean in practice?

There is no such thing as a **winner-takes-all** in ML!

In ML we always operate under some assumptions!

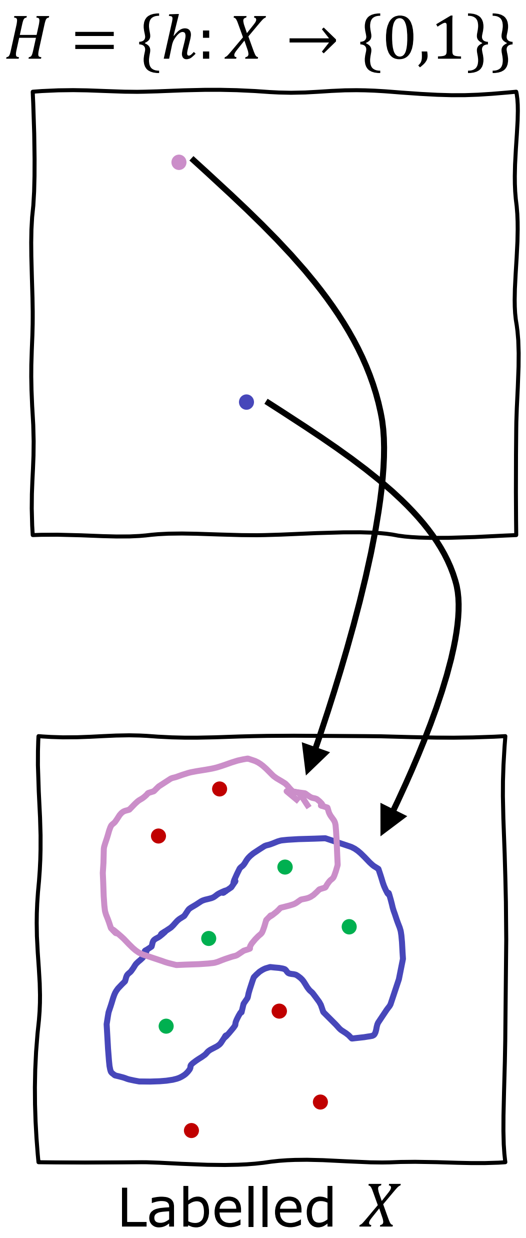
Probably Learning an Approximately Correct Hypothesis

Basics

- Problem setting
  - Let X be the instance space
  - Let $H = \{h: X \rightarrow \{0,1\}\}$ be the hypothesis space of L
  - Let $C = \{c: X \rightarrow \{0,1\}\}$ be the set of all the possible target functions (**concepts**) we might want to learn
  - Let be $\mathcal{D}$ be training data drawn from a **stationary** distribution $P(X)$ and labeled (**without noise**) according to a concept c we want to learn

- A learner L outputs a hypothesis $h \in H$ such that

$$h^* = \arg\min_{h \in H} error_{train}(h)$$



How do we compute the error?

- We compute the error of an hypothesis as the probability of misclassfyng a sample:

$$error_{\mathcal{D}}(h) = \Pr_{x \in \mathcal{D}}[h(x) \neq c(x)] = \frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} I(h(x) \neq c(x))$$

