Machine Learning Theory 2024
Lecture 3

Tim van Erven

Focus on binary classification:

- Review
- Shattering and VC-dimension
- The Fundamental Theorem of PAC-Learning
- VC-dimension of Linear Predictors

(Agnostic) PAC Learning

$\mathcal{H}$ is **agnostically PAC-learnable**:

Exist learner (selecting $h_S \in \mathcal{H}$) that achieves, for finite $m_{\mathcal{H}}(\epsilon, \delta)$,

$$L_{\mathcal{D}}(h_S) \leq \inf_{h \in \mathcal{H}} L_{\mathcal{D}}(h) + \epsilon \qquad \text{with probability} \geq 1 - \delta,$$

whenever $m \geq m_{\mathcal{H}}(\epsilon, \delta)$,

for all $\mathcal{D}, \epsilon, \delta$.

(Agnostic) PAC Learning

$\mathcal{H}$ is **agnostically PAC-learnable**:

Exist learner (selecting $h_S \in \mathcal{H}$) that achieves, for finite $m_{\mathcal{H}}(\epsilon, \delta)$,

$$L_{\mathcal{D}}(h_S) \leq \inf_{h \in \mathcal{H}} L_{\mathcal{D}}(h) + \epsilon \qquad \text{with probability} \geq 1 - \delta,$$

whenever $m \geq m_{\mathcal{H}}(\epsilon, \delta)$,

for all $\mathcal{D}, \epsilon, \delta$.

$\mathcal{H}$ is **PAC-learnable** (only for binary classification):

Same, except only for $\mathcal{D}$ for which realizability holds w.r.t. $\mathcal{H}$.

- Realizability: exists classifier $h^* \in \mathcal{H}$ that is perfect for $\mathcal{D}$
- Implies that $\inf_{h \in \mathcal{H}} L_{\mathcal{D}}(h) = 0$

What We Know So Far About Learnability

Theorem (Finite Hypothesis Classes)

Suppose loss range is $[0, 1]$*. Finite hypothesis classes* $\mathcal{H}$ *are* **agnostically PAC-learnable** *with ERM.*

What We Know So Far About Learnability

Theorem (Finite Hypothesis Classes)

Suppose loss range is $[0, 1]$. Finite hypothesis classes $\mathcal{H}$ are **agnostically PAC-learnable** *with ERM.*

- Does not cover e.g. linear predictors
  $\mathcal{H} = \{h_{\boldsymbol{w},b}(\boldsymbol{X}) = \mathrm{sign}(b + \langle \boldsymbol{w}, \boldsymbol{X} \rangle) \mid \boldsymbol{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$

What We Know So Far About Learnability

Theorem (Finite Hypothesis Classes)

Suppose loss range is $[0,1]$*. Finite hypothesis classes* $\mathcal{H}$ *are* **agnostically PAC-learnable** *with ERM.*

- Does not cover e.g. linear predictors
  $\mathcal{H} = \{h_{\boldsymbol{w},b}(\boldsymbol{X}) = \mathrm{sign}(b + \langle \boldsymbol{w}, \boldsymbol{X} \rangle) \mid \boldsymbol{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$

Let $\mathcal{H}_{\text{all}}$ = all (measurable) functions from $\mathcal{X}$ to $\{-1,+1\}$

Theorem (No-Free-Lunch)

Consider binary classification. For any $\epsilon < 1/8$*,* $\delta < 1/7$*,*
sample size $m \leq |\mathcal{X}|/2$ *is not enough to* **PAC-learn** $\mathcal{H}_{all}$*:*

$$m_{\mathcal{H}_{all}}(\epsilon, \delta) > \frac{|\mathcal{X}|}{2}.$$

Rest of today's lecture: focus on **binary classification**!

Shattering and VC-Dimension

- VC-dimension of $\mathcal{H}$ characterizes if $\mathcal{H}$ is (agnostic) PAC-learnable!

Consequences of No-Free-Lunch

No-Free-Lunch Theorem has **consequences even if $\mathcal{H} \neq \mathcal{H}_{\text{all}}$**:

Definition (Restriction of $\mathcal{H}$ to $\mathcal{C}$)

For finite $\mathcal{C} = \{c_1, \ldots, c_k\} \subset \mathcal{X}$, let $\mathcal{H}_{\mathcal{C}} = \{\big(h(c_1), \ldots, h(c_k)\big) \mid h \in \mathcal{H}\}$.

