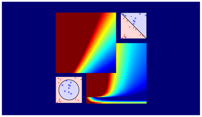
Machine Learning Foundations
(機器學習基石)



Lecture 5: Training versus Testing

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Roadmap

1. When Can Machines Learn?

   Lecture 4: Feasibility of Learning

   learning is **PAC-**possible
   if enough **statistical data** and **finite** $|\mathcal{H}|$

2. **Why** Can Machines Learn?

   Lecture 5: Training versus Testing

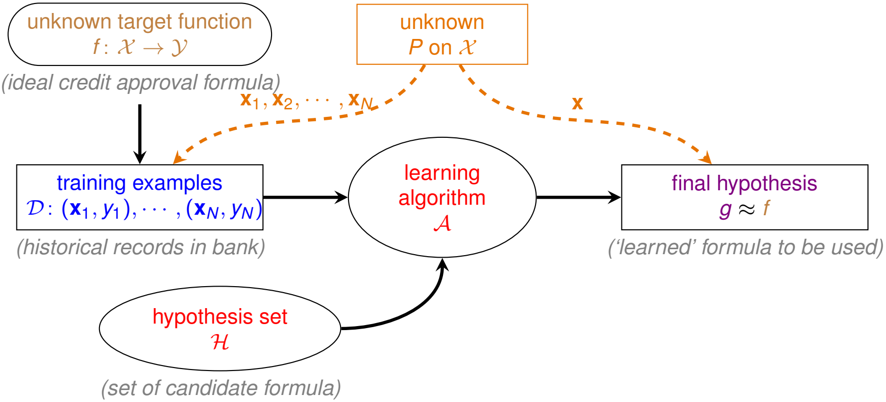
   - Recap and Preview
   - Effective Number of Lines
   - Effective Number of Hypotheses
   - Break Point

3. How Can Machines Learn?
4. How Can Machines Learn Better?

Recap: the 'Statistical' Learning Flow

if $|\mathcal{H}| = M$ finite, N large enough,

for whatever g picked by $\mathcal{A}$, $E_{\text{out}}(g) \approx E_{\text{in}}(g)$



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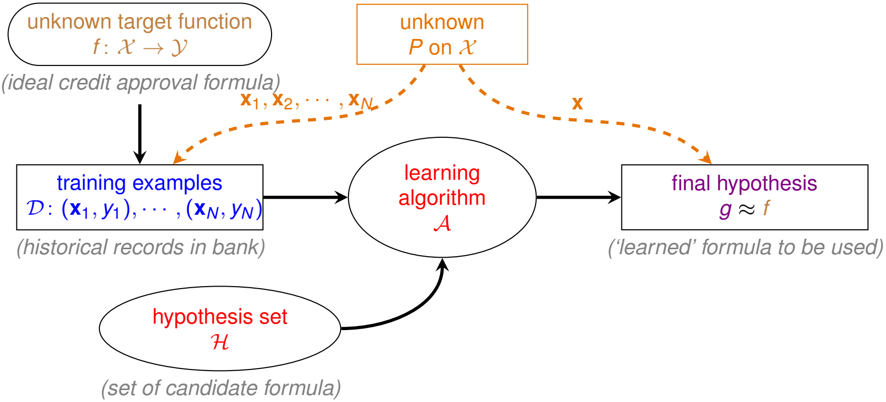
PAC guarantee for $E_{\text{out}}(g) \approx 0 \Longrightarrow$ **learning possible :-)**



