

COMP5212: Machine Learning

Lecture 9

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From last time

Shattered

- Given a set $S = \{x^{(i)}, \dots, x^{(d)}\}$ (no relation to the training set) of points $x^{(i)} \in \mathcal{X}$, we say that \mathcal{H} shatters S if \mathcal{H} can realize any labeling on S . I.e, if for any set of labels $\{y^{(i)}, \dots, y^{(d)}\}$, there exist some $h \in \mathcal{H}$ so that $h(x^{(i)}) = y^{(i)}$ for all $i = 1, \dots, d$

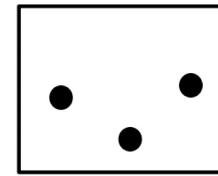
Break point of \mathcal{H}

- 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)

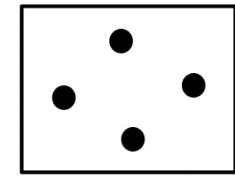
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- VC dimension of \mathcal{H} : $k - 1$ (the most points \mathcal{H} can shatter)
- For 2-D perceptron: $k = 4$, VC dimension = 3

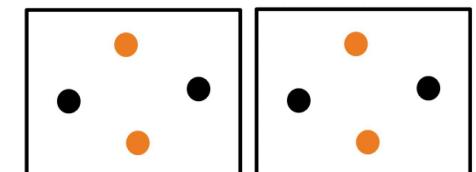
Shattered



Not Shattered



Can't generate



Break point - examples

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

Break point - examples

- 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 $k = 3, d_{VC} = 2$

Break point - examples

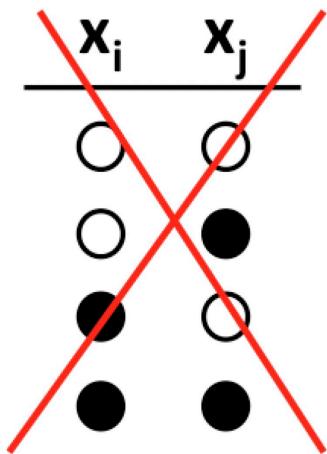
- Positive rays: $m_{\mathcal{H}}(N) = N + 1$
 - Break point $k = 2, d_{VC} = 1$
- Positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$
 - Break point $k = 3, d_{VC} = 2$
- Convex set: $m_{\mathcal{H}}(N) = 2^N$
 - Break point $k = \infty, d_{VC} = \infty$
- Connection to # of parameters

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

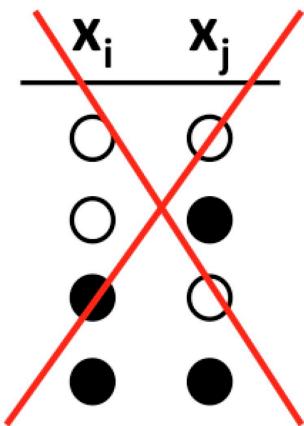
- Break point is $k = 2$



| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |

Puzzle

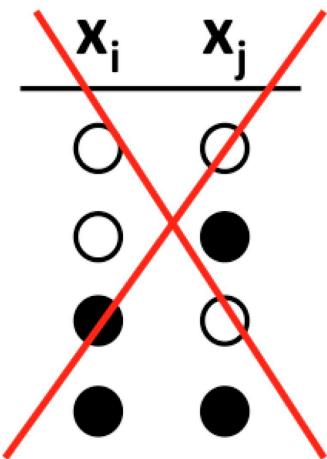
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |

Puzzle

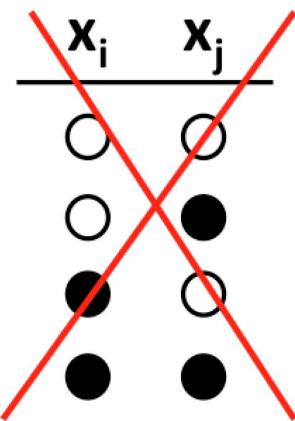
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |

Puzzle

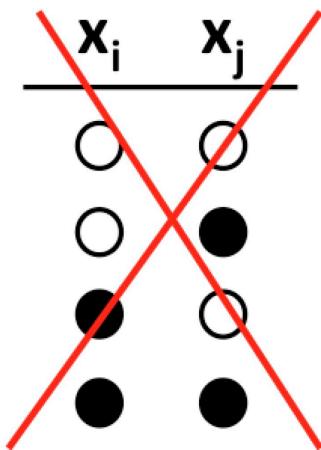
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| | x_1 | x_2 | x_3 |
|---|-------|-------|-------|
| 1 | ○ | ○ | ○ |
| 2 | ○ | ○ | ● |
| 3 | ○ | ● | ○ |
| 4 | ○ | ● | ● |

Puzzle

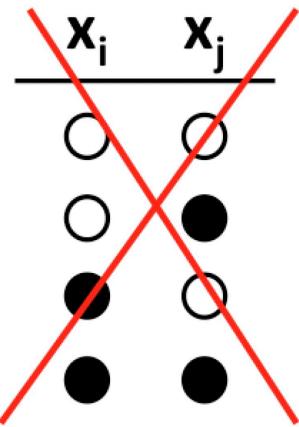
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ○ | ● | ● |

Puzzle

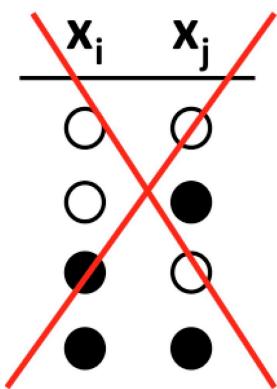
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |

Puzzle

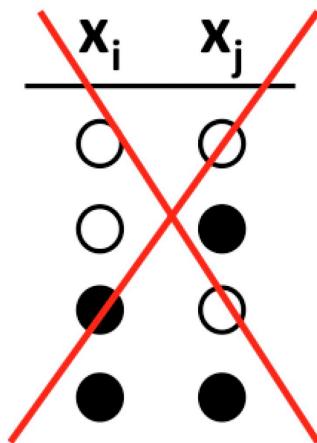
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |
| ● | ○ | ● |

Puzzle

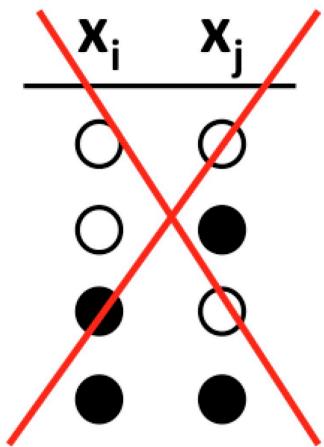
- Break point is $k = 2$



| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |
| ● | ○ | ● |

Puzzle

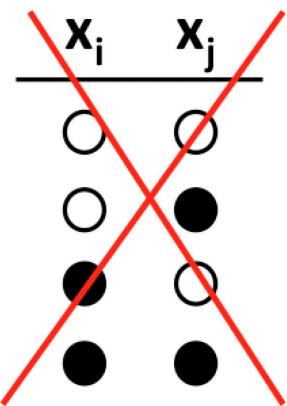
- Break point is $k = 2$



| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |
| ● | ● | ○ |

Puzzle

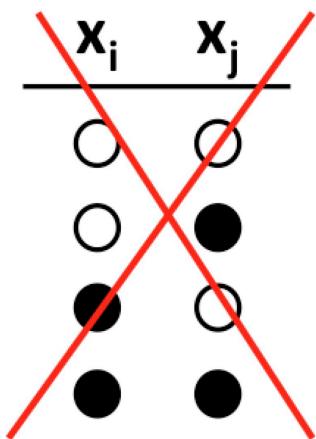
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
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| ● | ● | ○ |

Puzzle

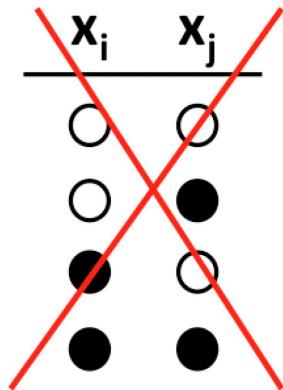
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |
| ● | ● | ● |