- Obtain $\mathcal{H}_{\mathcal{C}}$ by evaluating hypotheses in $\mathcal{H}$ only on inputs in $\mathcal{C}$.

Consequences of No-Free-Lunch

No-Free-Lunch Theorem has **consequences even if $\mathcal{H} \neq \mathcal{H}_{\textsf{all}}$**:

Definition (Restriction of $\mathcal{H}$ to $\mathcal{C}$)

For finite $\mathcal{C} = \{c_1, \ldots, c_k\} \subset \mathcal{X}$, let $\mathcal{H}_{\mathcal{C}} = \{\big(h(c_1), \ldots, h(c_k)\big) \mid h \in \mathcal{H}\}$.

- Obtain $\mathcal{H}_{\mathcal{C}}$ by evaluating hypotheses in $\mathcal{H}$ only on inputs in $\mathcal{C}$.

Corollary (Difficult Subsets of $\mathcal{H}$)

If exists finite $\mathcal{C} \subset \mathcal{X}$ s.t. $\mathcal{H}_{\mathcal{C}}$ **contains all functions from $\mathcal{C}$ to $\{-1, +1\}$**, *then sample size $m \leq |\mathcal{C}|/2$ is not enough to PAC-learn $\mathcal{H}$.*

Proof: Restrict attention to $\mathcal{D}$ supported on $\mathcal{C}$ and apply no-free-lunch.

Shattering

$\mathcal{H}_\mathcal{C}$: evaluate hypotheses in $\mathcal{H}$ only on inputs in $\mathcal{C}$

Definition (Shattering)

$\mathcal{H}$ **shatters** a finite set $\mathcal{C} \subset \mathcal{X}$ if $\mathcal{H}_\mathcal{C} =$ all functions from $\mathcal{C}$ to $\{-1, +1\}$, i.e. $|\mathcal{H}_\mathcal{C}| = 2^{|\mathcal{C}|}$.

Shattering

$\mathcal{H}_{\mathcal{C}}$: evaluate hypotheses in $\mathcal{H}$ only on inputs in $\mathcal{C}$

Definition (Shattering)

$\mathcal{H}$ **shatters** a finite set $\mathcal{C} \subset \mathcal{X}$ if $\mathcal{H}_{\mathcal{C}} =$ all functions from $\mathcal{C}$ to $\{-1, +1\}$, i.e. $|\mathcal{H}_{\mathcal{C}}| = 2^{|\mathcal{C}|}$.

Example (Axis-aligned Rectangles)

$\mathcal{H}^2_{\text{rec}} = \{h_{(a_1,b_1,a_2,b_2)} \mid a_1 \leq b_1, a_2 \leq b_2\}$, where

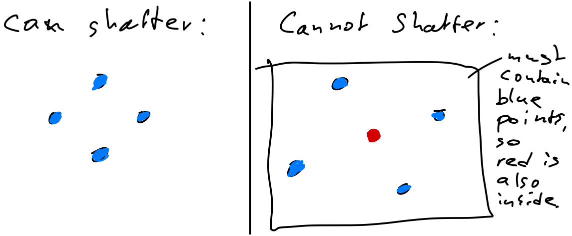
$$h_{(a_1,b_1,a_2,b_2)}(x_1, x_2) = \begin{cases} +1 & \text{if } a_1 \leq x_1 \leq b_1 \text{ and } a_2 \leq x_2 \leq b_2 \\ -1 & \text{otherwise} \end{cases}$$

Exists a $\mathcal{C}$ of size 4 that is shattered by $\mathcal{H}^2_{\text{rec}}$, but not of size 5.

Proof (Handwritten)

Need to show:

1. Exists $\mathcal{C}$ of size 4 that is shattered
2. No $\mathcal{C}$ of size 5 is shattered



Proof not size 5: if left-most, right-most, top-most and bottom-most point $+1$, then remaining point also $+1$

VC-Dimension

Definition (Shattering)

$\mathcal{H}$ **shatters** a finite set $\mathcal{C} \subset \mathcal{X}$ if $\mathcal{H}_{\mathcal{C}} =$ all functions.

Definition (Vapnik-Chervonenkis (VC) Dimension)

- VCdim$(\mathcal{H}) =$ **maximum size** of finite set $\mathcal{C} \subset \mathcal{X}$ **shattered** by $\mathcal{H}$
- VCdim$(\mathcal{H}) = \infty$ if there is no maximum

VC-Dimension

Definition (Shattering)

$\mathcal{H}$ **shatters** a finite set $\mathcal{C} \subset \mathcal{X}$ if $\mathcal{H}_{\mathcal{C}} =$ all functions.

