Machine Learning 5:
PAC learning, No-Free-Lunch theorem, uniform convergence

Master 2 Computer Science

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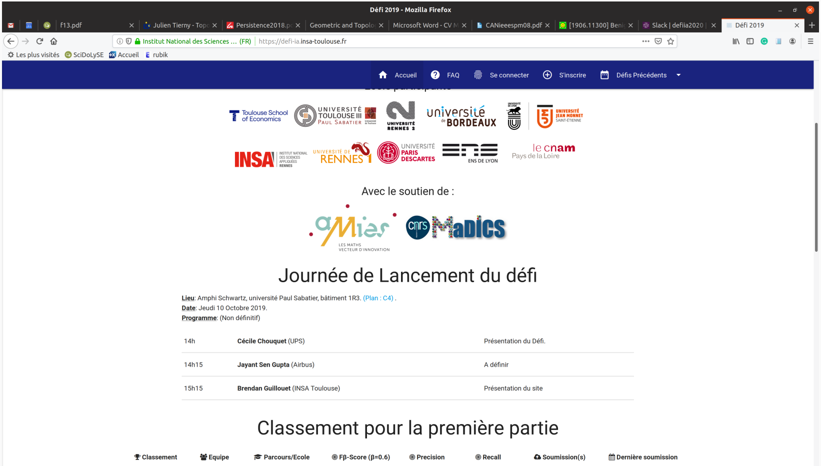

PAC learning

PAC learnability: "probably approximately correct"

Definition

A hypothesis class $\mathcal{H}$ is PAC learnable if there exists a function $m_{\mathcal{H}} : (0,1)^2 \to \mathbb{N}$ and a learning algorithm $S \mapsto \hat{h}_m$ such that for every $\epsilon, \delta \in (0,1)$, for every distribution D_X on $\mathcal{X}$ and for every labelling function $f : \mathcal{X} \to \{0,1\}$, if the realizable assumption holds with respect to $\mathcal{H}, D_X, f$ then when $S = \big((X_1, f(X_1)), \ldots, (X_m, f(X_m))\big)$ with $(X_i)_{1 \leq i \leq m} \overset{iid}{\sim} D_X$,

$$\mathbb{P}\Big(L_{(D_X,f)}\big(\hat{h}_m\big) \geq \epsilon\Big) \leq \delta$$

for all $m \geq m_{\mathcal{H}}(\epsilon, \delta)$.

The smallest possible function $m_{\mathcal{H}}$ is called the *sample complexity* of learning $\mathcal{H}$.

Remark: Valiant's PAC requires also sample complexity and running time polynomial in $1/\epsilon$ and $1/\delta$.

Finite hypothese classes are PAC-learnable

The sample complexity of finite hypothese classes in the realizable case is smaller than $\frac{\log \frac{|\mathcal{H}|}{\delta}}{\epsilon}$:

Theorem

Let $\mathcal{H}$ be a finite hypothesis class. Let $\epsilon, \delta \in (0, 1)$ and let m be an integer that satisfies

$$m \geq \frac{\log \frac{|\mathcal{H}|}{\delta}}{\epsilon} \; .$$

Then, for any labeling function f and for any distribution D_X on $\mathcal{X}$, under the realizability assumption, with probability at least $1 - \delta$ over the choice of iid sample S of size m, any ERM hypothesis $\hat{h}_m$ is such that

$$L_{(D_X, f)}(\hat{h}_m) \leq \epsilon \; .$$

Proof

The realizability assumption implies that an ERM $\hat{h}_S$ has empirical risk $L_S(\hat{h}_S) = 0$. Hence,

$$
\begin{aligned}
\mathbb{P}\left(L(\hat{h}_S) \geq \epsilon\right) &= D_X^{\otimes m}\Big(\big\{S \in \mathcal{X}^m : \exists h \in \mathcal{H}, L_S(h) = 0 \text{ and } L_D(h) \geq \epsilon\big\}\Big) \\
&= D_X^{\otimes m}\left(\bigcup_{h : L_D(h) \geq \epsilon} S_h\right) \quad \text{where } S_h = \big\{S \in \mathcal{X}^m : L_s(h) = 0\big\} \\
&\leq \sum_{h : L_D(h) \geq \epsilon} D_X^{\otimes m}(S_h) \\
&= \sum_{h : L_D(h) \geq \epsilon} \prod_{i=1}^{m} \underbrace{D_X\big(\{x \in \mathcal{X} : h(x) = f(x)\}\big)}_{= 1 - L_D(h) \leq 1 - \epsilon} \\
&\leq \sum_{h : L_{(D_X, f)}(h) \geq \epsilon} \prod_{i=1}^{m} (1 - \epsilon) \leq \big|\mathcal{H}\big|(1 - \epsilon)^m \leq \big|\mathcal{H}\big| \exp(-m\epsilon) \, .
\end{aligned}
$$

This quantity is smaller than δ for $m \geq \dfrac{\log \frac{|\mathcal{H}|}{\delta}}{\epsilon}$.

