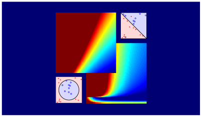
Machine Learning Foundations
(機器學習基石)



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

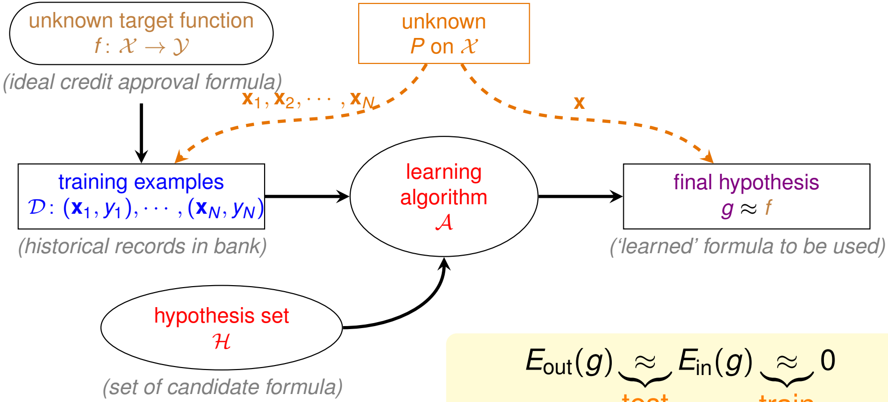
- Recap and Preview
- Effective Number of Lines
- Effective Number of Hypotheses
- Break Point

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 $\mathcal{A}$, $E_{\text{out}}(g) \approx E_{\text{in}}(g)$

if $\mathcal{A}$ finds one g with $E_{\text{in}}(g) \approx 0$,
PAC guarantee for $E_{\text{out}}(g) \approx 0 \Longrightarrow$ **learning possible :-)**



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

Two Central Questions

for $\underbrace{\text{batch \& supervised binary classification}}_{\text{lecture 3}}$, $\underbrace{g \approx f}_{\text{lecture 1}} \iff E_{\text{out}}(g) \approx 0$

achieved through $\underbrace{E_{\text{out}}(g) \approx E_{\text{in}}(g)}_{\text{lecture 4}}$ and $\underbrace{E_{\text{in}}(g) \approx 0}_{\text{lecture 2}}$

learning split to two central questions:

1. can we make sure that $E_{\text{out}}(g)$ is close enough to $E_{\text{in}}(g)$?
2. can we make $E_{\text{in}}(g)$ small enough?

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

Trade-off on M

1. can we make sure that $E_{\text{out}}(g)$ is close enough to $E_{\text{in}}(g)$?
2. can we make $E_{\text{in}}(g)$ small enough?

small M

1. Yes!,
   $\mathbb{P}[\textbf{BAD}] \leq 2 \cdot M \cdot \exp(\ldots)$
2. No!, too few choices

large M

1. No!,
   $\mathbb{P}[\textbf{BAD}] \leq 2 \cdot M \cdot \exp(\ldots)$
2. Yes!, many choices

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

Preview

Known

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

Todo

- establish **a finite quantity** that replaces M

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

- justify the feasibility of learning for infinite M
- study $m_{\mathcal{H}}$ to understand its trade-off for 'right' $\mathcal{H}$, just like M

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

Where Did M Come From?

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

- **$\mathcal{B}$AD events $\mathcal{B}_m$**: $|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon$
- to give $\mathcal{A}$ freedom of choice: bound $\mathbb{P}[\mathcal{B}_1$ or $\mathcal{B}_2$ or $\ldots \mathcal{B}_M]$
- worst case: all $\mathcal{B}_m$ non-overlapping

$$\mathbb{P}[\mathcal{B}_1 \text{ or } \mathcal{B}_2 \text{ or } \ldots \mathcal{B}_M] \quad \underbrace{\le}_{\textbf{union bound}} \quad \mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \ldots + \mathbb{P}[\mathcal{B}_M]$$

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

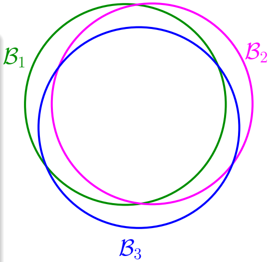
Where Did Uniform Bound Fail?

