CSE4088 Introduction to Machine Learning

The VC dimension

Slides are adopted from lecture notes of Yaser Abu-Mostafa

Outline

- The definition of VC dimension
- VC dimension of perceptrons
- Interpreting the VC dimension
- Generalization bounds

Definition of VC Dimension

The VC dimension of a hypothesis set $\mathcal{H}$, denoted by $d_{\text{VC}}(\mathcal{H})$, is

the largest value of N for which $m_{\mathcal{H}}(N) = 2^N$

"the most points $\mathcal{H}$ can shatter"

$N \leq d_{\text{VC}}(\mathcal{H}) \implies \mathcal{H}$ can shatter N points

$k > d_{\text{VC}}(\mathcal{H}) \implies k$ is a break point for $\mathcal{H}$

The growth function

In terms of a break point k:

$$m_{\mathcal{H}}(N) \leq \sum_{i=0}^{k-1} \binom{N}{i}$$

In terms of the VC dimension d_{VC}:

$$m_{\mathcal{H}}(N) \leq \underbrace{\sum_{i=0}^{d_{\text{VC}}} \binom{N}{i}}_{\text{maximum power is } N^{d_{\text{VC}}}}$$

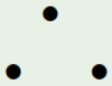
Examples

- $\mathcal{H}$ is positive rays:

$$d_{\text{VC}} = 1$$

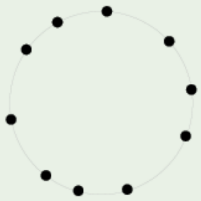
- $\mathcal{H}$ is 2D perceptrons:

$$d_{\text{VC}} = 3$$



- $\mathcal{H}$ is convex sets:

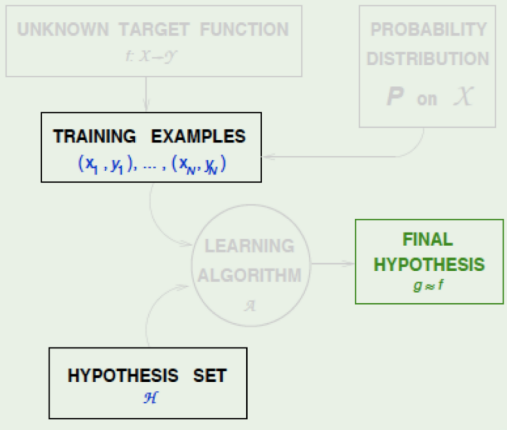
$$d_{\text{VC}} = \infty$$



VC dimension and learning

$d_{\text{VC}}(\mathcal{H})$ is finite $\implies$ $g \in \mathcal{H}$ will generalize

- Independent of the learning algorithm
- Independent of the input distribution
- Independent of the target function



VC dimension of perceptrons

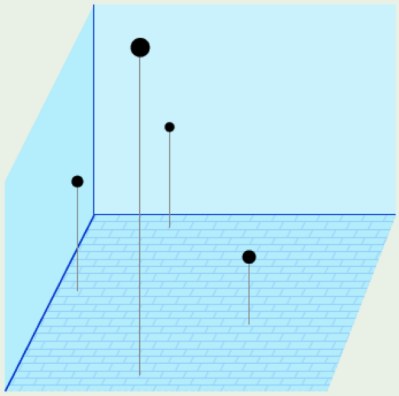
For $d = 2$, $d_{\text{VC}} = 3$

In general, $\boxed{d_{\text{VC}} = d + 1}$

We will prove two directions:

$$d_{\text{VC}} \leq d + 1$$

$$d_{\text{VC}} \geq d + 1$$



Here is one direction

A set of $N = d + 1$ points in $\mathbb{R}^d$ shattered by the perceptron:

$$\mathrm{X} = \begin{bmatrix} — \mathbf{x}_1^\intercal — \\ — \mathbf{x}_2^\intercal — \\ — \mathbf{x}_3^\intercal — \\ \vdots \\ — \mathbf{x}_{d+1}^\intercal — \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & & 0 \\ & \vdots & & \ddots & 0 \\ 1 & 0 & \dots & 0 & 1 \end{bmatrix}$$

X is invertible

Can we shatter this data set?