Agnostic PAC learnability

Definition

A hypothesis class $\mathcal{H}$ is *agnostic PAC learnable* if there exists a function $m_{\mathcal{H}} : (0,1)^2 \to \mathbb{N}$ and a learning algorithm $S \mapsto \hat{h}_m$ such that for every $\epsilon, \delta \in (0,1)$, for every distribution D on $\mathcal{X} \times \mathcal{Y}$ when $S = \big((X_1, Y_1), \ldots, (X_m, Y_m)\big) \overset{iid}{\sim} D$,

$$\mathbb{P}\Big(L_D(\hat{h}_m) \geq \min_{h' \in \mathcal{H}} L_D(h') + \epsilon\Big) \leq \delta$$

for all $m \geq m_{\mathcal{H}}(\epsilon, \delta)$.
The smallest possible function $m_{\mathcal{H}}$ is called the *sample complexity* of learning $\mathcal{H}$.

If the realizable assumption holds, boils down to PAC learnability.
Otherwise, recall that the best Bayes classifier has a risk not larger than $\min_{h' \in \mathcal{H}} L_D(h')$.

Learning via uniform convergence

Definition

A training set S is called ϵ-representative (wrt domain $\mathcal{X} \times \mathcal{Y}$, hypothese class $\mathcal{H}$, loss function l and distribution D) if

$$\forall h \in \mathcal{H}, \left| L_S(h) - L_D(h) \right| \leq \epsilon \,.$$

Lemma

If S is $\epsilon/2$-representative, then any ERM $\hat{h}_m$ defined by $\hat{h}_m \in \arg\min_{h \in \mathcal{H}} L_S(h)$ satisfies:

$$L_D\left(\hat{h}_m\right) \leq \min_{h \in \mathcal{H}} L_D(h) + \epsilon \,.$$

Proof: for every $h \in \mathcal{H}$,

$$L_D\left(\hat{h}_m\right) \leq L_S\left(\hat{h}_m\right) + \frac{\epsilon}{2} \leq L_S\left(h\right) + \frac{\epsilon}{2} \leq L_D\left(h\right) + \frac{\epsilon}{2} + \frac{\epsilon}{2} \,.$$

Uniform Convergence Property

Definition

A hypothesis class $\mathcal{H}$ has the *uniform convergence property* (wrt $\mathcal{X} \times \mathcal{Y}$ and l) if there exists a function $m_{\mathcal{H}}^{UC} : (0,1)^2 \to \mathbb{N}$ such that for every $\epsilon, \delta \in (0,1)$ and for every distribution D over $\mathcal{X} \times \mathcal{Y}$, a sample $S = \big((X_1, Y_1), \dots, (X_m, Y_m)\big) \overset{iid}{\sim} D$ of size $m \geq m_{\mathcal{H}}^{UC}(\epsilon, \delta)$ has probability at least $1 - \delta$ to be ϵ-representative.

Corollary

If $\mathcal{H}$ has the uniform convergence property with a function $m_{\mathcal{H}}^{UC}$, then $\mathcal{H}$ is agnostically PAC learnable with a sample complexity $m_{\mathcal{H}}(\epsilon, \delta) \leq m_{\mathcal{H}}^{UC}\left(\frac{\epsilon}{2}, \delta\right)$. Furthermore, the ERM is a successful PAC learner for $\mathcal{H}$.

Finite classes are agnostically PAC-learnable

Theorem

Let $\mathcal{H}$ be a finite hypothesis class. Then $\mathcal{H}$ enjoys the uniform convergence property with sample complexity

$$m_{\mathcal{H}}^{UC}(\epsilon, \delta) \leq \left\lceil \frac{\log \frac{2|\mathcal{H}|}{\delta}}{2\epsilon^2} \right\rceil .$$

Moreover, $\mathcal{H}$ is agnostically PAC learnable using an ERM algorithm with sample complexity

$$m_{\mathcal{H}}(\epsilon, \delta) \leq 2m_{\mathcal{H}}^{UC}\left(\frac{\epsilon}{2}, \delta\right) \leq \left\lceil \frac{2 \log \frac{2|\mathcal{H}|}{\delta}}{\epsilon^2} \right\rceil .$$

Proof: Hoeffding's inequality and the union bound.