Puzzle

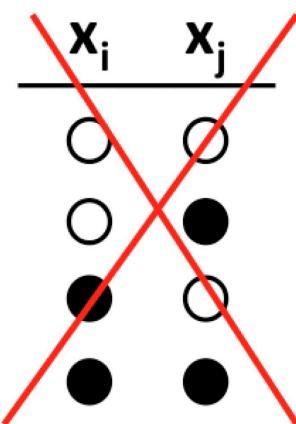
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| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |
| ● | ● | ● |

Puzzle

- Break point is $k = 2$



| x_1 | x_2 | x_3 |
|-------|-------|-------|
| ○ | ○ | ○ |
| ○ | ○ | ● |
| ○ | ● | ○ |
| ● | ○ | ○ |

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

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

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

- Key quantity:
 - $B(N, k)$: Maximum number of dichotomies on N points, with break 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, \dots, x_{N-1} only appears once
 - S_2^+, S_2^- : pattern of x_1, \dots, x_{N-1} only appears twice

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

Recursive bound on $B(N, k)$

- Focus on x_1, \dots, 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 | : |
| | | | +1 | -1 | \dots | -1 | -1 |
| | | | -1 | +1 | \dots | -1 | +1 |
| S_2^+ | β | | +1 | -1 | \dots | +1 | +1 |
| | | | -1 | -1 | \dots | +1 | +1 |
| | | | : | : | \vdots | \vdots | : |
| | | | +1 | -1 | \dots | +1 | +1 |
| | | | -1 | -1 | \dots | -1 | +1 |
| S_2 | β | | +1 | -1 | \dots | +1 | -1 |
| | | | -1 | -1 | \dots | +1 | -1 |
| | | | : | : | \vdots | \vdots | : |
| | | | +1 | -1 | \dots | +1 | -1 |
| | | | -1 | -1 | \dots | -1 | -1 |
| S_2^- | β | | +1 | -1 | \dots | +1 | -1 |
| | | | -1 | -1 | \dots | +1 | -1 |
| | | | : | : | \vdots | \vdots | : |
| | | | +1 | -1 | \dots | +1 | -1 |
| | | | -1 | -1 | \dots | -1 | -1 |

Recursive bound on $B(N, k)$

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

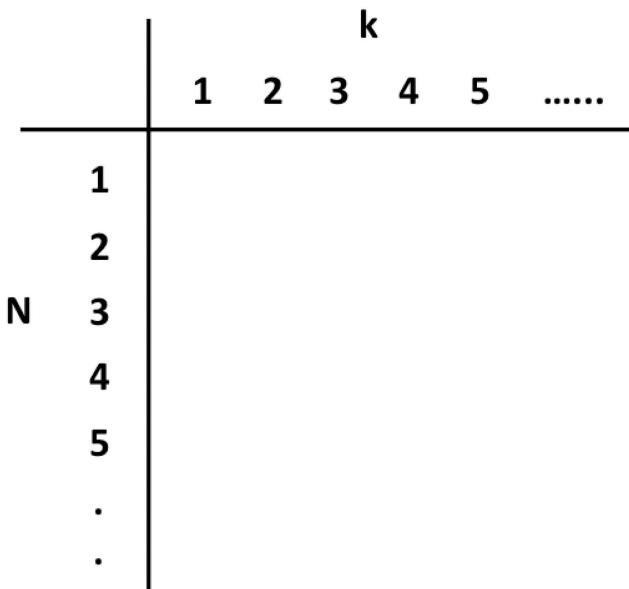
| | # of rows | \mathbf{x}_1 | \mathbf{x}_2 | \dots | \mathbf{x}_{N-1} | \mathbf{x}_N |
|---------|-----------|----------------|----------------|----------|--------------------|----------------|
| S_1 | α | +1 | +1 | \dots | +1 | +1 |
| | | -1 | +1 | \dots | +1 | -1 |
| | | \vdots | \vdots | \vdots | \vdots | \vdots |
| | | +1 | -1 | \dots | -1 | -1 |
| | | -1 | +1 | \dots | -1 | +1 |
| S_2^+ | 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^- | 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 $B(N, k)$

- $$B(N, k) = \alpha + \beta + \beta$$
- $\leq B(N - 1, k) + B(N - 1, k - 1)$
 - What's the upper bound for $B(N, k)$?