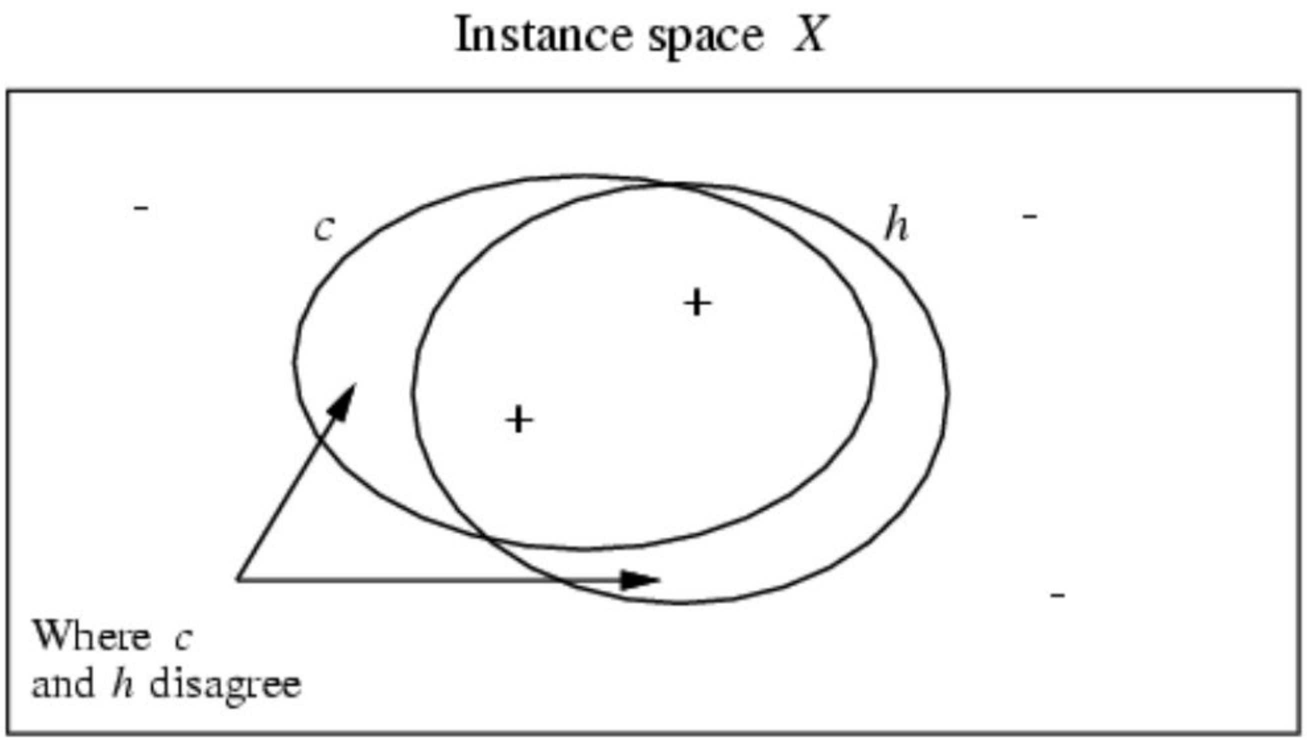
$\mathcal{D}$ is the training data

- This is the training error, instead we are interested in the **true error** of h:

$$error_{true}(h) = \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

$P(X)$ is the input space distribution

How do we compute the error?



- But we have to remember that...

$$error_{true}(h) = \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

What now?

- We say that h overfits the training data if $error_{true} > error_{\mathcal{D}}$ ...
- ... but can we bound $error_{true}$ given $error_{\mathcal{D}}$?
- Let assume...
  - $error_{true}$ is the probability of making a mistake on a sample
  - we can compute $error_{\mathcal{D}}$ that is the average error probability on $\mathcal{D}$
  - assuming a Bernoulli distribution for the error probability, the 95% CI is:

$$error_{true}(h) = error_{\mathcal{D}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

- Is this correct? No! Because $\mathcal{D}$ is the training data and not **independent** of h
- So, **we need to bound the error under more strict assumptions**

Version Space

- A hypothesis h is **consistent** with a training dataset $\mathcal{D}$ of the concept c if and only if $h(x) = c(x)$ for each training sample in $\mathcal{D}$

