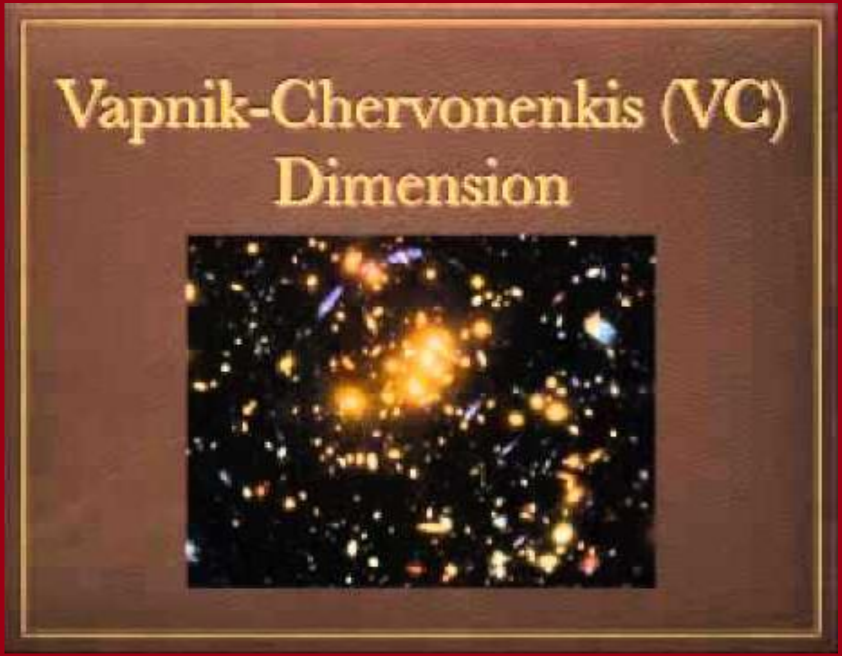
DIPARTIMENTO DI INGEGNERIA DELL'INFORMAZIONE

UNIVERSITÀ DEGLI STUDI DI PADOVA



VC Dimension

Machine Learning 2023-24

UML Book Chapter 6

Slides P. Zanuttigh (some slides from F. Vandin)

Which hypothesis classes are PAC learnable ?

Simplification: focus on binary classification and 0-1 loss

☑ Theorem (*uniform convergence*): finite classes are agnostic PAC learnable

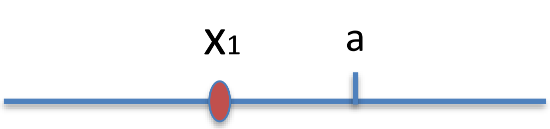
☒ Theorem (*corollary of NFL*): The set of all functions from an infinite domain set to {0,1} is not PAC learnable

- Up to now, if $|\mathcal{H}| < \infty \Rightarrow \mathcal{H}$ is PAC learnable (finite size classes are agnostic PAC learnable)
- What about infinite size classes ($|\mathcal{H}| = \infty$) ?

→ We'll demonstrate that the finite size is a sufficient but not necessary condition for agnostic PAC learnability

$$\mathcal{H} = \{h_a : a \in \mathbb{R}\}$$
$$h_a : \mathbb{R} \rightarrow \{0,1\}$$
$$h_A(x) = \begin{cases} 1 \; if \; x < a \\ 0 \; if \; x \geq a \end{cases}$$

Example: threshold function →it is PAC learnable with sample complexity $m_{\mathcal{H}}(\epsilon, \delta) = \left\lceil \frac{\log\left(\frac{2}{\delta}\right)}{\epsilon} \right\rceil$



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Restriction of a Function

Definition: Restriction of $\mathcal{H}$ to $\mathcal{C}$

- Let $\mathcal{H}$ be a class of functions from $\mathcal{X}$ to {0,1}
- Let $C = \{c_1, \dots, c_m\} \subset \mathcal{X}$ (i.e., a subset of the data domain)

The restriction $\mathcal{H}_c$ of $\mathcal{H}$ to $\mathcal{C}$ is the set of functions from $\mathcal{C}$ to *{0,1}* that can be derived from $\mathcal{H}$:

$$\mathcal{H}_c = \{ \boxed{[h(c_1), \dots, h(c_m)] :} \, h \in \mathcal{H} \}$$

Each entry: A vector of 0s and 1s of length m with the output for each c_i

Notes:

- We can represent each function h from $\mathcal{C}$ to *{0,1}* as $[h(c_1), \dots, h(c_m)]$, i.e., as a vector in $\{0,1\}^{|C|}$ with the output for each c_i
- *No Free Lunch theorem*: the idea is to select a distribution concentrated on a set C (→restriction) on which the algorithm A fails

Shattering

Definition (Shattering)

Given $C \subset X, \mathcal{H}$ shatters C if $\mathcal{H}_c$ contains all the $2^{|C|}$ functions from C to {0,1}

Corollary (of No Free Lunch)

Let $\mathcal{H}$ be a hypothesis class of functions from $\mathcal{X}$ to {0,1}. Let *m* be a training set size. Assume that there exist a set $C \subset \mathcal{X}$ of size 2*m* that is shattered by $\mathcal{H}$. Then for any learning algorithm A there exist a distribution *D* over $\mathcal{X}\ x\ \{0,1\}$ and a predictor $h \in \mathcal{H}$ such that $L_d(h) = 0$ but with probability at least 1/7 over the choice of S we have that $L_D\big(A(S)\big) \geq \frac{1}{8}$

Demonstration (intuition): on set C all functions from C to {0,1} can be chosen and we fall back into the situation of the NFL corollary

VC Dimension (1)

Definition (VC-dimension)

The VC-dimension $VCdim(\mathcal{H})$ of a hypothesis class $\mathcal{H}$, is the maximal size of a set $C \subset X$ that can be shattered by $\mathcal{H}$

Note: if $\mathcal{H}$ can shatter sets of arbitrarily large size then $VCdim(\mathcal{H}) = +\infty$

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VC Dimension (2)

Definition (VC-dimension): The VC-dimension $VCdim(\mathcal{H})$ of a hypothesis class $\mathcal{H}$, is the maximal size of a set $C \subset X$ that can be shattered by $\mathcal{H}$

- *In the case of finite class hypotheses:*
  1. They are agnostic PAC learnable (already demonstrated)
  2. To shatter a set of size $|C|$ → at least $2^{|C|}$ functions (need all combinations)
  3. With $|\mathcal{H}|$ functions → the largest set that can be shattered has size $\log_2|\mathcal{H}|$
  4. To have $VCdim(\mathcal{H}) = d \Longrightarrow$ shatter a set of size $d \Longrightarrow$ $VCdim(\mathcal{H}) \leq \log_2|\mathcal{H}|$

- *If $\mathcal{H}$ has an infinite VC dimension: it is not PAC learnable*
  1. $VCdim(\mathcal{H}) = \infty \Longrightarrow \forall m$: ∃ a shattered set of size 2m (can shatter any size)
  2. Apply NFL corollary: $\exists D$ on which A does not work (for any possible A)
  3. $\exists D$ with probability $\geq \frac{1}{7}$ $L_D \geq \frac{1}{8} \Longrightarrow$ it is not PAC learnable (for ∀ A)

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Compute VC Dimension

VC-dimension: The VC-dimension $VCdim(\mathcal{H})$ of a hypothesis class $\mathcal{H}$, is the maximal size of a set $C \subset X$ that can be shattered by $\mathcal{H}$

To show that $VCdim(\mathcal{H}) = d$ we need to show that:

1. $VCdim(\mathcal{H}) \geq d$: there exists a set C of size *d* which is shattered by $\mathcal{H}$

2. $VCdim(\mathcal{H}) < (d + 1)$: every set of size *d + 1* is not shattered by $\mathcal{H}$

Note: need to shatter a single set of size d but must not shatter any possible set of size d+1

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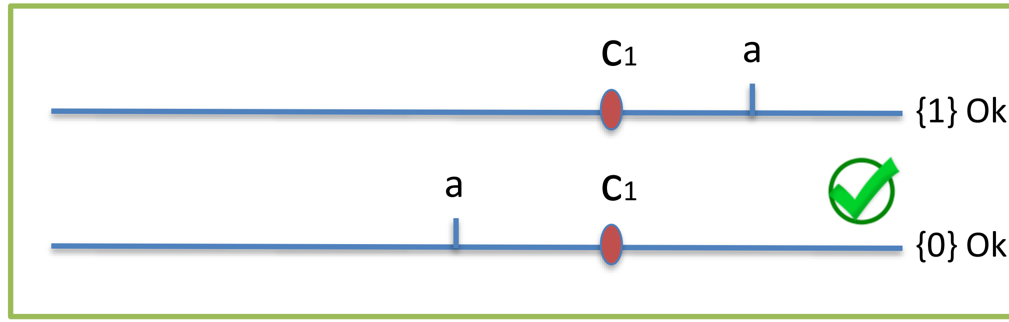
Compute VC Dimension: Example (1)

