CS260: Machine Learning Algorithms

Lecture 7: VC Dimension

Cho-Jui Hsieh
UCLA

Jan 30, 2019

Reducing M to finite number

Where did the M come from?

- The $\mathcal{B}$ad events $\mathcal{B}_m$:
  "$|E_{\text{tr}}(h_m) - E(h_m)| > \epsilon$" with probability $\leq 2e^{-2\epsilon^2 N}$

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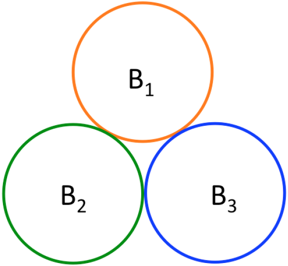
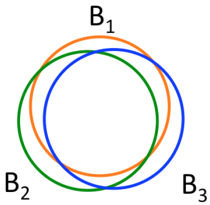
- The union bound:

  $$\mathbb{P}[\mathcal{B}_1 \text{ or } \mathcal{B}_2 \text{ or } \cdots \text{ or } \mathcal{B}_M]$$
  $$\leq \underbrace{\mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \cdots + \mathbb{P}[\mathcal{B}_M]}_{\text{consider worst case: no overlaps}} \leq 2Me^{-2\epsilon^2 N}$$

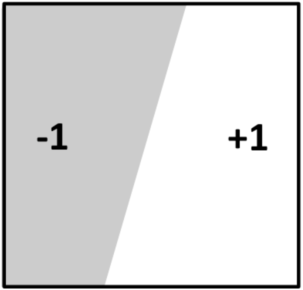


No overlap: bound is tight



Large overlap

Can we improve on M?



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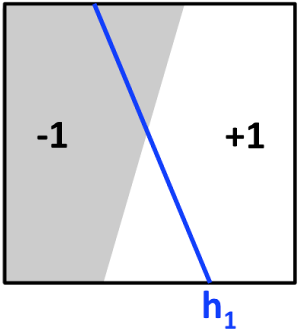

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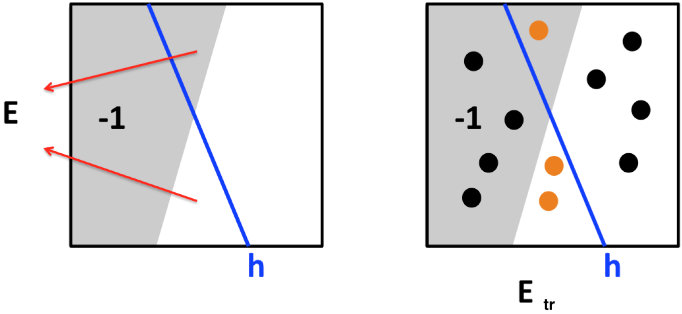

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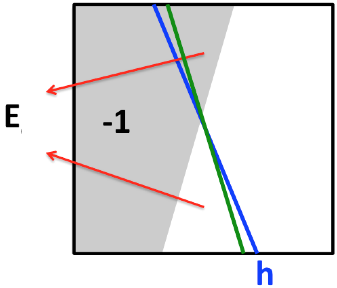
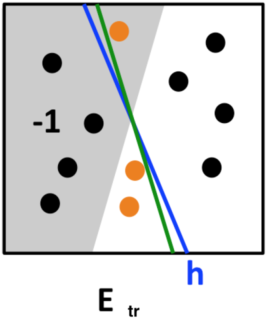
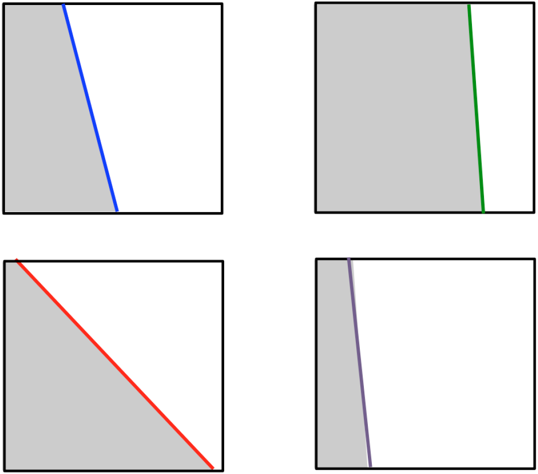




- The event that $|E_{\text{tr}}(h_1) - E(h_1)| > \epsilon$ and $|E_{\text{tr}}(h_2) - E(h_2)| > \epsilon$ are largely overlapped.