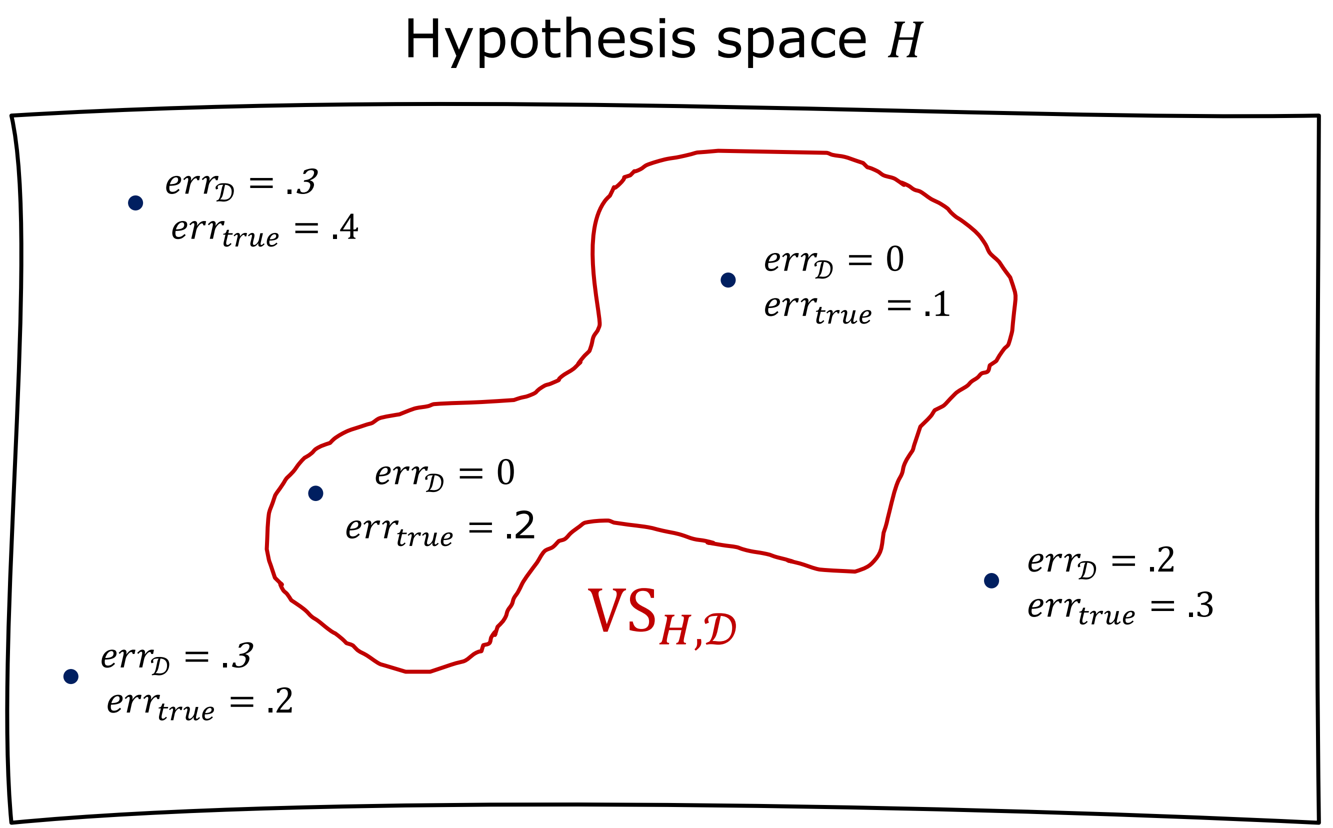
$$Consistent(h, \mathcal{D}) \stackrel{\text{def}}{=} \forall \langle x, c(x) \rangle \in \mathcal{D}, h(x) = c(x)$$

- The version space, $VS_{H,\mathcal{D}}$ with respect to hypothesis space H and labelled dataset $\mathcal{D}$, is the subset of hypotheses in H consistent with $\mathcal{D}$

$$VS_{h,\mathcal{D}} \stackrel{\text{def}}{=} \{h \in H | Consistent(h, \mathcal{D})\}$$

- From now on, we consider only **consistent learners**, that always output a **consistent** hypothesis, i.e., an hypothesis in $VS_{H,\mathcal{D}}$, **assuming it is not empty**
- Can we bound the $error_{true}$ of a consistent learner?