For any $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{d+1} \end{bmatrix} = \begin{bmatrix} \pm 1 \\ \pm 1 \\ \vdots \\ \pm 1 \end{bmatrix}$, can we find a vector $\mathbf{w}$ satisfying

$$\text{sign}(\mathrm{X}\mathbf{w}) = \mathbf{y}$$

Easy! Just make $\mathrm{X}\mathbf{w} = \mathbf{y}$

which means $\mathbf{w} = \mathrm{X}^{-1}\mathbf{y}$

We can shatter these $d+1$ points

This implies what?

[a] $d_{\text{VC}} = d + 1$

[b] $d_{\text{VC}} \geq d + 1$ ✓

[c] $d_{\text{VC}} \leq d + 1$

[d] No conclusion

Now, to show that $d_{\text{vc}} \leq d + 1$

We need to show that:

[a] There are $d + 1$ points we cannot shatter

[b] There are $d + 2$ points we cannot shatter

[c] We cannot shatter *any* set of $d + 1$ points

[d] We cannot shatter *any* set of $d + 2$ points ✓

Take any $d + 2$ points

For any $d + 2$ points,

$$\mathbf{x}_1, \cdots, \mathbf{x}_{d+1}, \mathbf{x}_{d+2}$$

More points than dimensions $\implies$ we must have

$$\mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{x}_i$$

where not all the a_i's are zeros

So?

$$\mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{x}_i$$

Consider the following dichotomy:

$\mathbf{x}_i$'s with non-zero a_i get $y_i = \text{sign}(a_i)$

and $\mathbf{x}_j$ gets $y_j = -1$

No perceptron can implement such dichotomy!

This is a dichotomy

Why?

$$\mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{x}_i \implies \mathbf{w}^\intercal \mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{w}^\intercal \mathbf{x}_i$$

If $y_i = \text{sign}(\mathbf{w}^\intercal \mathbf{x}_i) = \text{sign}(a_i)$, then $a_i \, \mathbf{w}^\intercal \mathbf{x}_i > 0$

This forces $\mathbf{w}^\intercal \mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{w}^\intercal \mathbf{x}_i > 0$

Therefore, $y_j = \text{sign}(\mathbf{w}^\intercal \mathbf{x}_j) = +1$

Putting it together

We proved $d_{\text{VC}} \leq d+1$ and $d_{\text{VC}} \geq d+1$

$$\boxed{d_{\text{VC}} = d+1}$$

What is $d+1$ in the perceptron?

It is the number of parameters $w_0, w_1, \cdots, w_d$

Outline

- The definition of VC dimension
- VC dimension of perceptrons
- Interpreting the VC dimension
  1. What does the VC dimension signify?
  2. Is VC dimension useful in practice?
- Generalization bounds

1. Degrees of freedom

Parameters create degrees of freedom

# of parameters: **analog** degrees of freedom

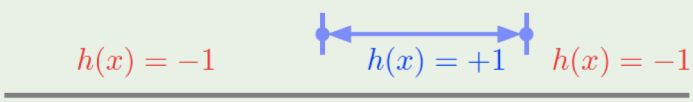
d_{VC}: equivalent '**binary**' degrees of freedom

- VC dimension represents how many different dichotomies We can get.
- VC dimension abstracts how expressive the model is.

The usual suspects

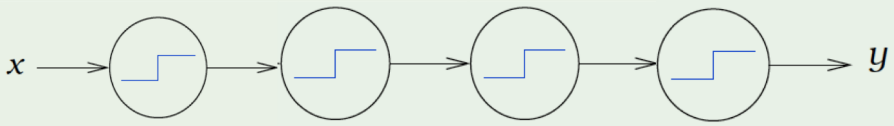
Positive rays ($d_{\text{VC}} = 1$):

Positive intervals ($d_{\text{VC}} = 2$):



Not just parameters

Parameters may not contribute degrees of freedom:



- 1-D perceptron has 2 parameters: the weight and the threshold.
- If we cascade 4 perceptrons, we have 2 x 4 = 8 parameters
- Does it have 8 degrees of freedom?
- NO!: It is equivalent to a single perceptron.

d_{VC} measures the **effective** number of parameters

2. Number of data points needed

Two small quantities in the VC inequality:

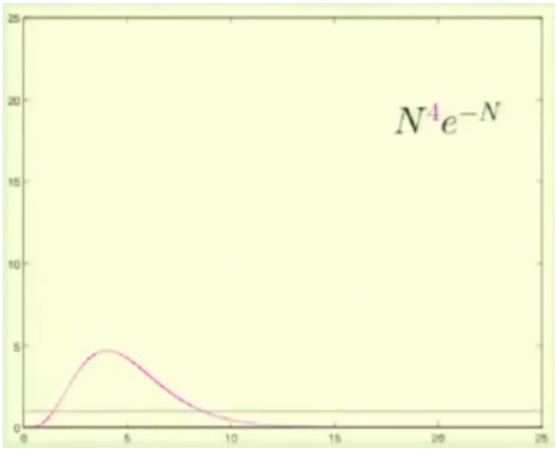
$$\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq \underbrace{4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N}}_{\delta}$$

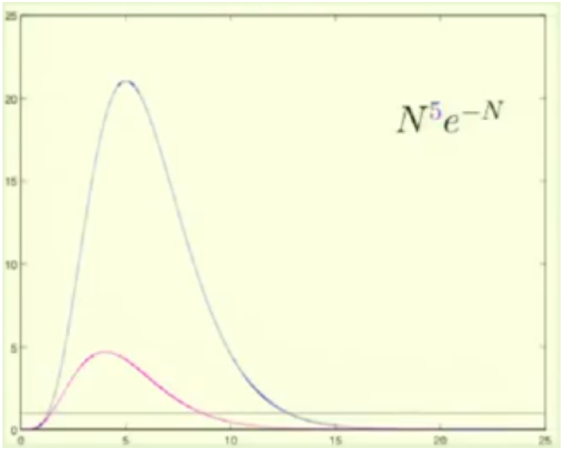
If we want certain ϵ and δ, how does N depend on d_{VC}?

E.g. If we want E_{in} and E_{out} to be within 10% of each other 95% of the time, how many examples do we need?
$(\in = 0.1, \delta = 0.05)$

Let us look at $N^d e^{-N}$

$$N^d e^{-N}$$





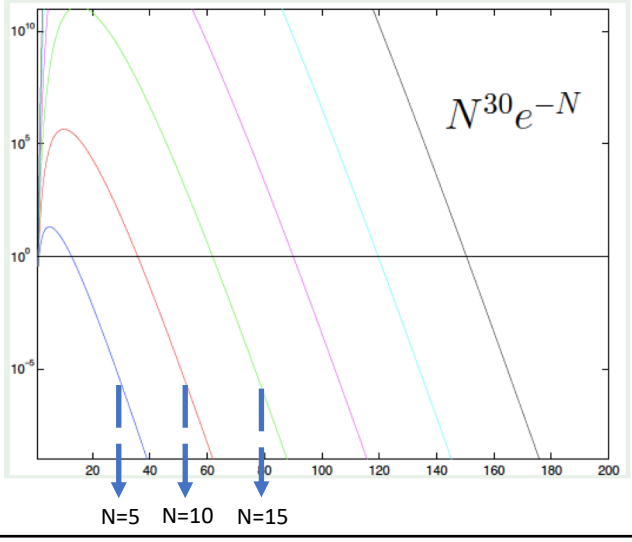
$$N^d e^{-N}$$

Fix $N^d e^{-N}$ = small value

How does N change with d?

Rule of thumb:

$$N \geq 10\, d_{\text{VC}}$$



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Rearranging things

Start from the VC inequality:

$$\mathbb{P}\left[|E_{\text{out}} - E_{\text{in}}| > \epsilon\right] \leq \underbrace{4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N}}_{\delta}$$

Get ϵ in terms of δ:

$$\delta = 4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N} \implies \epsilon = \underbrace{\sqrt{\frac{8}{N}\ln\frac{4m_{\mathcal{H}}(2N)}{\delta}}}_{\Omega}$$

With probability $\geq 1 - \delta$, $\quad |E_{\text{out}} - E_{\text{in}}| \leq \Omega(N, \mathcal{H}, \delta)$

Generalization bound

With probability $\geq 1 - \delta$, $\underbrace{E_{\text{out}} - E_{\text{in}}}_{\text{Generalization error}} \leq \Omega$

$\Longrightarrow$

With probability $\geq 1 - \delta$,

$$E_{\text{out}} \leq E_{\text{in}} + \Omega$$