No-Free-Lunch theorems: when learning is not possible

The No-Free-Lunch theorem

Theorem

Let A be any learning algorithm for binary classification over a domain $\mathcal{X}$. If the training set size is $m \leq |\mathcal{X}|/2$, then there exists a distribution $\mathcal{D}$ over $\mathcal{X} \times \{0,1\}$ such that:

- there exists a function $f : \mathcal{X} \to \{0,1\}$ with $L_D(f) = 0$;
- with probability at least $1/7$ over the choice of $S \sim \mathcal{D}^{\otimes m}$,

$$L_{\mathcal{D}}\big(A(S)\big) \geq \frac{1}{8} \, .$$

Note that the ERM over $\mathcal{H} = \{f\}$, or over any set $\mathcal{H}$ such that $m \geq 8 \log(7|\mathcal{H}|/6)$, is a successful learner in that setting.

Proof

Take $C \subset \mathcal{X}$ of cardinality $2m$, and $\{0,1\}^C = \{f_1, \dots, f_T\}$ where $T = 2^{2m}$. For each $1 \le i \le T$, we denote by D_i the probability distribution on $C \times \{0,1\}$ defined by

$$D_i(\{x,y\}) = \begin{cases} \frac{1}{2m} \text{ if } y = f_i(x) \ , \\ 0 \text{ otherwise.} \end{cases}$$

We will show that $\max_{1 \le i \le T} \mathbb{E}\left[L_{D_i}(A(S))\right] \ge 1/4$, which entails the result thanks to the small lemma: if $P(0 \le Z \le 1) = 1$ and $\mathbb{E}[Z] \ge 1/4$, then $\mathbb{P}(Z \ge 1/8) \ge 1/7$. Indeed, $1/4 \le \mathbb{E}[Z] \le \mathbb{P}(Z < 1/8)/8 + \mathbb{P}(Z \ge 1/8) = 1/8 - 7\,\mathbb{P}(Z \ge 1/8)/8$.

All the X-samples $S_1^X, \dots, S_k^X$, for $k = m^{2m}$, are equaly likely. For $1 \le j \le k$, if $S_j^X = (x_1, \dots, x_m)$ we denote by $S_j^i = \big((x_1, f_i(x_1)), \dots, (x_m, f_i(x_m)\big)$, and $\hat{f}_j^i = A(S_j^i)$.

$$\begin{aligned} \max_{1 \le i \le T} \mathbb{E}\Big[L_{D_i}(A(S))\Big] &= \max_{1 \le i \le T} \frac{1}{k} \sum_{j=1}^{k} L_{D_i}\left(\hat{f}_j^i\right) \ge \frac{1}{T} \sum_{i=1}^{T} \frac{1}{k} \sum_{j=1}^{k} L_{D_i}\left(\hat{f}_j^i\right) \\ &= \frac{1}{k} \sum_{j=1}^{k} \frac{1}{T} \sum_{i=1}^{T} L_{D_i}\left(\hat{f}_j^i\right) \ge \min_{1 \le j \le k} \frac{1}{T} \sum_{i=1}^{T} L_{D_i}\left(\hat{f}_j^i\right) \ . \end{aligned}$$

Fix $1 \le j \le k$, denote $S_j^X = (x_1, \dots, x_m)$ and define $\{v_1, \dots, v_p\} = C \setminus \{x_1, \dots, x_m\}$, where $p \ge m$. Then

$$L_{D_i}\left(\hat{f}_j^i\right) = \frac{1}{2m} \sum_{x \in C} \mathbb{1}\{\hat{f}_j^i(x) \ne f_i(x)\} \ge \frac{1}{2p} \sum_{r=1}^{p} \mathbb{1}\{\hat{f}_j^i(v_r) \ne f_i(v_r)\}$$

and hence

$$\frac{1}{T} \sum_{i=1}^{T} L_{D_i}\left(\hat{f}_j^i\right) \ge \frac{1}{T} \sum_{i=1}^{T} \frac{1}{2p} \sum_{r=1}^{p} \mathbb{1}\{\hat{f}_j^i(v_r) \ne f_i(v_r)\} \ge \frac{1}{2} \min_{1 \le r \le p} \frac{1}{T} \sum_{i=1}^{T} \mathbb{1}\{\hat{f}_j^i(v_r) \ne f_i(v_r)\} \ .$$