Version Space (2)



- If we wish to bound the $error_{true}$ of a consistent learner, we need to find a bound for all the hypotheses in $VS_{H,\mathcal{D}}$

Bound for Consistent Learners

If the hypothesis space H is **finite** and $\mathcal{D}$ is a sequence of $N \geq 1$ independent random examples of some target concept c, then for any $0 \leq \varepsilon \leq 1$, the probability that $VS_{H,\mathcal{D}}$ contains a hypothesis error greater then ε is less than $|H|e^{-\varepsilon N}$

$$Pr(\exists h \in H : error_{\mathcal{D}}(h) = 0 \wedge error_{true}(h) \geq \varepsilon) \leq |H|e^{-\varepsilon N}$$

Proof

$$
\begin{aligned}
& Pr((error_{\mathcal{D}}(h_1) = 0 \wedge error_{true}(h_1) \geq \varepsilon) \vee \cdots \vee (error_{\mathcal{D}}(h_{|VS_{H,\mathcal{D}}|}) = 0 \wedge error_{true}(h_{|VS_{H,\mathcal{D}}|}) \geq \varepsilon)) \\
& \quad \leq \sum_{h \in VS_{H,\mathcal{D}}} Pr(error_{\mathcal{D}}(h) = 0 \wedge error_{true}(h) \geq \varepsilon) && \text{(Union bound)} \\
& \quad \leq \sum_{h \in VS_{H,\mathcal{D}}} Pr(error_{\mathcal{D}}(h) = 0 | error_{true}(h) \geq \varepsilon) && \text{(Bound using Bayes' rule)} \\
& \quad \leq \sum_{h \in VS_{H,\mathcal{D}}} (1 - \varepsilon)^N && \text{(Bound on individual } h\text{)} \\
& \quad \leq |H|(1 - \varepsilon)^N && (|VS_{H,\mathcal{D}}| \leq |H|) \\
& \quad \leq |H|e^{-\varepsilon N} && (1 - \varepsilon \leq e^{-\varepsilon}, \text{ for } 0 \leq \varepsilon \leq 1)
\end{aligned}
$$

What does it mean in practice?

- Let say that δ is the probability to have $error_{true} > \varepsilon$ for a consistent hypotesis:

$$|H|e^{-\varepsilon N} \leq \delta$$

- We can bound N after setting ε and δ:

$$N \geq \frac{1}{\varepsilon}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

- We can bound ε after setting N and δ:

$$\varepsilon \geq \frac{1}{N}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

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- We can bound ε after setting N and δ:

Can be expeonential in #features

$$\varepsilon \geq \frac{1}{N}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

Example: Conjunction of up to N Boolean Literals

- Consider a classification problem
  - Instance space is $\mathrm{X} = < \mathrm{x}_1, \mathrm{x}_2, \mathrm{x}_3, \mathrm{x}_4 >$, where x_i is a boolean variable
  - Each hypothesis h is a rule like this:

$$if\ (x_1 = 1, x_2 =?, x_3 = 0, x_4 = 1)\ then\ y = 1, otherwise\ y = 0$$

- How many samples N are necessary to guarantee that, with a probability at least of 0.99, the error of a consistent hypothesis is not greater than 0.05?

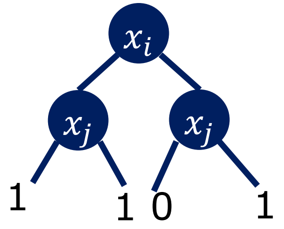
$$N \geq \frac{1}{\underbrace{\varepsilon}_{0.05}}\left(\ln|\underbrace{H}_{3^4}| + \ln\left(\frac{1}{\underbrace{\delta}_{0.01}}\right)\right)$$

N≥180

- How does it scale with respect to the number of variables (M)?
  - M=10 → N≥312
  - M=100 → N≥2290

Example: Decision Tree (depth=2)

- Consider a classification problem
  - Instance space is $X = < x_1, \ldots, x_M >$, where x_i is a boolean variable
  - Each hypothesis h is a rule is a decision trees of depth 2 using only two variables:



- How many samples N are necessary to guarantee that, with a probability at least of 0.99, the error of a consistent hypothesis is not greater than 0.05?