What can we replace M with?

Instead of the whole input space



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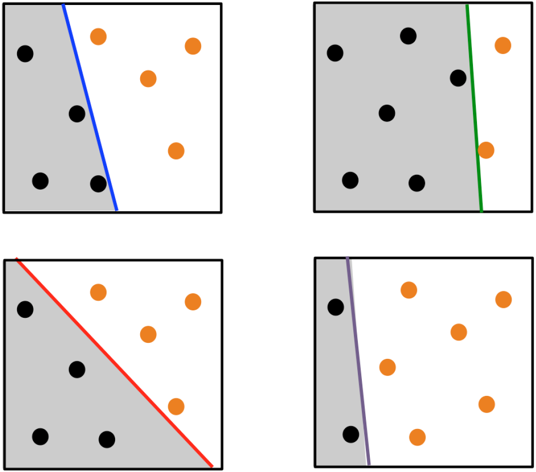
Let's consider a finite set of input points

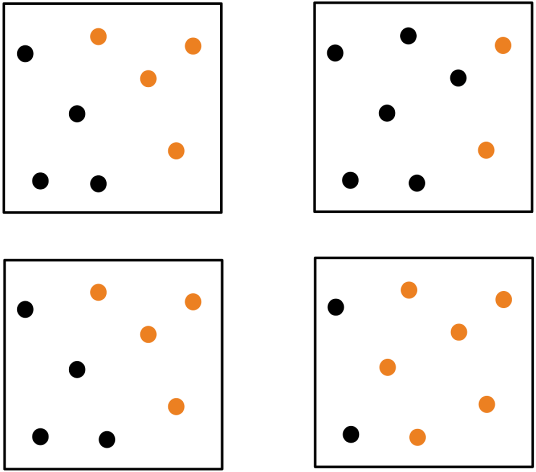


What can we replace M with?

Instead of the whole input space

Let's consider a finite set of input points

How many patterns of colors can you get?



Dichotomies: mini-hypotheses

- A hypothesis: $h : \mathcal{X} \to \{-1, +1\}$
- A dichotomy: $h : \{\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_N\} \to \{-1, +1\}$

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  $\Rightarrow$Candidate for replacing M

The growth function

- The growth function counts the most dichotomies on any N points:

$$m_{\mathcal{H}}(N) = \max_{\boldsymbol{x}_1,\cdots,\boldsymbol{x}_N \in \mathcal{X}} |\mathcal{H}(\boldsymbol{x}_1,\cdots,\boldsymbol{x}_N)|$$

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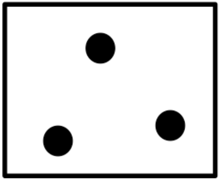
- The growth function satisfies:

$$m_{\mathcal{H}}(N) \leq 2^N$$

Growth function for linear classifiers

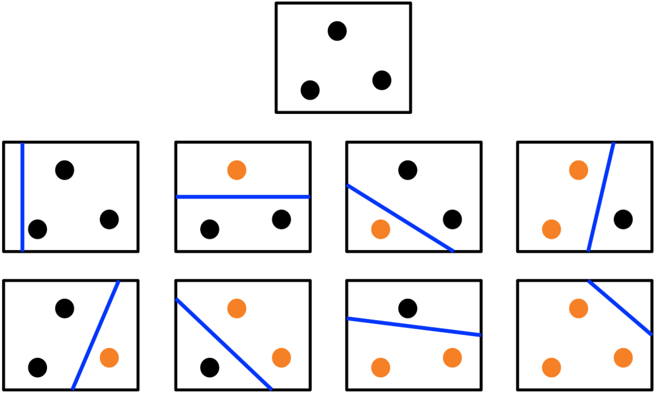
Compute $m_{\mathcal{H}}(3)$ in 2-D space



What's $|\mathcal{H}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)|$?