Fix $1 \le r \le p$. Then the functions $\{f_i : 1 \le i \le T\}$ can be grouped into $T/2$ pairs of functions $\left(\tilde{f}_i^0, \tilde{f}_i^1\right)$, $1 \le i \le T/2$ which agree on all $x \in C$ except on v_r, and for all $1 \le i \le T/2$ it holds that $\mathbb{1}\{\hat{f}_j^i(v_r) \ne \tilde{f}_i^0(v_r)\} + \mathbb{1}\{\hat{f}_j^i(v_r) \ne \tilde{f}_i^1(v_r)\} = 1$. Hence, $\sum_{i=1}^{T} \mathbb{1}\{\hat{f}_j^i(v_r) \ne f_i(v_r)\} = \sum_{i=1}^{T/2} \mathbb{1}\{\hat{f}_j^i(v_r) \ne \tilde{f}_i^0(v_r)\} + \mathbb{1}\{\hat{f}_j^i(v_r) \ne \tilde{f}_i^1(v_r)\} = T/2$, which concludes the proof.

Consequence: Curse of Dimensionality

Theorem

Let $c > 1$ be a Lipschitz constant. Let A be any learning algorithm for binary classification over a domain $\mathcal{X} = [0,1]^d$. If the training set size is $m \leq (c+1)^d/2$, then there exists a distribution $\mathcal{D}$ over $[0,1]^d \times \{0,1\}$ such that:

- $\eta(x)$ is c-Lipschitz;
- the Bayes error of the distribution is 0;
- with probability at least $1/7$ over the choice of $S \sim \mathcal{D}^{\otimes m}$,

$$L_{\mathcal{D}}\big(A(S)\big) \geq \frac{1}{8} \, .$$

Uniform convergence for infinite classes: VC dimension

Shattering

Definition

Let $\mathcal{H}$ be a class of functions $\mathcal{X} \to \{0,1\}$ and let $C = \{c_1, \ldots, c_m\} \subset \mathcal{X}$. The *restriction* of $\mathcal{H}$ to C is the set of functions $C \to \{0,1\}$ that can be derived from $\mathcal{H}$:

$$\mathcal{H}_C = \Big\{ (c_1, \ldots, c_m) \to \big(h(c_1), \ldots, h(c_m)\big) : h \in \mathcal{H} \Big\} .$$

Shattering

A hypothesis class $\mathcal{H}$ *shatters* a finite set $C \subset \mathcal{X}$ if $\mathcal{H}_C = \{0,1\}^C$.

Example:

- $\mathcal{H} = \big\{ h_a : a \in \mathbb{R} \big\}$.
- $\mathcal{H}^2_{\mathrm{rec}} = \big\{ h_{(a_1,b_1,a_2,b_2)} : a_1 \leq b_1 \text{ and } a_2 \leq b_2 \big\}$ where

$$h_{(a_1,b_1,a_2,b_2)}(x_1, x_2) = \begin{cases} 1 & \text{if } a_1 \leq x_1 \leq b_1 \text{ and } a_2 \leq x_2 \leq b_2 \, ; \\ 0 & \text{otherwise} . \end{cases}$$

VC dimension

Definition

The *Vapnik Chervonenkis dimension* $\mathrm{VCdim}(\mathcal{H})$ of a hypothesis class $\mathcal{H}$ is the maximal size of a set $C \subset \mathcal{X}$ that can be shattered by $\mathcal{H}$. If $\mathcal{H}$ can shatter sets of arbitrarily large size we say that $\mathrm{VCdim}(\mathcal{H}) = \infty$.

Theorem

Let $\mathcal{H}$ be a class of infinite VC-dimension. Then $\mathcal{H}$ is not PAC-learnable.

Proof: for every training size m, there exists a set C of size $2m$ that is shattered by $\mathcal{H}$. By the NFL theorem, for every learning algorithm A there exists a probability distribution D over $\mathcal{X} \times \{0, 1\}$ such that $L_D(h) = 0$ but with probability at least $1/7$ over the training set, we have $L_D\big(A(S)\big) \geq 1/8$.