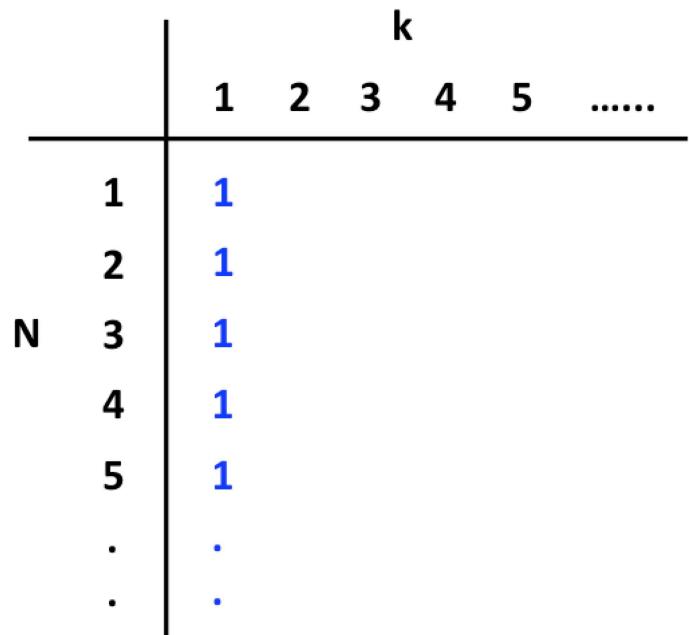
Recursive bound on $B(N, k)$

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



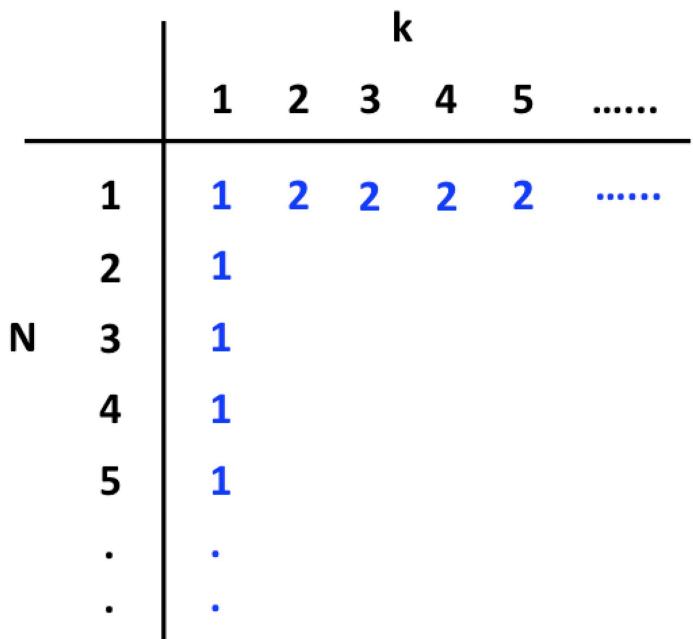
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Recursive bound on $B(N, k)$

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

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

Recursive bound on $B(N, k)$

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

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

Recursive bound on $B(N, k)$

- $$B(N, k) = \alpha + \beta + \beta$$
- $\leq B(N - 1, k) + B(N - 1, k - 1)$

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

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

- $B(N, k)$ is upper bounded by $C(N, k)$
 - $C(N, 1) = 1, N = 1, 2, \dots$
 - $C(1, k) = 2, k = 2, 3, \dots$
 - $C(N, k) = C(N - 1, k) + C(N - 1, k - 1)$
 - Theorem: $C(N, k) = \sum_{i=0}^{k=1} \binom{N}{i}$

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

- $B(N, k)$ is upper bounded by $C(N, k)$
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 - $C(1, k) = 2, k = 2, 3, \dots$
 - $C(N, k) = C(N - 1, k) + C(N - 1, k - 1)$
- Sauer's Lemma: $C(N, k) = \sum_{i=0}^{k-1} \binom{N}{i}$
- Boundary conditions: (easy to check)