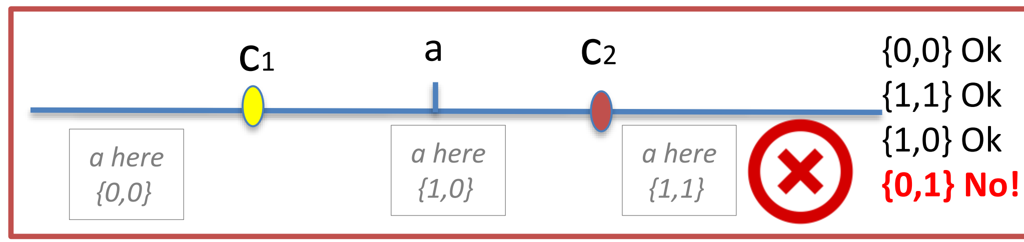
Threshold function

$$\mathcal{H} = \{h_a : a \in \mathbb{R}\}$$

$h_a : \mathbb{R} \rightarrow \{0,1\}$ is:

$$h_A(x) = \begin{cases} 1 \; if \; x < a \\ 0 \; if \; x \geq a \end{cases}$$





$$VCdim(\mathcal{H}) \geq 1$$

$$VCdim(\mathcal{H}) < 2$$

$$\boldsymbol{VCdim(\mathcal{H}) = 1}$$

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Compute VC Dimension: Example (2)

Interval

$$\mathcal{H} = \{h_{a,b} : a, b \in \mathbb{R} \ , a < b\}$$

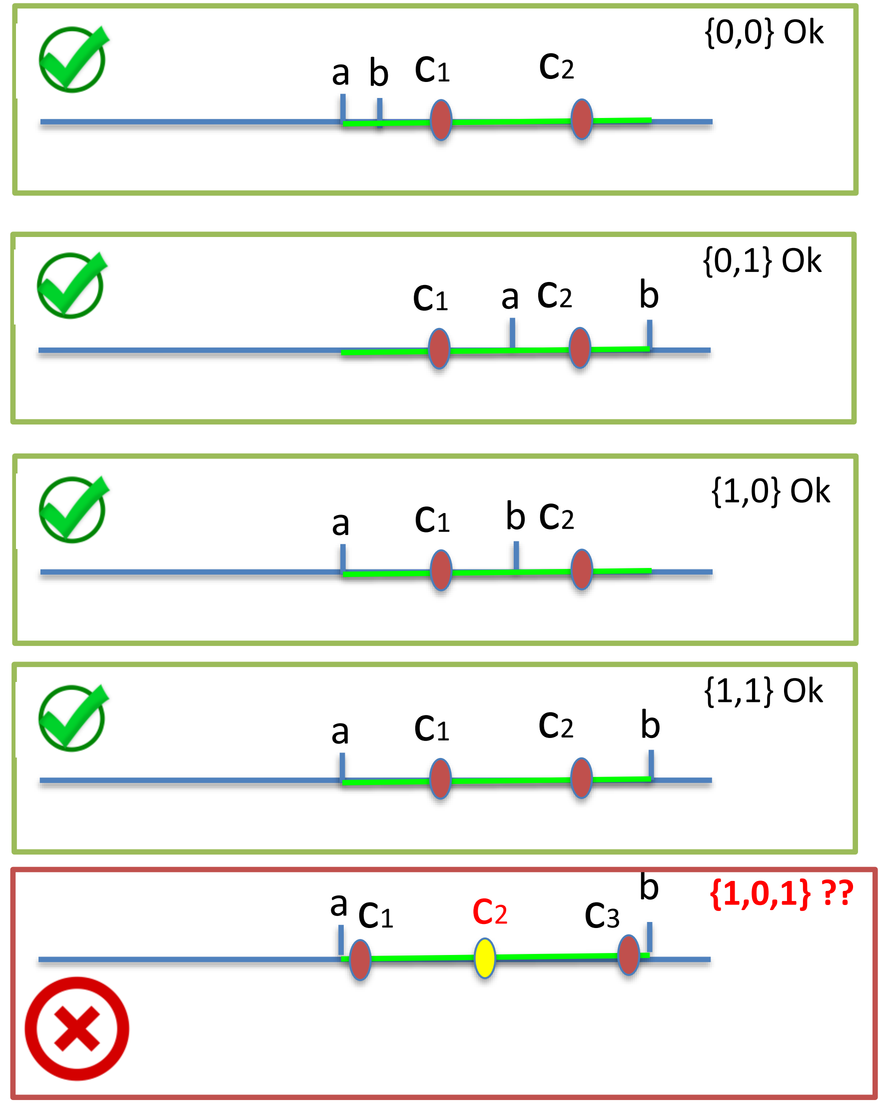
$h_{a,b} : \mathbb{R} \to \{0,1\}$ is:

$$h_{a,b}(x) = \begin{cases} 1 \ if \ a < x < b \\ 0 \quad otherwise \end{cases}$$

$$VCdim(\mathcal{H}) \geq 2$$

$$VCdim(\mathcal{H}) < 3$$

$$\boldsymbol{VCdim(\mathcal{H}) = 2}$$



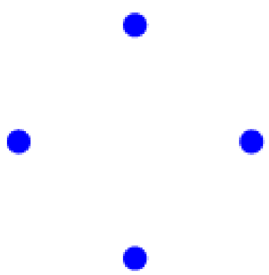
Compute VC Dimension: Exercise – Try to do it !!

Axis aligned rectangle

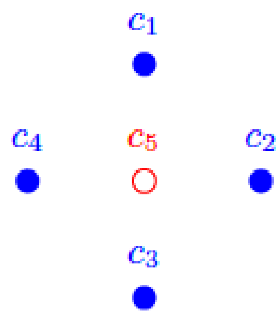
$$\mathcal{H} = \{h_{a_1,a_2,b_1,b_2} : a_1, a_2, b_1, b_2 \in \mathbb{R} \ , a_1 \le a_2, b_1 \le b_2 \}$$

$h_{a_1,a_2,b_1,b_2} : \mathbb{R} \to \{0,1\}$ is:

$$h_{a_1,a_2,b_1,b_2}(x_1, x_2) = \begin{cases} 1 \ if \ a_1 \le x_1 \le a_2, b_1 \le \ x_2 \le b_2 \\ \quad 0 \quad otherwise \end{cases}$$



The set can be shattered



{1,1,1,1,0} No!!

$VCdim(\mathcal{H}) \ge 4$

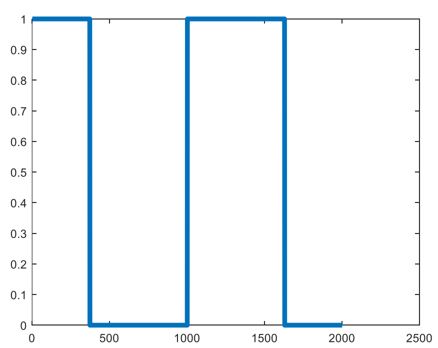
$VCdim(\mathcal{H}) < 5$

$\boldsymbol{VCdim(\mathcal{H}) = 4}$

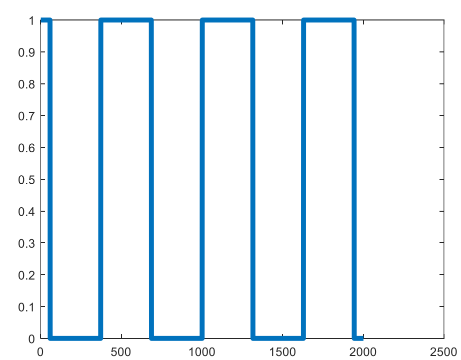
Case 5 points: define c_1 top point, c_2 rightmost, c_3 bottom, c_4 leftmost, c_5 the remaining one. If different labeling just swaps the case that can not be obtained.

Compute VC Dimension: Example (4)

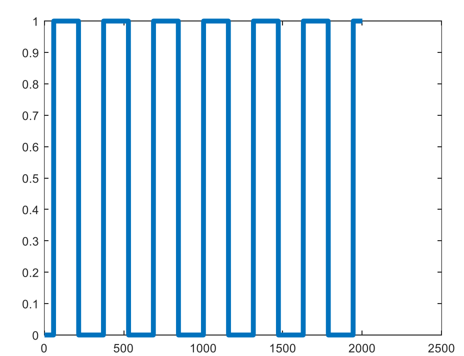
- *Recall*: for finite classes: $VCdim(\mathcal{H}) \leq \log_2(|\mathcal{H}|)$ ...
- ... but VC dimension does not always correspond to the number of parameters !!
- Example $\mathcal{H} = \{h_\theta : \theta \in \mathbb{R}\}, \; h_\theta : \mathcal{X} \to \{0,1\} \; h_\theta = [0.5\sin(\theta x)]$
  - It has infinite VC dimension !!