Growth function for linear classifiers

Compute $m_{\mathcal{H}}(3)$ in 2-D space when $\mathcal{H}$ is perceptron (linear hyperplanes)



$$m_{\mathcal{H}}(3) = 8$$

Growth function for linear classifiers

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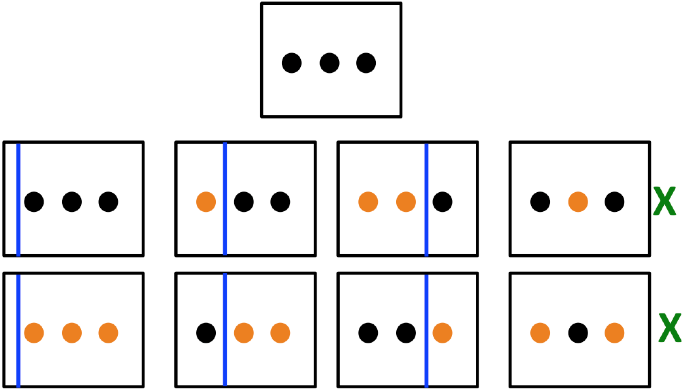

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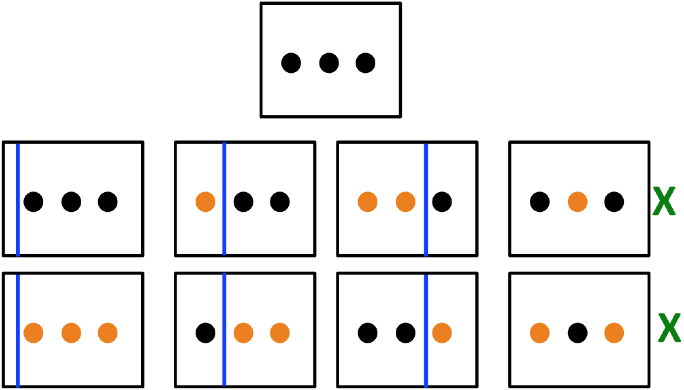

Doesn't matter because we only counts the most dichotomies

Growth function for linear classifiers

- What's $m_{\mathcal{H}}(4)$?

Growth function for linear classifiers

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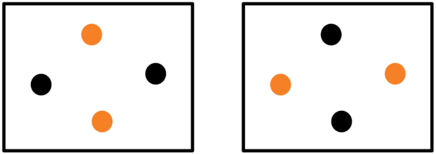
- (At least) missing two dichotomies:



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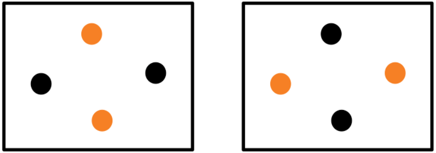
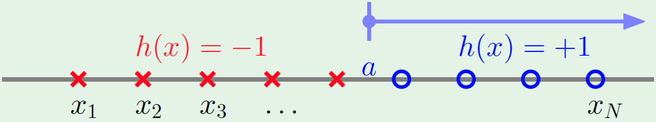


- $m_{\mathcal{H}}(4) = 14 < 2^4$

Example I: positive rays

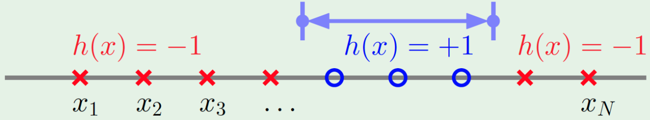


$\mathcal{H}$ is set of $h\colon \mathbb{R} \to \{-1, +1\}$

$h(x) = \mathrm{sign}(x - a)$

$m_{\mathcal{H}}(N) = N + 1$

Example II: positive intervals



$\mathcal{H}$ is set of $h \colon \mathbb{R} \to \{-1, +1\}$

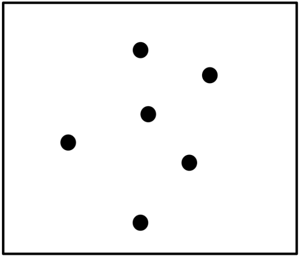
Place interval ends in two of $N + 1$ spots

$m_{\mathcal{H}}(N) = \binom{N+1}{2} + 1 = \frac{1}{2}N^2 + \frac{1}{2}N + 1$

Example III: convex sets

- $\mathcal{H}$ is set of $h : \mathbb{R}^2 \to \{-1, +1\}$

  $h(\boldsymbol{x}) = +1$ is convex
- How many dichotomies can we generate?