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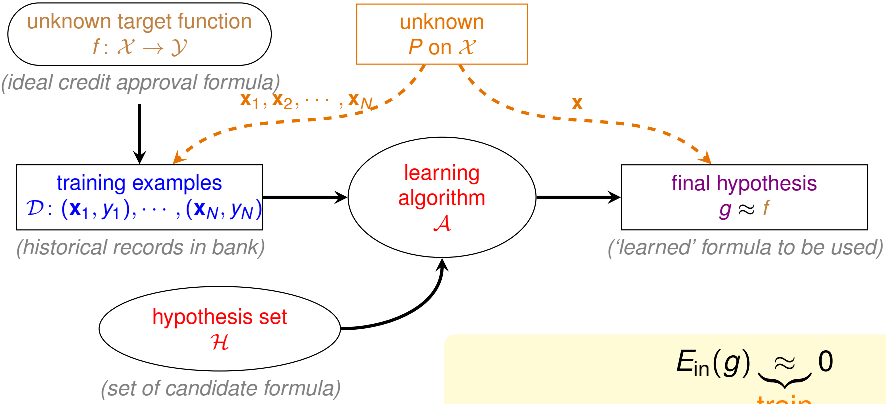

$$\underbrace{E_{\text{in}}(g) \approx 0}_{\text{train}}$$

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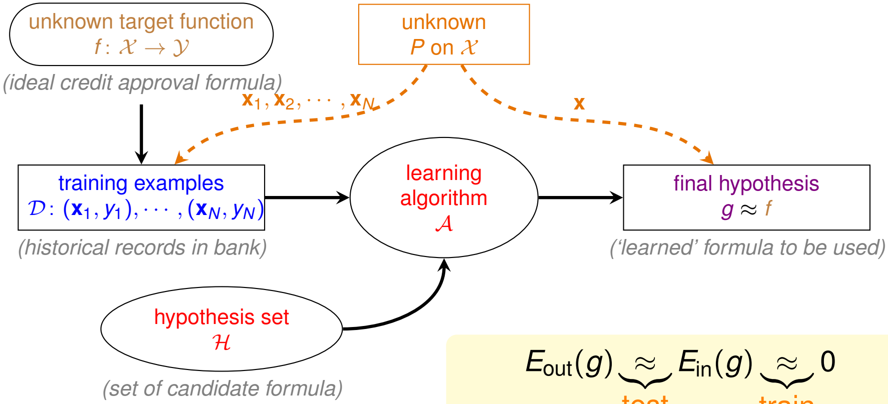

$$E_{\text{out}}(g) \underbrace{\approx}_{\text{test}} E_{\text{in}}(g) \underbrace{\approx}_{\text{train}} 0$$

Two Central Questions

$$\underbrace{g \approx f}_{\text{lecture 1}} \iff E_{\text{out}}(g) \approx 0$$

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what role does $\underbrace{M}_{|\mathcal{H}|}$ play for the two questions?

Trade-off on M

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small M

large M

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using the right M (or $\mathcal{H}$) is important
$M = \infty$ **doomed?**

Preview

Known

$$\mathbb{P}\left[\left|E_{\text{in}}(g) - E_{\text{out}}(g)\right| > \epsilon\right] \leq 2 \cdot M \cdot \exp\left(-2\epsilon^2 N\right)$$

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mysterious PLA to be fully resolved
after 3 more lectures :-)

Fun Time

Data size: how large do we need?

One way to use the inequality

$$\mathbb{P}\left[\left|E_{\text{in}}(g) - E_{\text{out}}(g)\right| > \epsilon\right] \leq \underbrace{2 \cdot M \cdot \exp\left(-2\epsilon^2 N\right)}_{\delta}$$

is to pick a tolerable difference ϵ as well as a tolerable **BAD** probability δ, and then gather data with size (N) large enough to achieve those tolerance criteria. Let $\epsilon = 0.1$, $\delta = 0.05$, and $M = 100$. What is the data size needed?

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2. 415
3. 615
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Reference Answer: 2

We can simply express N as a function of those 'known' variables. Then, the needed $N = \frac{1}{2\epsilon^2} \ln \frac{2M}{\delta}$.

Where Did M Come From?

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where did **union bound fail** to consider for $M = \infty$?

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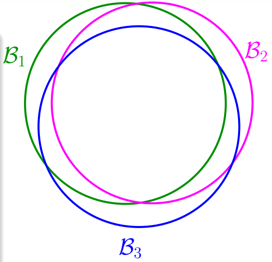

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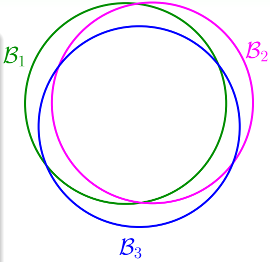

to account for overlap,
can we group similar hypotheses by **kind**?