union bound $\mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \ldots + \mathbb{P}[\mathcal{B}_M]$

- **$\mathcal{B}$AD events $\mathcal{B}_m$**: $|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon$

  overlapping for similar hypotheses $h_1 \approx h_2$
- why? 1 $E_{\text{out}}(h_1) \approx E_{\text{out}}(h_2)$

  2 for most $\mathcal{D}$, $E_{\text{in}}(h_1) = E_{\text{in}}(h_2)$
- union bound **over-estimating**

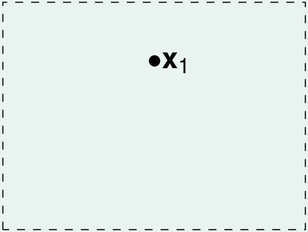


to account for overlap,
can we group similar hypotheses by **kind**?

How Many Lines Are There? (1/2)

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

- how many lines? ∞
- how many **kinds of** lines if viewed from one input vector $\mathbf{x}_1$?



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

How Many Lines Are There? (1/2)

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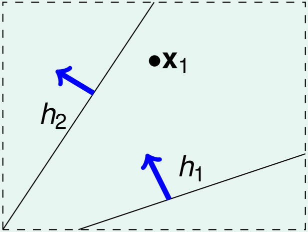
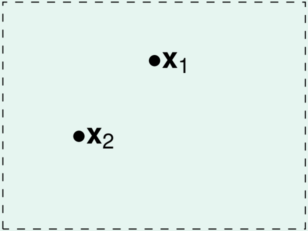


2 kinds: h_1-like$(\mathbf{x}_1) = \circ$ or h_2-like$(\mathbf{x}_1) = \times$

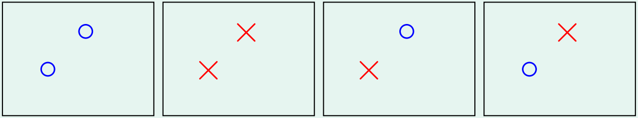
How Many Lines Are There? (2/2)

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

- how many **kinds of** lines if viewed from two inputs $\mathbf{x}_1, \mathbf{x}_2$?



4:



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

How Many Lines Are There? (2/2)

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

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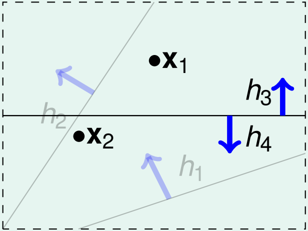
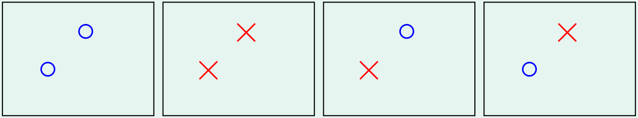


4:

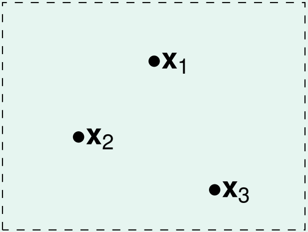


one input: 2; two inputs: 4; **three inputs?**

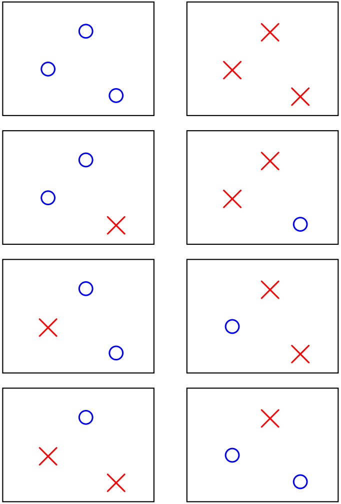
How Many Kinds of Lines for Three Inputs? (1/2)

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

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



8:

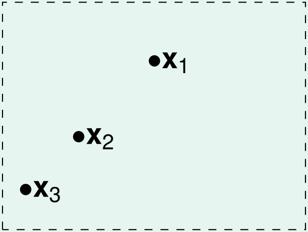


always 8 **for three inputs**?