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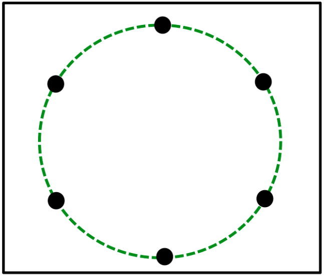

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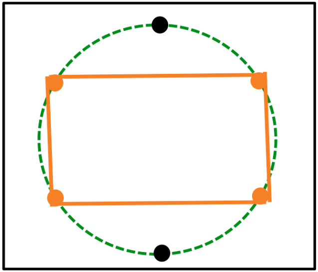

Example III: convex sets

- $\mathcal{H}$ is set of $h : \mathbb{R}^2 \to \{-1, +1\}$

  $h(\boldsymbol{x}) = +1$ is convex
- $m_{\mathcal{H}}(N) = 2^N$ for any N

  $\Rightarrow$ We say the N points are "shattered" by h

The 3 growth functions

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

$$m_{\mathcal{H}}(N) = N + 1$$

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

$$m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

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

$$m_{\mathcal{H}}(N) = 2^N$$

What's next?

- Remember the inequality

$$\mathbb{P}[|E_{\text{in}} - E_{\text{out}}| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$$

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- What happens if we replace M by $m_{\mathcal{H}}(N)$?
  $m_{\mathcal{H}}(N)$ polynomial $\Rightarrow$ Good!

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$$\mathbb{P}[|E_{\text{in}} - E_{\text{out}}| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$$

- What happens if we replace M by $m_{\mathcal{H}}(N)$?
  $m_{\mathcal{H}}(N)$ polynomial $\Rightarrow$ Good!
- How to show $m_{\mathcal{H}}(N)$ is polynomial?

When will $m_{\mathcal{H}}(N)$ be polynomial

Break point of $\mathcal{H}$

- If no data set of size k can be shattered by $\mathcal{H}$, then k is a break point for $\mathcal{H}$

$$m_{\mathcal{H}}(k) < 2^k$$

- VC dimension of $\mathcal{H}$: $k - 1$ (the most points $\mathcal{H}$ can shatter)

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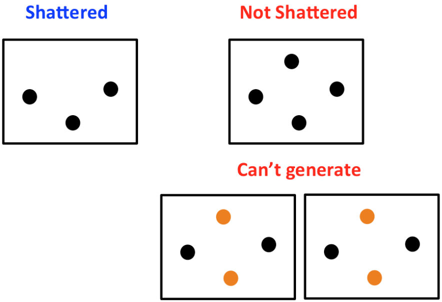
- For 2-D perceptron: $k = 4$, VC dimension $= 3$



Break point - examples

- Positive rays: $m_{\mathcal{H}}(N) = N + 1$

  Break point $k = 2$, $d_{VC} = 1$

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- Positive rays: $m_{\mathcal{H}}(N) = N + 1$

  Break point $k = 2$, $d_{VC} = 1$
- Positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$

  Break point $k = 3$, $d_{VC} = 2$
- Convex set: $m_{\mathcal{H}}(N) = 2^N$

  Break point $k = \infty$, $d_{VC} = \infty$

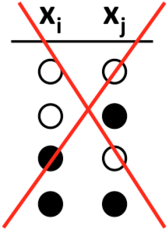
We will show

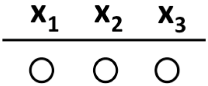
No break point $\Rightarrow m_{\mathcal{H}}(N) = 2^N$