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$$\mathcal{H} = \left\{\text{all lines in } \mathbb{R}^2\right\}$$

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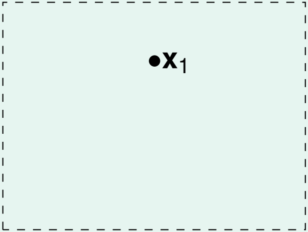

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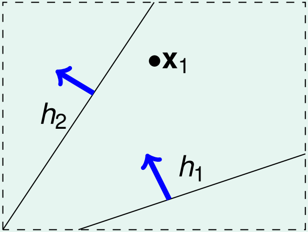

2 kinds: h_1-like$(\mathbf{x}_1) = \circ$ or h_2-like$(\mathbf{x}_1) = \times$

How Many Lines Are There? (2/2)

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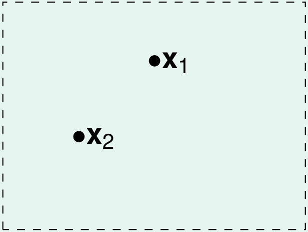

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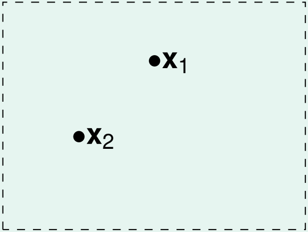
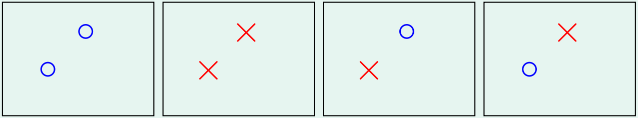


4: 

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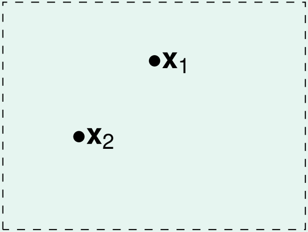

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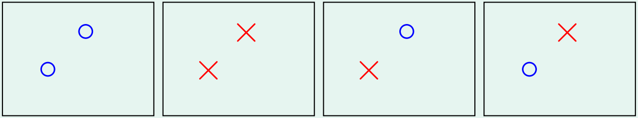

one input: 2; two inputs: 4; **three inputs?**

How Many Kinds of Lines for Three Inputs? (1/2)

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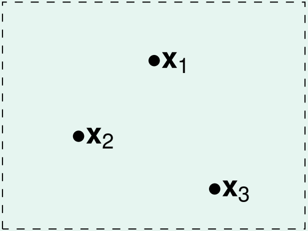
for three inputs $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$



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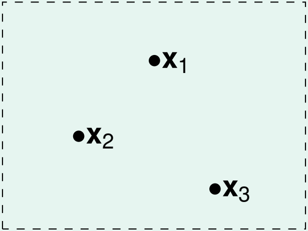

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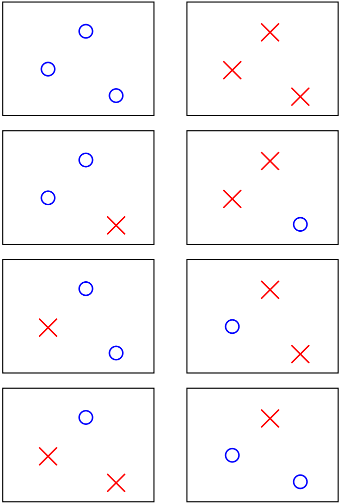

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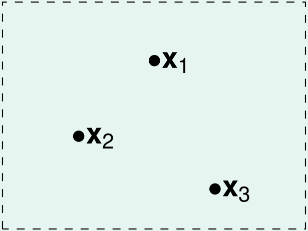

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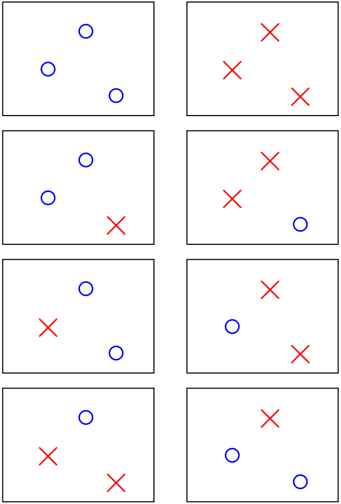

always 8 **for three inputs**?