$\theta = 0.5$



$\theta = 1$



$\theta = 2$

Fundamental Theorem of Statistical Learning

Let $\mathcal{H}$ be a hypothesis class of functions from $\mathcal{X}$ to {0,1} and let the loss function be the 0-1 loss

Then, the following statements are equivalent:

1. $\mathcal{H}$ has the uniform convergence property
2. Any ERM rule is a successful agnostic PAC learner for $\mathcal{H}$
3. $\mathcal{H}$ is agnostic PAC learnable
4. $\mathcal{H}$ is PAC learnable
5. Any ERM rule is a successful PAC learner for $\mathcal{H}$
6. $\mathcal{H}$ has finite VC dimension

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Theorem of Statistical Learning: Notes on the demonstration

1. We have already seen that 1 → 2 → 3 (uniform convergence implies agnostic PAC learnable and ERM rule is PAC learner)
2. 3 → 4 is trivial (if realizable they are the same if not PAC condition does not apply)
3. 2 → 5 also trivial (ERM rule, if realizable same target)
4. 4 → 6 and 5 → 6 follow from corollary of No-Free-Lunch (by contradiction, if $VCdim(\mathcal{H}) = \infty$, $\mathcal{H}$ is not PAC learnable)
5. The challenging part is how to close the loop (6 → 1, from finite VC dimension to uniform convergence)

The proof 6 → 1 (not part of the course) can be divided in two main parts:

- *If VCdim($\mathcal{H}$) = d, then even though |$\mathcal{H}$| might be infinite, when restricting $\mathcal{H}$ to a finite set C, its "effective size" $|\mathcal{H}_C|$, is only $O(|C|^d)$. That is, $|\mathcal{H}_C|$ grows polynomially rather than exponentially with |C| (Sauer's lemma)*
- *Recall that finite hypothesis classes enjoy the uniform convergence property. This result can be generalized by showing that uniform convergence holds whenever the hypothesis class has a "small effective size" (i.e., classes for which $|\mathcal{H}_C|$ grows polynomially with |C|)*

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Theorem of Statistical Learning: Quantitative Version

Not part of the course, just notice how the number of samples depend on $VCdim(\mathcal{H}) = d$

Let $\mathcal{H}$ be a hypothesis class of functions from $\mathcal{X}$ to {0,1} and let the loss function be the 0-1 loss. Assume that $VCdim(\mathcal{H}) = d < \infty$

Then, there are absolute constants C_1 and C_2 such that:

1. $\mathcal{H}$ has the uniform convergence property with sample complexity

$$C_1 \frac{d + \log(\frac{1}{\delta})}{\epsilon^2} \leq m_{\mathcal{H}}^{UC}(\epsilon, \delta) \leq C_2 \frac{d + \log(\frac{1}{\delta})}{\epsilon^2}$$

2. $\mathcal{H}$ is agnostic PAC learnable with sample complexity

$$C_1 \frac{d + \log(\frac{1}{\delta})}{\epsilon^2} \leq m_{\mathcal{H}}^{UC}(\epsilon, \delta) \leq C_2 \frac{d + \log\left(\frac{1}{\delta}\right)}{\epsilon^2}$$

3. $\mathcal{H}$ is PAC learnable with sample complexity

$$C_1 \frac{d + \log(\frac{1}{\delta})}{\epsilon} \leq m_{\mathcal{H}}^{UC}(\epsilon, \delta) \leq C_2 \frac{d\ log(\frac{1}{\epsilon}) + \log(\frac{1}{\delta})}{\epsilon}$$

$$\log\left(\frac{2|\mathcal{H}|}{\delta}\right) = \log 2|\mathcal{H}| + \log\frac{1}{\delta}$$

Recall:

(notice the role of $|\mathcal{H}|$ and of the VC dimension d)

Proposition

Let $\mathcal{H}$ be a finite hypothesis class, let Z be a domain, and let $\ell : \mathcal{H} \times Z \to [0,1]$ be a loss function. Then:

- $\mathcal{H}$ enjoys the uniform convergence property with sample complexity

$$m_{\mathcal{H}}^{UC}(\varepsilon, \delta) \leq \left\lceil \frac{\log(2|\mathcal{H}|/\delta)}{2\varepsilon^2} \right\rceil$$