Any break point $\Rightarrow m_{\mathcal{H}}(N)$ is polynomial in N

Puzzle

- Break point is $k = 2$





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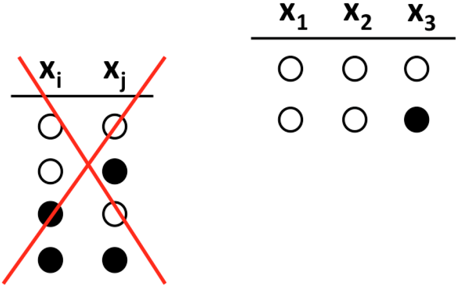

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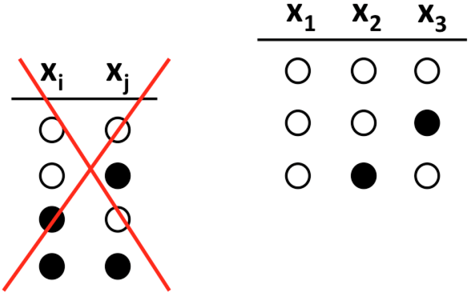

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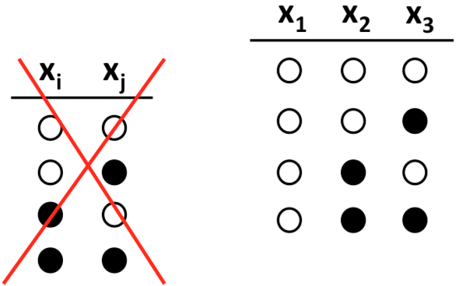

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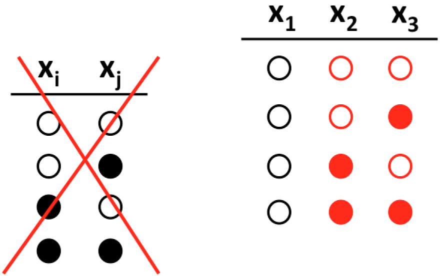

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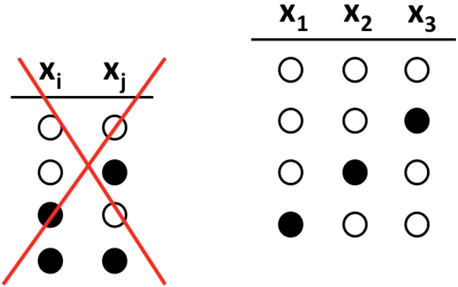

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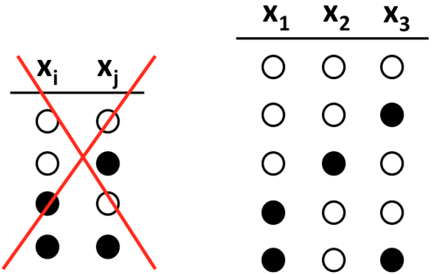

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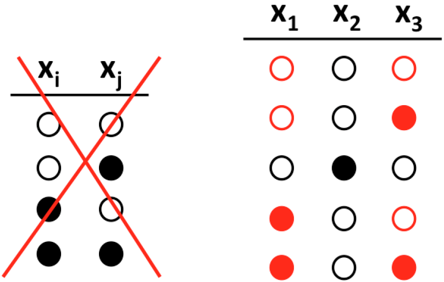

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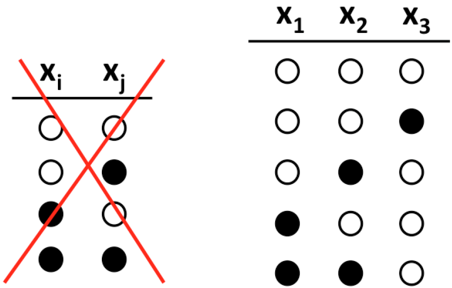

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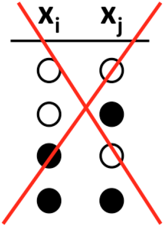

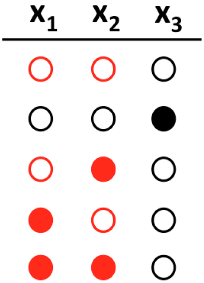

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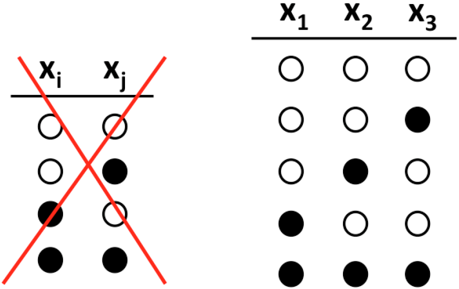