$$N \geq \frac{1}{\underbrace{\varepsilon}_{0.05}} \left(\ln \underbrace{|H|}_{\frac{M(M-1)}{2}16} + \ln \left(\frac{1}{\underbrace{\delta}_{0.01}} \right) \right)$$

Probably Learning an Approximately Correct Hypothesis

- Considering a class C of possible target concepts defined over an instance space X with an encoding lenght M, and a learner L using an hypotesis space H we define:

  C is PAC-learnable by L using H if for all $c \in C$, for any distribution $P(X)$, ε (such that $0 < \varepsilon < 1/2$), and δ (such that $0 < \delta < 1/2$), learner L will with a probability at least $(1 - \delta)$ output a hypotehsis $h \in H$ such that $error_{true}(h) \leq \varepsilon$, in time that is polynomial in $1/\varepsilon$, $1/\delta$, M, and $size(c)$.

- So, PAC-learnability is only about computational complexity? What about the complexity with respect to the number of training samples N?

- **A sufficient condition to prove PAC-learnability is proving that a learner L requires only a polynomial number of training examples, and processing per example is polynomial**

Agnostic Learning

- So far, we assumed that $c \in H$, or at least that $VS_{H,\mathcal{D}}$ is not empty, and the learner L will always output a hypothesis h such that $error_{\mathcal{D}}(h) = 0$
- But in general (**agnostic**) leaner will output a hypothesis h such that $error_{\mathcal{D}}(h) > 0$
- Can we bound $error_{true}(h)$ given $error_{\mathcal{D}}(h)$?

If the hypothesis space H is **finite** and $\mathcal{D}$ is a sequence of $N \geq 1$ i.i.d. examples of some target concept c, then for any $0 \leq \varepsilon \leq 1$, and for any learned hypothesis h, the probability that $error_{true}(h) - error_{\mathcal{D}}(h) > \varepsilon$ is less than $|H|e^{-2N\varepsilon^2}$

$$Pr(\exists h \in H : error_{true}(h) > error_{\mathcal{D}}(h) + \varepsilon) \leq |H|e^{-2N\varepsilon^2}$$

Agnostic Learning - Proof

- **Additive Hoeffding Bound**: let $\hat{\theta}$ be the empirical mean of N i.i.d. Bernoulli random variables with mean θ:

$$Pr(\theta > \hat{\theta} + \varepsilon) \leq e^{-2N\varepsilon^2}$$

- So for any **single** hypothesis h:

$$Pr(error_{true}(h) > error_{\mathcal{D}}(h) + \varepsilon) \leq e^{-2N\varepsilon^2}$$

- As we want this to be true for all the hypothesis in H:

$$Pr(\exists h \in H : error_{true}(h) > error_{\mathcal{D}}(h) + \varepsilon) \leq |H| e^{-2N\varepsilon^2}$$

Bounds for Agnostic Learning

- Similarly to what done before, we can bound the sample complexity:

$$N \geq \frac{1}{2\varepsilon^2}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

- We can also bound the true error of the hypotesis as:

$$error_{true}(h) \leq error_{\mathcal{D}}(h) + \sqrt{\frac{\ln|H| + \ln\frac{1}{\delta}}{2N}}$$

- We found the bias and variance decomposition we previously saw in the course!