How Many Kinds of Lines for Three Inputs? (2/2)

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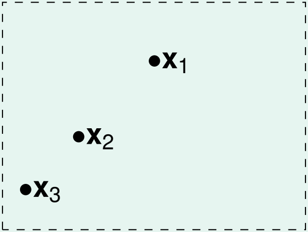
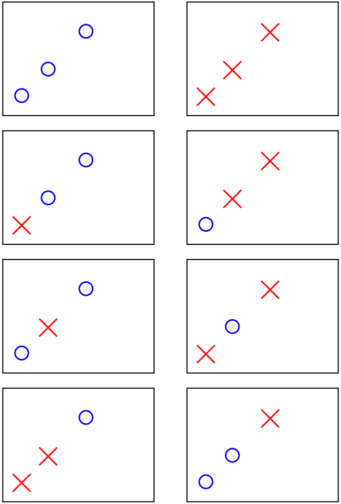
for another three inputs $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$



6:



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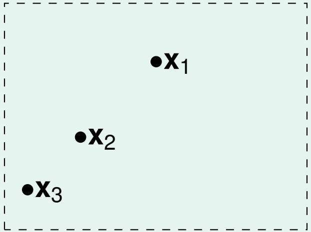

‘fewer than 8’ when degenerate
(e.g. collinear or same inputs)

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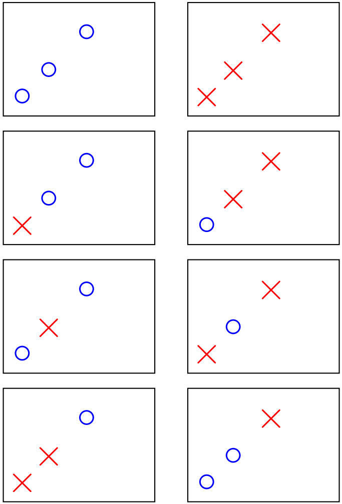

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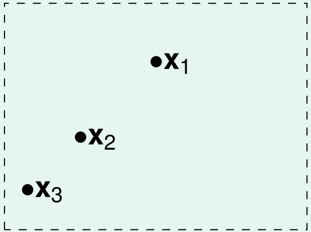
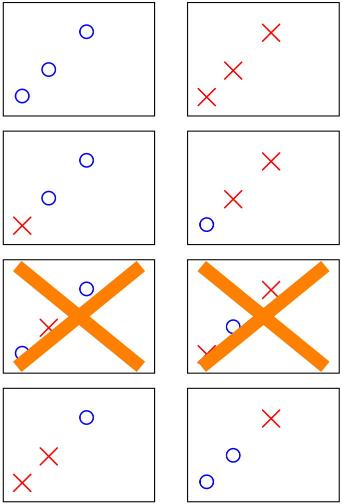
for another three inputs $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$



6:

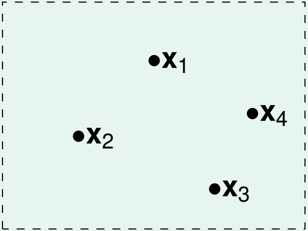


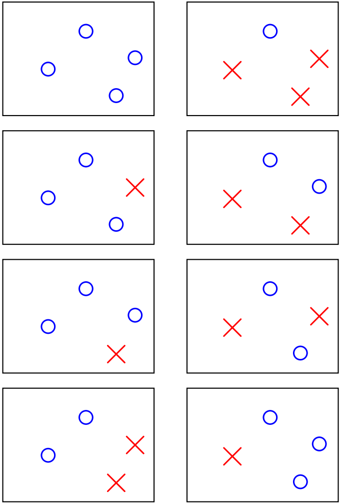
'fewer than 8' when degenerate (e.g. collinear or same inputs)

How Many Kinds of Lines for Four Inputs?