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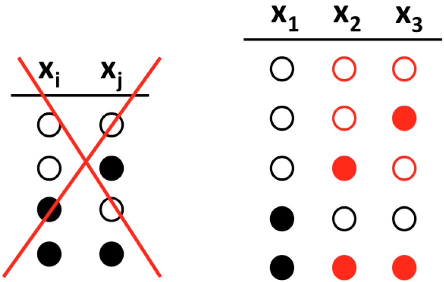

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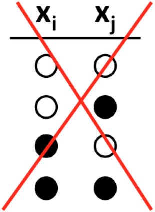

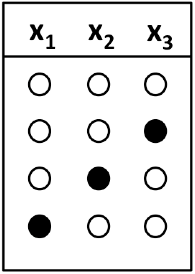

Bounding $m_{\mathcal{H}}(N)$

- Key quantity:

  $B(N, k)$: Maximum number of dichotomies on N points, with break point k

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- Key quantity:

  $B(N, k)$: Maximum number of dichotomies on N points, with break point k
- If the hypothesis space has break point k, then

$$m_{\mathcal{H}}(N) \leq B(N, k)$$

Recursive bound on $B(N, k)$

- For any "valid" set of dichotomies, reorganize rows by
  - S_1: pattern of $x_1, \cdots, x_{N-1}$ only appears once
  - S_2^+, S_2^-: pattern of $x_1, \cdots, x_{N-1}$ appears twice

		# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\ldots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
			$+1$	$+1$	$\ldots$	$+1$	$+1$
			-1	$+1$	$\ldots$	$+1$	-1
	S_1	α	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	-1	-1
			-1	$+1$	$\ldots$	-1	$+1$
			$+1$	-1	$\ldots$	$+1$	$+1$
			-1	-1	$\ldots$	$+1$	$+1$
	S_2^+	β	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	$+1$	$+1$
S_2			-1	-1	$\ldots$	-1	$+1$
			$+1$	-1	$\ldots$	$+1$	-1
			-1	-1	$\ldots$	$+1$	-1
	S_2^-	β	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	$+1$	-1
			-1	-1	$\ldots$	-1	-1

Recursive bound on $B(N, k)$

- Focus on $x_1, x_2, \cdots, x_{N-1}$ columns:
  $\alpha + \beta \leq B(N-1, k)$

	# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\dots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
S_1	α	$+1$	$+1$	$\dots$	$+1$	$+1$
		-1	$+1$	$\dots$	$+1$	-1
		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
		$+1$	-1	$\dots$	-1	-1
		-1	$+1$	$\dots$	-1	$+1$
S_2: S_2^+	β	$+1$	-1	$\dots$	$+1$	$+1$
		-1	-1	$\dots$	$+1$	$+1$
		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
		$+1$	-1	$\dots$	$+1$	$+1$
		-1	-1	$\dots$	-1	$+1$
S_2: S_2^-	β	$+1$	-1	$\dots$	$+1$	-1
		-1	-1	$\dots$	$+1$	-1
		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
		$+1$	-1	$\dots$	$+1$	-1
		-1	-1	$\dots$	-1	-1

Recursive bound on $B(N, k)$

- Now focus on the $S_2 = S_2^+ \cup S^- + 2$ rows
  $\beta \leq B(N-1, k-1)$

		# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\ldots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
S_1		α	$+1$	$+1$	$\ldots$	$+1$	$+1$
			-1	$+1$	$\ldots$	$+1$	-1
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	-1	-1
			-1	$+1$	$\ldots$	-1	$+1$
S_2	S_2^+	β	$+1$	-1	$\ldots$	$+1$	$+1$
			-1	-1	$\ldots$	$+1$	$+1$
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	$+1$	$+1$
			-1	-1	$\ldots$	-1	$+1$
	S_2^-	β	$+1$	-1	$\ldots$	$+1$	-1
			-1	-1	$\ldots$	$+1$	-1
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	$+1$	-1
			-1	-1	$\ldots$	-1	-1

Recursive bound on $B(N, k)$

$$\begin{aligned} B(N,k) &= \alpha + \beta + \beta \\ &\leq B(N-1,k) + B(N-1,k-1) \end{aligned}$$

What's the upper bound for $B(N, k)$?