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

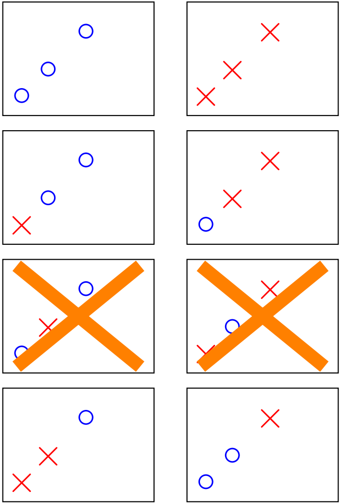
$$\mathcal{H} = \left\{\text{all lines in } \mathbb{R}^2\right\}$$

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



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

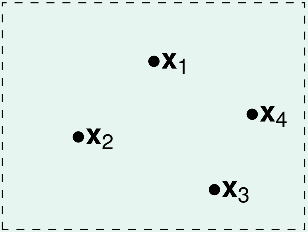
6:



How Many Kinds of Lines for Four Inputs?

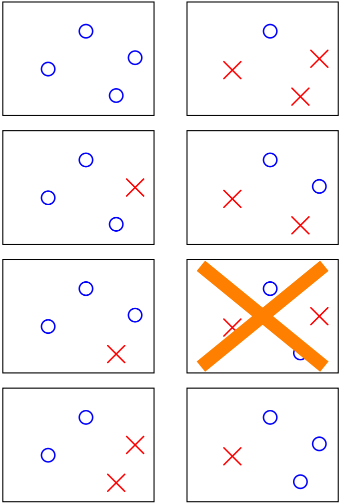
$$\mathcal{H} = \left\{ \text{all lines in } \mathbb{R}^2 \right\}$$

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



for any four inputs
at most 14

14: 2×



Effective Number of Lines

maximum kinds of lines with respect to N inputs $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N$
$\Longleftrightarrow$ **effective number of lines**

- must be $\leq 2^N$ (why?)
- finite 'grouping' of infinitely-many lines $\in \mathcal{H}$
- wish:

$$\begin{aligned} & \mathbb{P}\left[\left|E_{\text{in}}(g) - E_{\text{out}}(g)\right| > \epsilon\right] \\ \leq \quad & 2 \cdot \text{effective}(N) \cdot \exp\left(-2\epsilon^2 N\right) \end{aligned}$$

lines in 2D

N	effective(N)
1	2
2	4
3	8
4	$14 < 2^N$

if (1) effective(N) can replace M and
(2) effective(N) $\ll 2^N$
learning possible with infinite lines :-)

Dichotomies: Mini-hypotheses

$$\mathcal{H} = \{\text{hypothesis } h\colon \mathcal{X} \to \{\times, \circ\}\}$$

- call

$$h(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = (h(\mathbf{x}_1), h(\mathbf{x}_2), \ldots, h(\mathbf{x}_N)) \in \{\times, \circ\}^N$$

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

- $\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$:
  all dichotomies 'implemented' by $\mathcal{H}$ on $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$

	hypotheses $\mathcal{H}$	dichotomies $\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$
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

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

Growth Function

- $|\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)|$: depend on inputs $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$
- growth function: remove dependence by **taking** max **of all possible** $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$

$$m_{\mathcal{H}}(N) = \max_{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in \mathcal{X}} |\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)|$$

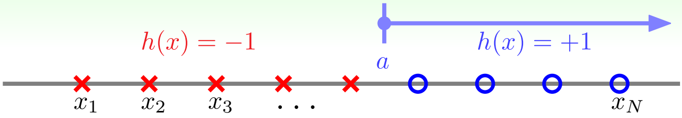
- finite, upper-bounded by 2^N

lines in 2D

N	$m_{\mathcal{H}}(N)$
1	2
2	4
3	$\max(\ldots, 6, 8)$ $= 8$
4	$14 < 2^N$

how to 'calculate' the growth function?