$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

for four inputs $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4$





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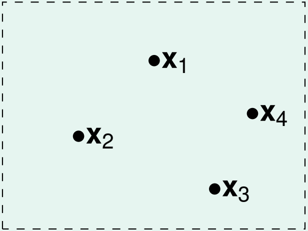
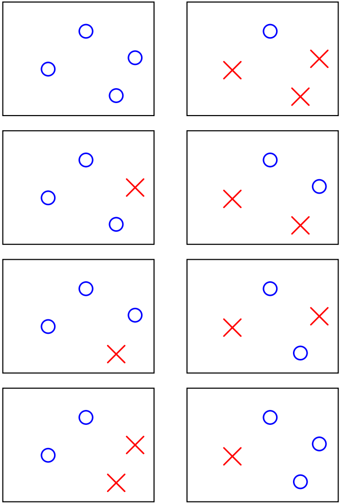


14: 2×



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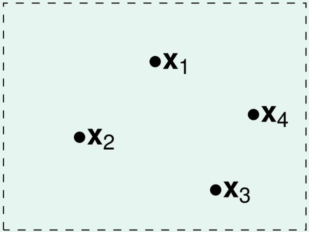
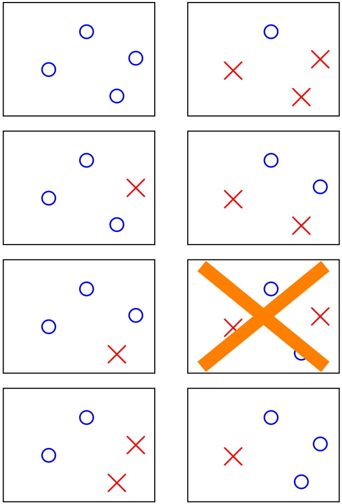


for any four inputs
at most 14

14: 2×



Effective Number of Lines

maximum kinds of lines with respect to N inputs $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N$
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2	4
3	8
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if (1) effective(N) can replace M and
(2) effective(N) $\ll 2^N$

learning possible with infinite lines :-)

Fun Time

What is the effective number of lines for five inputs $\in \mathbb{R}^2$?

1. 14
2. 16
3. 22
4. 32

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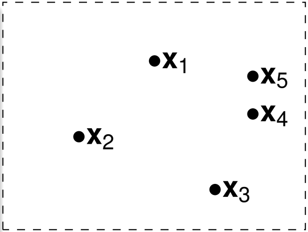
Reference Answer: ③

If you put the inputs roughly around a circle, you can then pick any consecutive inputs to be on one side of the line, and the other inputs to be on the other side. The procedure leads to effectively 22 kinds of lines, which is **much smaller than $2^5 = 32$**. You shall find it difficult to generate more kinds by varying the inputs, and we will give a formal proof in future lectures.



Dichotomies: Mini-hypotheses

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- call

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a **dichotomy**: hypothesis 'limited' to the eyes of $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$

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e.g.	all lines in $\mathbb{R}^2$	$\{\circ\circ\circ\circ, \circ\circ\circ\times, \circ\circ\times\times, \ldots\}$
size	possibly infinite	upper bounded by 2^N

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$|\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)|$: candidate for **replacing M**

Growth Function

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1	2
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3	$\max(\ldots, 6, 8) = 8$
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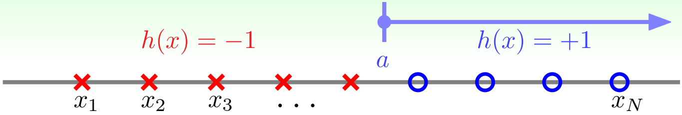
how to 'calculate' the growth function?