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		k					
		1	2	3	4	5	......
	1						
	2						
N	3						
	4						
	5						
	.						
	.						

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$$

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		1	2	3	4	5	......
	1	1					
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	.	.					
	.	.					

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	1	1	2	2	2	2	......
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	.	.					
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N \ k	1	2	3	4	5	......
1	1	2	2	2	2	......
2	1	3				
3	1					
4	1					
5	1					
.	.					
.	.					

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		1	2	3	4	5	......
	1	1	2	2	2	2	......
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	.	.					
	.	.					

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		k					
		1	**2**	**3**	**4**	**5**	**......**
	1	1	2	2	2	2	......
	2	1	3	4	4	4	......
N	**3**	1	4	7	8	8	......
	4	1	5	11	......		
	5	1	6	.	.		
	.	.	.	.		.	
	.	.	.				

Analytic solution for $B(N, k)$ bound

$B(N, k)$ is upper bounded by $C(N, k)$:

$$
\begin{aligned}
&C(N, 1) = 1, \;\; N = 1, 2, \cdots \\
&C(1, k) = 2, \;\; k = 2, 3, \cdots \\
&C(N, k) = C(N-1, k) + C(N-1, k-1)
\end{aligned}
$$

- Theorem: $C(N, k) = \sum_{i=0}^{k-1} \binom{N}{i}$

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- Boundary conditions: (easy to check)
- Induction:

$$\underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}_{\text{select } < k \text{ from } N \text{ items}} = \underbrace{\sum_{i=0}^{k-1} \binom{N-1}{i}}_{N\text{-th item not chosen}} + \underbrace{\sum_{i=0}^{k-2} \binom{N-1}{i}}_{N\text{-th item chosen}}$$

It is polynomial!

- For a given $\mathcal{H}$, the break point k is fixed:

$$m_{\mathcal{H}}(N) \leq \underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}_{\text{Polynomial with degree } k-1}$$

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$$m_{\mathcal{H}}(N) \leq \frac{1}{6}N^3 + \frac{5}{6}N + 1$$

Replace M by $m_{\mathcal{H}}(N)$

- Original bound:

$$\mathbf{P}[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{tr}}(h) - E(h)| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$$

- Replace M by $m_{\mathcal{H}}(N)$

$$\underbrace{\mathbf{P}[\exists h \in \mathcal{H} \text{ s.t. } |E_{\text{tr}}(h) - E(h)| > \epsilon]}_{\text{BAD}} \leq 2 \cdot 2m_{\mathcal{H}}(2N) \cdot e^{-\frac{1}{8}\epsilon^2 N}$$

Vapnik-Chervonenkis (VC) bound

VC Dimension

Definition

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

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

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

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- $N \leq d_{\mathrm{VC}}(\mathcal{H}) \Rightarrow \mathcal{H}$ can shatter N points
- $k > d_{\mathrm{VC}}(\mathcal{H}) \Rightarrow \mathcal{H}$ cannot be shattered
- The smallest **break point** is 1 above VC-dimension

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}:

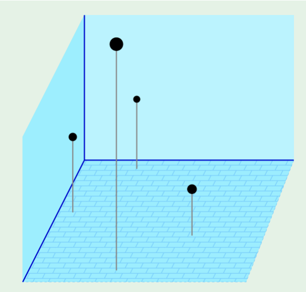
$$m_{\mathcal{H}}(N) \leq \sum_{i=0}^{d_{\text{VC}}} \binom{N}{i}$$

VC dimension of linear classifiers

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

VC dimension of linear classifiers

- For $d = 2$, $d_{\mathrm{VC}} = 3$
- What if $d > 2$?