Growth Function for Positive Rays



- $\mathcal{X} = \mathbb{R}$ (one dimensional)
- $\mathcal{H}$ contains h, where **each** $h(x) = \text{sign}(x - a)$ **for threshold** a
- 'positive half' of 1D perceptrons

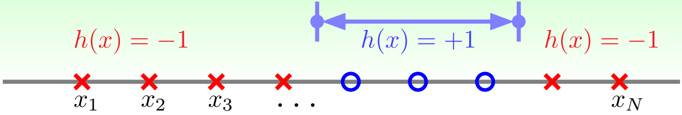
one dichotomy for $a \in$ each spot (x_n, x_{n+1}):

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

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

x_1	x_2	x_3	x_4
○	○	○	○
×	○	○	○
×	×	○	○
×	×	×	○
×	×	×	×

Growth Function for Positive Intervals



- $\mathcal{X} = \mathbb{R}$ (one dimensional)
- $\mathcal{H}$ contains h, where **each $h(x) = +1$ iff $x \in [\ell, r)$, -1 otherwise**

one dichotomy for each 'interval kind'

$$m_{\mathcal{H}}(N) = \underbrace{\binom{N+1}{2}}_{\text{interval ends in } N+1 \text{ spots}} + \underbrace{1}_{\text{all } \times}$$

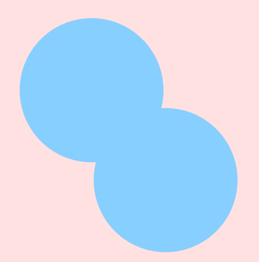
$$= \frac{1}{2}N^2 + \frac{1}{2}N + 1$$

x_1	x_2	x_3	x_4
○	×	×	×
○	○	×	×
○	○	○	×
○	○	○	○
×	○	×	×
×	○	○	×
×	○	○	○
×	×	○	×
×	×	○	○
×	×	×	○
×	×	×	×

$\left(\frac{1}{2}N^2 + \frac{1}{2}N + 1\right) \ll 2^N$ when N large!

Growth Function for Convex Sets (1/2)

convex region in blue



non-convex region

- $\mathcal{X} = \mathbb{R}^2$ (two dimensional)
- $\mathcal{H}$ contains h, where **$h(\mathbf{x}) = +1$ iff x in a convex region, -1 otherwise**

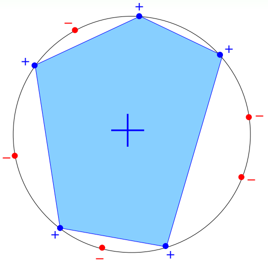
what is $m_{\mathcal{H}}(N)$?

Growth Function for Convex Sets (2/2)

- one possible set of N inputs: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ on a big circle
- **every dichotomy can be implemented** by $\mathcal{H}$ using a convex region slightly extended from contour of positive inputs

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

- call those N inputs **'shattered' by $\mathcal{H}$**



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

1. N
2. $N+1$
3. $2N$
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: $m_{\mathcal{H}}(N) = N + 1$
- positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$
- convex sets: $m_{\mathcal{H}}(N) = 2^N$
- 2D perceptrons: $m_{\mathcal{H}}(N) < 2^N$ **in some cases**

what if $m_{\mathcal{H}}(N)$ replaces M?

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

polynomial: good; **exponential: bad**

for 2D or general perceptrons,
$m_{\mathcal{H}}(N)$ **polynomial**?

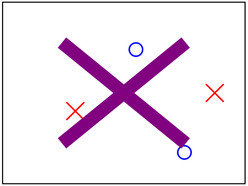
Break Point of $\mathcal{H}$

what do we know about 2D perceptrons now?

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

if no k inputs can be shattered by $\mathcal{H}$,
call k a **break point** for $\mathcal{H}$

- $m_{\mathcal{H}}(k) < 2^k$
- $k+1$, $k+2$, $k+3$, $\ldots$ also break points!
- will study minimum break point k



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

The Four Break Points

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

  break point at 2
- positive intervals: $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1 = O(N^2)$

  break point at 3
- convex sets: $m_{\mathcal{H}}(N) = 2^N$

  no break point
- 2D perceptrons: $m_{\mathcal{H}}(N) < 2^N$ **in some cases**

  break point at 4

conjecture:

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

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

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?