Definition (Vapnik-Chervonenkis (VC) Dimension)

- VCdim($\mathcal{H}$) = **maximum size** of finite set $\mathcal{C} \subset \mathcal{X}$ **shattered** by $\mathcal{H}$
- VCdim($\mathcal{H}$) $= \infty$ if there is no maximum

Corollary (Difficult Subsets of $\mathcal{H}$)

If exists finite $\mathcal{C} \subset \mathcal{X}$ such that $\mathcal{H}$ shatters $\mathcal{C}$, then sample size $m \leq |\mathcal{C}|/2$ is not enough to PAC-learn $\mathcal{H}$.

VC-Dimension

Definition (Shattering)

$\mathcal{H}$ **shatters** a finite set $\mathcal{C} \subset \mathcal{X}$ if $\mathcal{H}_{\mathcal{C}} =$ all functions.

Definition (Vapnik-Chervonenkis (VC) Dimension)

- $\mathrm{VCdim}(\mathcal{H}) =$ **maximum size** of finite set $\mathcal{C} \subset \mathcal{X}$ **shattered** by $\mathcal{H}$
- $\mathrm{VCdim}(\mathcal{H}) = \infty$ if there is no maximum

Corollary (Difficult Subsets of $\mathcal{H}$)

If exists finite $\mathcal{C} \subset \mathcal{X}$ such that $\mathcal{H}$ shatters $\mathcal{C}$, then sample size $m \leq |\mathcal{C}|/2$ is not enough to PAC-learn $\mathcal{H}$.

- Sample size $m \leq \mathrm{VCdim}(\mathcal{H})/2$ is not enough to PAC-learn $\mathcal{H}$.
- **If $\mathrm{VCdim}(\mathcal{H}) = \infty$, then $\mathcal{H}$ is not PAC-learnable.**

VC-Dimension: Examples

Definition (Vapnik-Chervonenkis (VC) Dimension)

- $\mathsf{VCdim}(\mathcal{H}) =$ **maximum size** of finite set $\mathcal{C} \subset \mathcal{X}$ **shattered** by $\mathcal{H}$
- $\mathsf{VCdim}(\mathcal{H}) = \infty$ if there is no maximum

Example (Axis-Aligned Rectangles)

$\mathsf{VCdim}(\mathcal{H}^2_{\mathsf{rect}}) = 4$

VC-Dimension: Examples

Definition (Vapnik-Chervonenkis (VC) Dimension)

- $\mathsf{VCdim}(\mathcal{H})$ = **maximum size** of finite set $\mathcal{C} \subset \mathcal{X}$ **shattered** by $\mathcal{H}$
- $\mathsf{VCdim}(\mathcal{H}) = \infty$ if there is no maximum

Example (Axis-Aligned Rectangles)

$\mathsf{VCdim}(\mathcal{H}^2_{\mathsf{rect}}) = 4$

Example (Finite Hypothesis Classes)

$\mathsf{VCdim}(\mathcal{H}) \leq \log_2(|\mathcal{H}|)$

The Fundamental Theorem of PAC-Learning

Theorem

For binary classification, the following are equivalent:

1. *$\mathcal{H}$ has the* **uniform convergence** *property.*
2. *Any* **ERM** *rule is a successful agnostic PAC-learner for $\mathcal{H}$.*
3. *$\mathcal{H}$ is* **agnostic PAC-learnable**.
4. *$\mathcal{H}$ is* **PAC-learnable**.
5. *Any* **ERM** *rule is a successful PAC-learner for $\mathcal{H}$.*
6. $\mathcal{H}$ **has finite VC-dimension.**

The Fundamental Theorem of PAC-Learning

Theorem

For binary classification, the following are equivalent:

1. $\mathcal{H}$ *has the* **uniform convergence** *property.*
2. *Any* **ERM** *rule is a successful agnostic PAC-learner for* $\mathcal{H}$*.*
3. $\mathcal{H}$ *is* **agnostic PAC-learnable***.*
4. $\mathcal{H}$ *is* **PAC-learnable***.*
5. *Any* **ERM** *rule is a successful PAC-learner for* $\mathcal{H}$*.*
6. $\mathcal{H}$ **has finite VC-dimension.**

Main Points:

- PAC-learnability and agnostic PAC-learnability are equivalent
- VC-dimension characterizes both!