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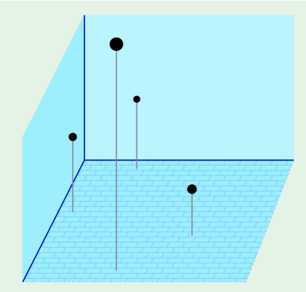

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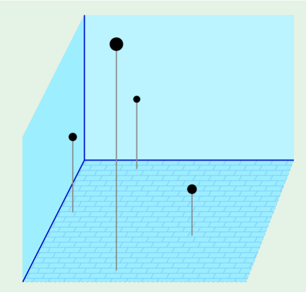

- In general,

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

- We will prove $d_{\text{VC}} \geq d + 1$ and $d_{\text{VC}} \leq d + 1$

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- To prove $d_{\mathrm{VC}} \geq d + 1$
- A set of $N = d + 1$ points in $\mathbb{R}^d$ shattered by the linear hyperplane

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

VC dimension of linear classifiers

- To prove $d_{\mathrm{VC}} \geq d+1$
- A set of $N = d+1$ points in $\mathbb{R}^d$ shattered by the linear hyperplane

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

- X is invertible!

Can we shatter the dataset?

- 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 $\boldsymbol{w}$ satisfying

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- So, $d_{\text{VC}} \geq d + 1$

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We cannot shatter any set of $d+2$ points

- For any $d+2$ points

$$\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_{d+1}, \boldsymbol{x}_{d+2}$$

- More points than dimensions $\Rightarrow$ linear dependent

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

where not all a_i's are zeros

VC dimension of linear classifiers

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

- Now we construct a dichotomy that cannot be generated:

$$y_i = \begin{cases} \text{sign}(a_i) & \text{if } i \neq j \\ -1 & \text{if } i = j \end{cases}$$

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  $\Rightarrow a_i \boldsymbol{w}^T \boldsymbol{x}_i > 0$
- For j-th data,

$$\boldsymbol{w}^T \boldsymbol{x}_j = \sum_{i \neq j} a_i \boldsymbol{w}^T \boldsymbol{x}_i > 0$$

- Therefore, $y_j = \text{sign}(\boldsymbol{w}^T \boldsymbol{x}_j) = +1$ (cannot be -1)

Putting it together

- We proved for d-dimensional linear hyperplane

$$d_{\mathrm{VC}} \leq d+1 \text{ and } d_{\mathrm{VC}} \geq d+1 \Rightarrow \qquad d_{\mathrm{VC}} = d+1$$

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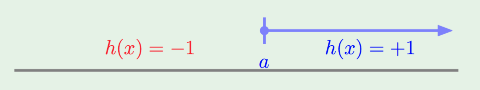
- Parameters create degrees of freedom

Examples

- Positive rays: 1 parameters, $d_{\text{VC}} = 1$



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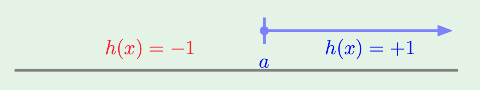
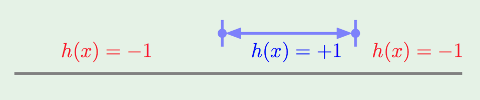


- Positive intervals: 2 parameters, $d_{\mathrm{VC}} = 2$



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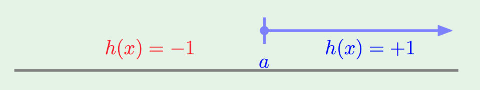

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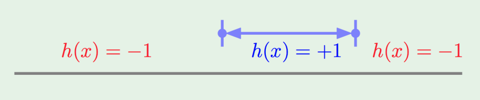

- Not always true $\cdots$

  d_{VC} measures the effective number of parameters

Number of data points needed

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

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

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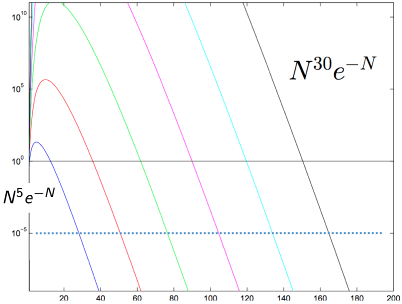

N is almost linear with d_{VC}

Conclusions

- VC dimension

Questions?