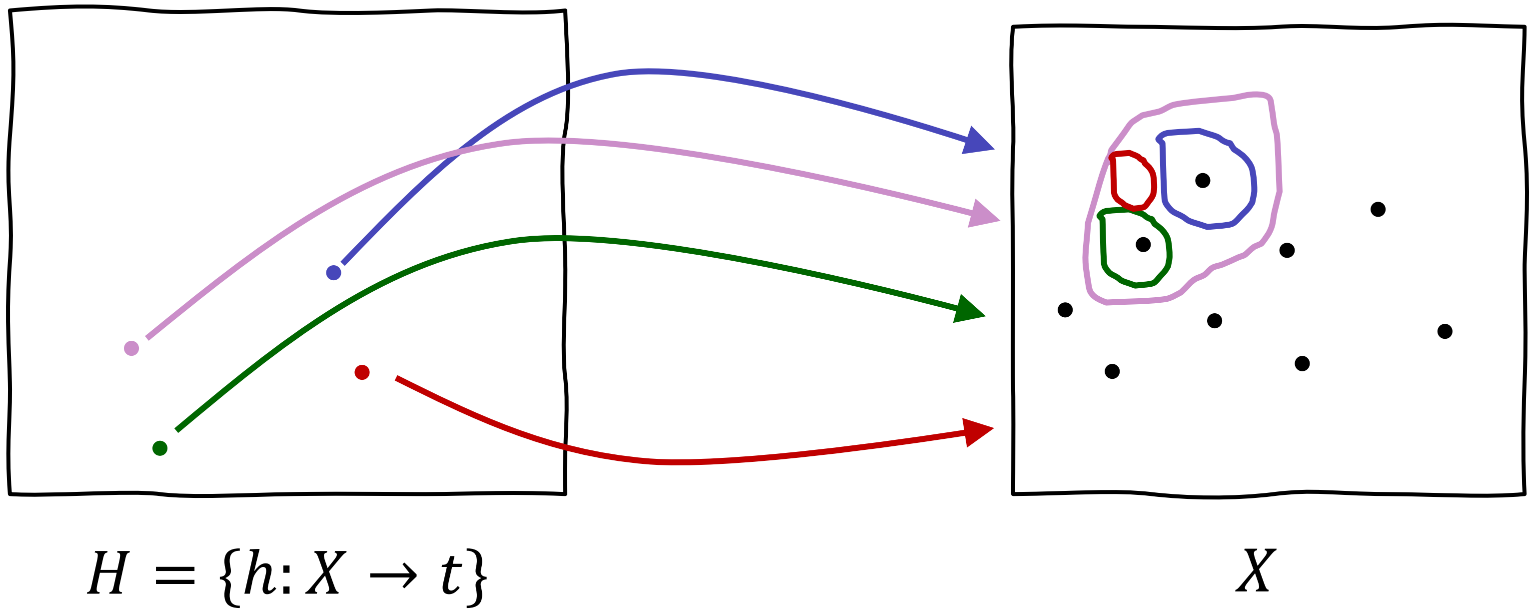
PAC-Learning with Infinite Hypotheses Spaces

- Previously we found this PAC-Learning bound for the number of samples:

$$N \geq \frac{1}{\varepsilon}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

- If |H| is infinite, what does this mean? What can we used instead of |H|?
- The answer is the largest subset of X for which |H| can guarantee a zero training error (regardless of the target function c)
- We call **VC dimension** the size of this subset

Intuition Behind Using VC Dimension



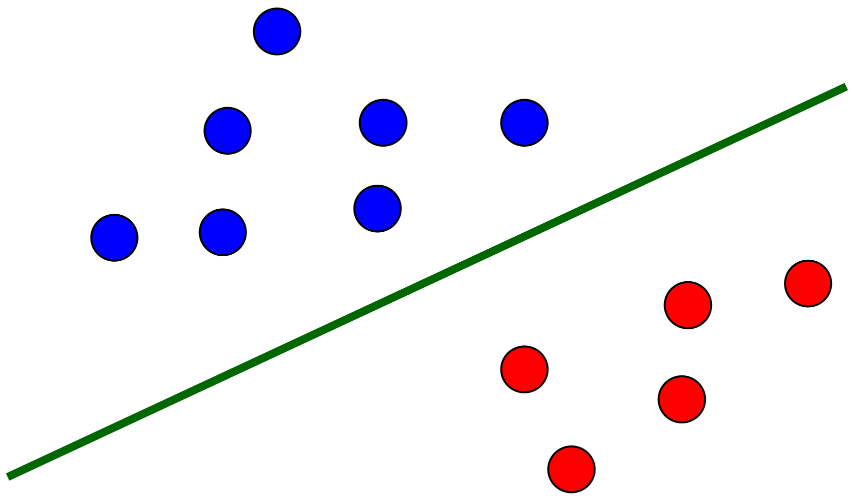
- Let assume that |X|=N, how big is |C|?
- Assuming |H| = 2^N, we can always find $h \in H$ with $error_{\mathcal{D}}(h)$=0
- Does $error_{\mathcal{D}}(h)$ tells something more on the error on other samples in X?
- What happens instead if with H we can classify correctly no more than 2 training samples?