Growth Function for Positive Rays



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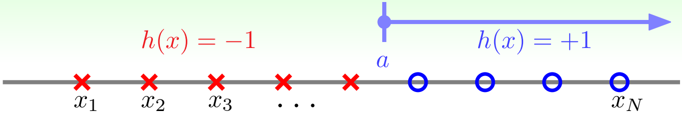

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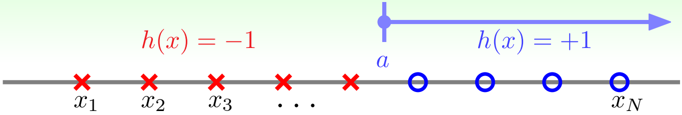

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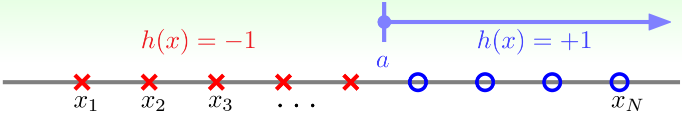

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×	○	○	○
×	×	○	○
×	×	×	○
×	×	×	×

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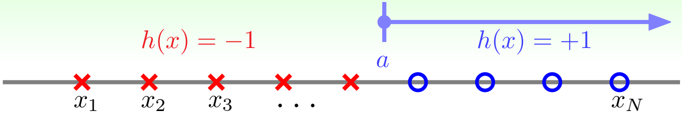

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$(N + 1) \ll 2^N$ when N large!

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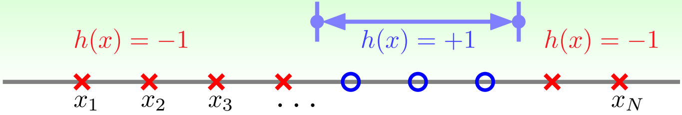
×	○	○	○
×	×	○	○
×	×	×	○
×	×	×	×

Growth Function for Positive Intervals



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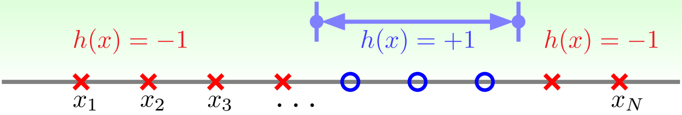
Growth Function for Positive Intervals



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one dichotomy for each 'interval kind'

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$$= \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

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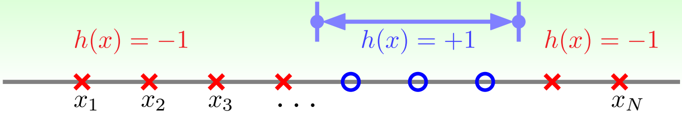

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○	○	×	×
○	○	○	×
○	○	○	○
×	○	×	×
×	○	○	×
×	○	○	○
×	×	○	×
×	×	○	○
×	×	×	○
×	×	×	×

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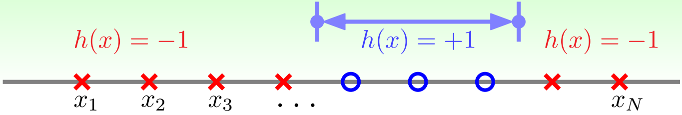

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×	○	○	×
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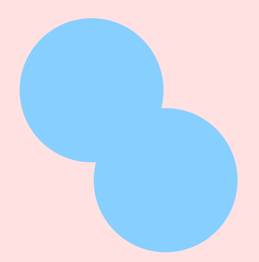
×	×	○	×
×	×	○	○
×	×	×	○
×	×	×	×

Growth Function for Convex Sets (1/2)

convex region in blue



non-convex region

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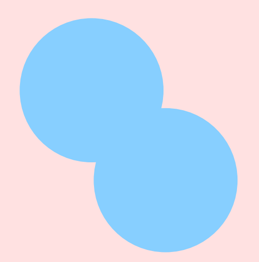

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what is $m_{\mathcal{H}}(N)$?