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

- $B(N, k)$ is upper bounded by $C(N, k)$
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 - $C(1, k) = 2, k = 2, 3, \dots$
 - $C(N, k) = C(N - 1, k) + C(N - 1, k - 1)$
- Sauer's Theorem: $C(N, k) = \sum_{i=0}^{k-1} \binom{N}{i}$
- Boundary conditions: (easy to check)
- Induction:
 - $$\sum_{i=0}^{k-1} \binom{N}{i} = \underbrace{\sum_{i=0}^{k-1} \binom{N-1}{i}}_{\text{select } < k \text{ from } N \text{ items}} + \underbrace{\sum_{i=0}^{k-2} \binom{N-1}{i}}_{\text{N-th item not chosen}}$$

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

- \mathcal{H} is positive rays: (break point $k = 2$)
 - $m_{\mathcal{H}}(N) = N + 1$

It is polynomial!

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

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

- \mathcal{H} is 2D perceptrons: (break point $k = 4$)
 - $m_{\mathcal{H}}(N) = ?$

It is polynomial!

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

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

- \mathcal{H} is 2D perceptrons: (break point $k = 4$)

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

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

- Original bound:

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

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

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

$$\underbrace{\quad\quad\quad}_{BAD}$$

- Vapnik-Chervonenkis (VC) bound

VC dimension

Definition

- 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”

VC dimension

Definition

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

VC dimension

Definition

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

VC dimension

The growth function

- In terms of a break point k :

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

- In terms of the VC dimension d_{VC} :

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

VC dimension

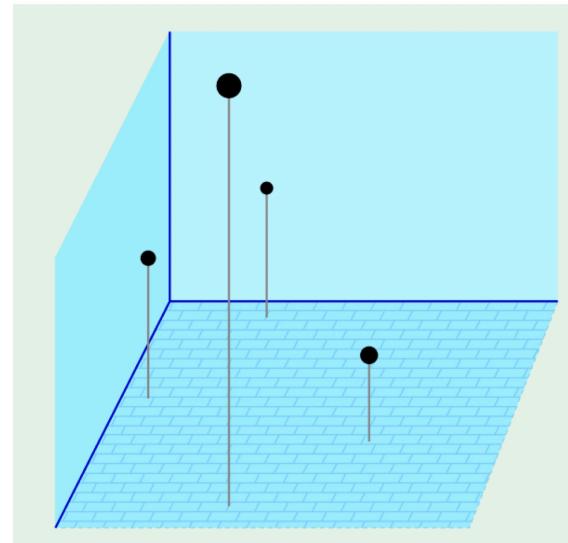
VC dimension of linear classifier

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

VC dimension

VC dimension of linear classifier

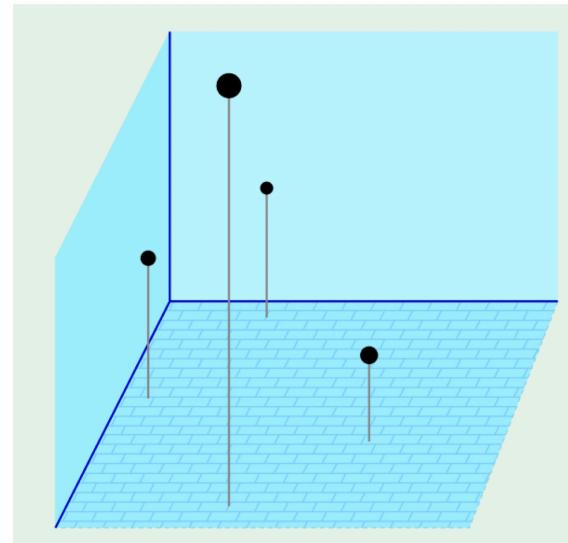
- For $d = 2$, $d_{VC} = 3$
- What if $d > 2$?



VC dimension

VC dimension of linear classifier

- For $d = 2$, $d_{\text{VC}} = 3$
- What if $d > 2$?
- In general,
 - $d_{\text{VC}} = d + 1$



VC dimension

VC dimension of linear classifier

- For $d = 2$, $d_{VC} = 3$
- What if $d > 2$?
- In general,
 - $d_{VC} = d + 1$
- We will prove $d_{VC} \geq d + 1$ and $d_{VC} \leq d + 1$