VC Dimension

- We define a **dichotomy** of a set S of instances as a partition of S into two disjoint subsets, i.e., labeling each instance in S as positive or negative
- We say that 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
- The **Vapnik-Chervonenkis dimension**, VC(H), of hypothesis space H over instance space X, is the largest finite subset of X shattered by H

Example: VC dimension of linear classifier

- What about a linear classifier in 2D input space?



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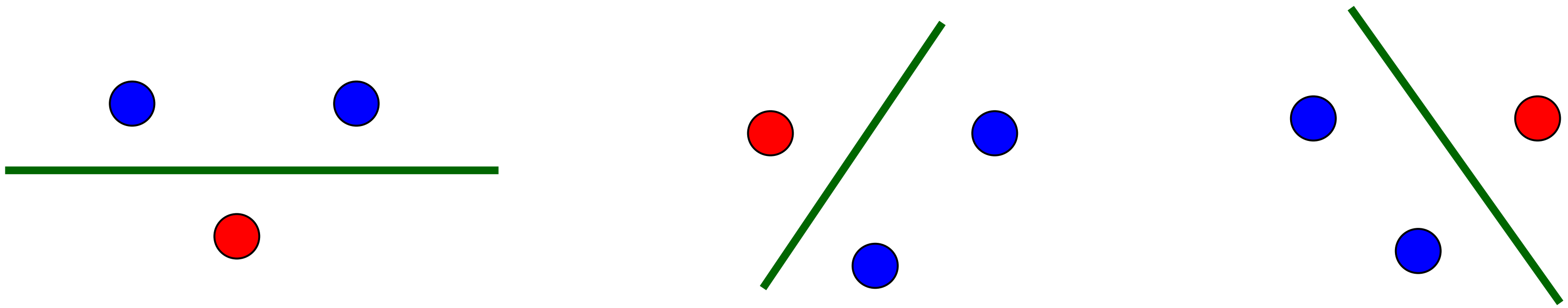

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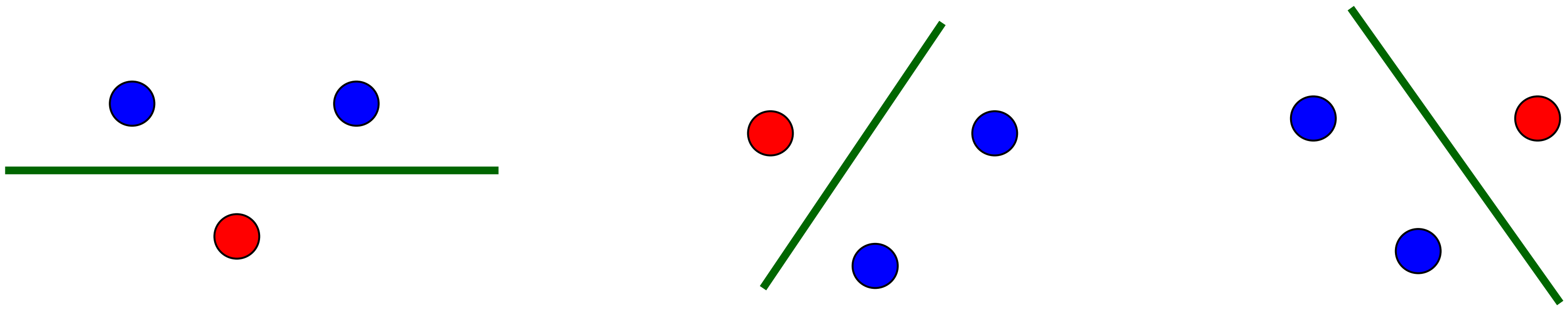

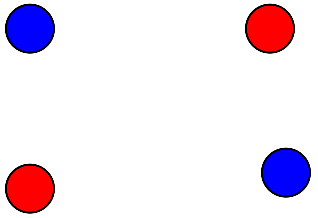

Cannot be correctly classified!