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- one possible set of N inputs: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ on a big circle

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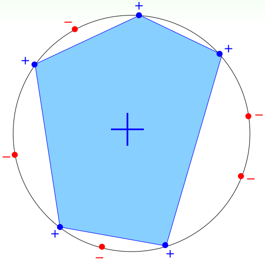
$$m_{\mathcal{H}}(N) = 2^N$$



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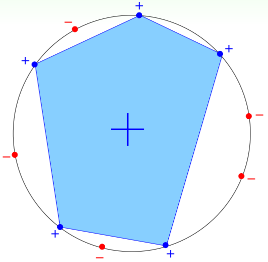

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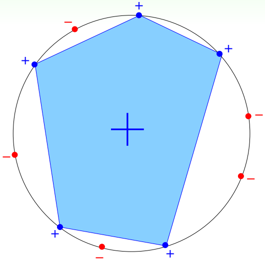

$$m_{\mathcal{H}}(N) = 2^N \iff$$

exists N inputs that can be shattered

Fun Time

Consider positive **and negative** rays as $\mathcal{H}$, which is equivalent to the perceptron hypothesis set in 1D. The hypothesis set is often called **'decision stump'** to describe the shape of its hypotheses. What is the growth function $m_{\mathcal{H}}(N)$?

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4. 2^N

Reference Answer: ③

Two dichotomies when threshold in each of the $N - 1$ 'internal' spots; two dichotomies for the all-$\circ$ and all-$\times$ cases.

The Four Growth Functions

- positive rays: $m_{\mathcal{H}}(N) = N + 1$
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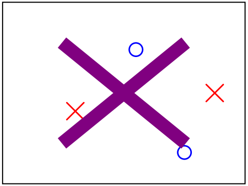
for 2D or general perceptrons,
$m_{\mathcal{H}}(N)$ **polynomial**?

Break Point of $\mathcal{H}$

what do we know about 2D perceptrons now?

three inputs: 'exists' shatter;
four inputs, 'for all' no shatter



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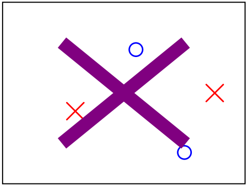

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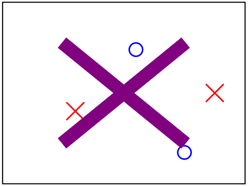

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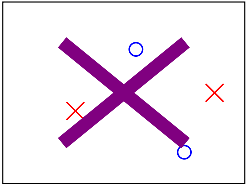

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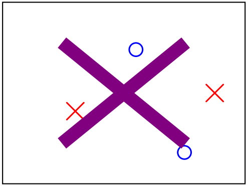

2D perceptrons: **break point at** 4

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conjecture:

- no break point: $m_{\mathcal{H}}(N) = 2^N$ (sure!)
- break point k: $m_{\mathcal{H}}(N) = O(N^{k-1})$

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excited? wait for next lecture :-)

Fun Time

Consider positive **and negative** rays as $\mathcal{H}$, which is equivalent to the perceptron hypothesis set in 1D. As discussed in an earlier quiz question, the growth function $m_{\mathcal{H}}(N) = 2N$. What is the minimum break point for $\mathcal{H}$?

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

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4. 4

Reference Answer: ③

At $k = 3$, $m_{\mathcal{H}}(k) = 6$ while $2^k = 8$.

Summary

1. When Can Machines Learn?

Lecture 4: Feasibility of Learning

2. **Why** Can Machines Learn?

Lecture 5: Training versus Testing

- Recap and Preview
  two questions: $E_{\text{out}}(g) \approx E_{\text{in}}(g)$, **and** $E_{\text{in}}(g) \approx 0$
- Effective Number of Lines
  at most 14 **through the eye of** 4 **inputs**
- Effective Number of Hypotheses
  at most $m_{\mathcal{H}}(N)$ **through the eye of** N **inputs**
- Break Point
  when $m_{\mathcal{H}}(N)$ **becomes 'non-exponential'**

- **next:** $m_{\mathcal{H}}(N) = poly(N)$**?**

3. How Can Machines Learn?
4. How Can Machines Learn Better?