The Fundamental Theorem of PAC-Learning

Theorem

For binary classification, the following are equivalent:

1. *$\mathcal{H}$ has the* **uniform convergence** *property.*
2. *Any* **ERM** *rule is a successful agnostic PAC-learner for $\mathcal{H}$.*
3. *$\mathcal{H}$ is* **agnostic PAC-learnable**.
4. *$\mathcal{H}$ is* **PAC-learnable**.
5. *Any* **ERM** *rule is a successful PAC-learner for $\mathcal{H}$.*
6. *$\mathcal{H}$* **has finite VC-dimension.**

Main Points:

- PAC-learnability and agnostic PAC-learnability are equivalent
- VC-dimension characterizes both!

Other Observations:

- Finite VC-dimension is equivalent to uniform convergence
- ERM always works for (agnostic) PAC-learning

VC-Dimension of Linear Predictors (Halfspaces)

$$\mathcal{H}^d_{\text{lin}} = \{h_{\boldsymbol{w},b} \mid \boldsymbol{w} \in \mathbb{R}^d, b \in \mathbb{R}\},$$

where

$$h_{\boldsymbol{w},b}(\boldsymbol{X}) = \begin{cases} +1 & \text{if } b + \langle \boldsymbol{w}, \boldsymbol{X} \rangle \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

for $\boldsymbol{X} \in \mathbb{R}^d$

Theorem

$\text{VCdim}(\mathcal{H}^d_{lin}) = d + 1$

- For many (but not all!) hypothesis classes VC-dimension equals number of parameters

VC-dim for halfspaces

$x \in \mathbb{R}^d$

$$h_{w,b}(x) = \begin{cases} +1 & \text{if } b + \langle w, x \rangle \geq 0 \\ -1 & \text{o.w.} \end{cases}$$

$\mathcal{H} = \{h_{w,b} : w \in \mathbb{R}^d, b \in \mathbb{R}\}$

I. VC-dim $\geq d+1$

To show: exists $C \subset \mathbb{R}^d$ of size $|C| = d+1$ that is shattered by $\mathcal{H}$.

Take $C = \{0, e_1, \ldots, e_d\}$.

Let $y_0, y_1, \ldots, y_d \in \{-1, +1\}$ be arbitrary.

Now take $b = \frac{y_0}{2}$, $w = (y_1, \dots, y_d)$

Then

$$\left.\begin{aligned} b + \langle w, 0 \rangle &= \frac{y_0}{2} \\ b + \langle w, e_i \rangle &= \frac{y_0}{2} + y_i \end{aligned}\right\} \text{correct sign.}$$

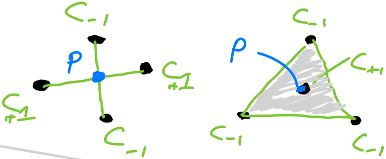
II. VC-dim < d+2:

To show: If $C \subset \mathbb{R}^d$ of size $|C| = d+2$,

then $\underbrace{C \text{ is not shattered by } \mathcal{H}.}_{\text{exist labels } y_1, \dots, y_{d+2} \text{ that cannot be realized by any } h_{w,b}.}$

Let $C = \{x_1, \dots, x_{d+2}\}$ be arbitrary.
To choose: $y_1, \dots, y_{d+2}$

$C_{-1} = \{x_i \in C : y_i = -1\}$
$C_{+1} = \{x_i \in C : y_i = +1\}$



C_j classified correctly

⇓ (linearity)

all points in convex hull of C_j
assigned class j

⇓

contradiction for p
in intersection of
convex hulls of C_{-1} and C_{+1}.

Can we always find C_{-1} and C_{+1} for which
convex hulls intersect? Yes!

Radon's Theorem: Any $C = \{x_1, \dots, x_{d+2}\} \subset \mathbb{R}^d$ can be partitioned into two (disjoint) subsets C_{-1} and C_{+1} whose convex hulls intersect.

Proof: Let $a_1, \dots, a_{d+2}$ (not all zero) be a solution to

$$\sum_{i=1}^{d+2} a_i x_i = 0 \quad , \qquad \sum_{i=1}^{d+2} a_i = 0$$

d constraints   1 constraint

Let $C_{-1} = \{x_i : a_i < 0\}$

$C_{+1} = \{x_i : a_i \geq 0\}$

Then both convex hulls contain

$$P = \sum_{x_i \in C_{+1}} \frac{a_i}{A} x_i = \sum_{x_j \in C_{-1}} \frac{-a_j}{A} x_j$$

where $A = \sum_{x_i \in C_{+1}} a_i = \sum_{x_j \in C_{-1}} -a_j$ $\square$