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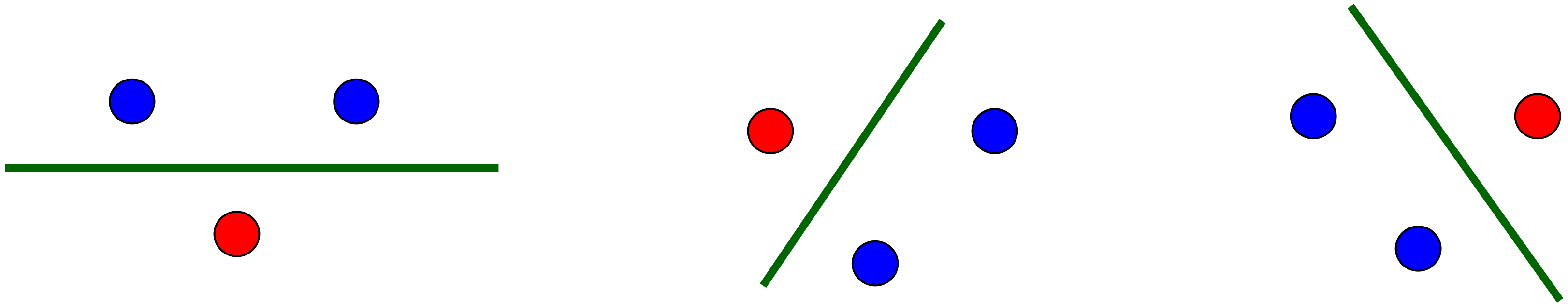

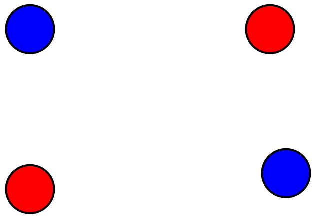

Cannot be correctly classified!

- A linear classifier in a 2D input space has VC(h)=3
- We can prove that a linear classifier in M-D input space has VC(h)=M+1

VC Dimension

- We define a **dichotomy** of a set S of instances as a partition of S into two disjoint subsets, i.e., labeling each instance in S as positive or negative
- We say that 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
- The **Vapnik-Chervonenkis dimension**, VC(H), of hypothesis space H over instance space X, is the largest finite subset of X shattered by H
- If an arbitrarily large set of X can be shattered by H, VC(H)=∞
- If $|H| < \infty$ then $VC(H) \leq \log_2(|H|)$
  - If $VC(H) = d$ it means there are in H at least 2^d hypotheses to label d instances
  - Thus, $|\mathrm{H}| \geq 2^d$

Sample Complexity based on VC-Dimension

- How many randomly drawn examples suffice to guarantee that any hypothesis that perfectly fits the training data is probably $(1-\delta)$ approximately (ε) correct ?

$$N \geq \frac{1}{\varepsilon}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

$$\Downarrow$$

$$N \geq \frac{1}{\varepsilon}\left(8VC(H)\log_2(13/\varepsilon) + 4\log_2(2/\delta)\right)$$

Agnostic Learning: VC Bounds

- With probability at least $(1-\delta)$ every $h \in H$ satisfies the following inequality:

$$error_{true}(h) \leq error_{\mathcal{D}}(h) + \sqrt{\frac{\ln|H| + \ln\frac{1}{\delta}}{2N}}$$

$$\Downarrow$$

$$error_{true}(h) \leq error_{\mathcal{D}}(h) + \sqrt{\frac{VC(H)(\ln\frac{2N}{VC(H)} + 1) + \ln\frac{4}{\delta}}{N}}$$