Statistical Machine Learning (BE4M33SSU) Lecture 4: Probably Approximately Correct Learning

Czech Technical University in Prague V. Franc

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• $R^* = \inf_{h \in \mathcal{Y}^{\mathcal{X}}} R(h)$ best attainable risk









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Error decomposition:

$$R(h_m) = \underbrace{\left(R(h_m) - R(h_{\mathcal{H}})\right)}_{\text{estimation error}} + \underbrace{\left(R(h_{\mathcal{H}}) - R^*\right)}_{\text{approximation error}} + R^*$$





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2/13

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• The approximation error: depends on $\mathcal H$ chosen prior to learning.

• The estimation error: depends on \mathcal{H} , data \mathcal{T} and the algorithm A.

Probably Approximately Correct (PAC) learning

Successful PAC learning algorithm

- Given a hypothesis space \mathcal{H} and the loss ℓ , the algorithm with high probability learns a predictor that has low estimation error.
- The following can be arbitrary: desired estimation error $\varepsilon > 0$, probability of failure $\delta \in (0, 1)$, and data distribution p(x, y).



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Definition. Algorithm is a successful PAC learner for hypothesis space \mathcal{H} w.r.t. loss $\ell: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ if there exists a function (called sample complexity) $m_{\mathcal{H}}^{\text{pac}}: \mathbb{R}_{>0} \times (0,1) \to \mathbb{N}$ such that: For every $\varepsilon > 0$, $\delta \in (0,1)$, and every distribution p(x,y), when running the algorithm on $m \ge m_{\mathcal{H}}^{\text{pac}}(\varepsilon, \delta)$ examples \mathcal{T}^m i.i.d. drawn from p(x,y), then the algorithm returns $h_m = A(\mathcal{T}^m)$ such that

$$\mathbb{P}\Big(R(h_m) - R(h_{\mathcal{H}}) \le \varepsilon\Big) \ge 1 - \delta.$$



ULLN implies that ERM is successful PAC learner

ULLN applies for $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$: there exists $m_{\mathcal{H}}^{\mathrm{ul}} \colon \mathbb{R}_{>0} \times (0,1) \to \mathbb{N}$ such that for every $\varepsilon > 0, \delta \in (0,1)$, every distribution p(x,y) and every $m \ge m_{\mathcal{H}}^{\mathrm{ul}}(\varepsilon,\delta)$ it holds that

$$\mathbb{P}\left(\sup_{h\in\mathcal{H}}\left|R(h)-R_{\mathcal{T}^m}(h)\right|\geq\varepsilon\right)\leq\delta.$$

ER can fail



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Successful PAC learner for $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$: there exists $m_{\mathcal{H}}^{\text{pac}} \colon \mathbb{R}_{>0} \times (0,1) \to \mathbb{N}$ such that when running the algorithm on $m \geq m_{\mathcal{H}}^{\text{pac}}(\varepsilon, \delta)$ examples $\mathcal{T}^m \sim p^m$ then it returns $h_m = A(\mathcal{T}^m)$ such that

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4/13

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Theorem: If ULLN applies for $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$ with a function $m_{\mathcal{H}}^{\mathrm{ul}}$ then ERM is a successful PAC learner for \mathcal{H} with the sample complexity $m_{\mathcal{H}}^{\mathrm{pac}}(\varepsilon, \delta) = m_{\mathcal{H}}^{\mathrm{ul}}(\frac{\varepsilon}{2}, \delta).$



















$$\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} = ?$$

 $\mathcal{H} = \{h(x) = \operatorname{sign}(x - \theta) | \theta \in \mathbb{R}\}, \ \ell(y, y') = [y \neq y']$ R(h) $R_{T^m}(h)$ m=100 $R(h_m)$ $R(h_H)$ $R_{T^m}(h_m)$ h_H h_m





estimation error









ULLN:
$$m \ge m_{\mathcal{H}}^{\mathrm{ul}}(\varepsilon, \delta) \implies \mathbb{P}\left(\sup_{h \in \mathcal{H}} \left| R(h) - R_{\mathcal{T}^m}(h) \right| > \varepsilon\right) \le \delta$$

ER can fail

$$\underbrace{R(h_m) - R(h_{\mathcal{H}})}_{\text{estimation error}} \leq 2 \sup_{h \in \mathcal{H}} \left| R(h) - R_{\mathcal{T}^m}(h) \right|$$



ULLN:
$$m \ge m_{\mathcal{H}}^{\mathrm{ul}}(\varepsilon, \delta) \Rightarrow \mathbb{P}\left(\sup_{h \in \mathcal{H}} \left| R(h) - R_{\mathcal{T}^m}(h) \right| > \varepsilon\right) \le \delta$$

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$$R(h_m) - R(h_{\mathcal{H}}) > \overline{\varepsilon} \quad \Rightarrow \quad \sup_{h \in \mathcal{H}} |R(h) - R_{\mathcal{T}^m}(h)| > \frac{\overline{\varepsilon}}{2}$$









Successful PAC: $m \ge m_{\mathcal{H}}^{\mathrm{pac}}(\bar{\varepsilon}, \delta) \Rightarrow \mathbb{P}\Big(R(h_m) - R(h_{\mathcal{H}}) \le \bar{\varepsilon}\Big) \le 1 - \delta$ where $m_{\mathcal{H}}^{\mathrm{pac}}(\bar{\varepsilon}, \delta) = m_{\mathcal{H}}^{\mathrm{ul}}(\frac{\bar{\varepsilon}}{2}, \delta)$



For fixed \mathcal{T}^m and $h_m \in \operatorname{Argmin}_{h \in \mathcal{H}} R_{\mathcal{T}^m}(h)$ we have:

$$R(h_m) - R(h_{\mathcal{H}}) = \left(R(h_m) - R_{\mathcal{T}^m}(h_m) \right) + \left(R_{\mathcal{T}^m}(h_m) - R(h_{\mathcal{H}}) \right)$$
$$\leq \left(R(h_m) - R_{\mathcal{T}^m}(h_m) \right) + \left(R_{\mathcal{T}^m}(h_{\mathcal{H}}) - R(h_{\mathcal{H}}) \right)$$
$$\leq 2 \sup_{h \in \mathcal{H}} \left| R(h) - R_{\mathcal{T}^m}(h) \right|$$

ERM is successful PAC learner for finite hypothesis space

• We showed that for finite hypothesis space $\mathcal{H} = \{h_1, \ldots, h_K\}$ it holds

$$\mathbb{P}\Big(\max_{h\in\mathcal{H}}|R_{\mathcal{T}^m}(h)-R(h)|\geq\varepsilon\Big)\leq 2|\mathcal{H}|e^{-\frac{2m\varepsilon^2}{(\ell_{\max}-\ell_{\min})^2}}=\delta$$

and hence ULLN applies with $m_{\mathcal{H}}^{\mathrm{ul}}(\varepsilon, \delta) = \frac{\log 2|H| - \log \delta}{2 \varepsilon^2} (\ell_{\mathrm{max}} - \ell_{\mathrm{min}})^2$.



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Therefore ERM is successful PAC learner for \mathcal{H} with sample complexity

$$m_{\mathcal{H}}^{\mathrm{pac}}(\bar{\varepsilon},\delta) = 2 \frac{\log 2|H| - \log \delta}{\bar{\varepsilon}^2} (\ell_{\mathrm{max}} - \ell_{\mathrm{min}})^2,$$

that is, when running ERM on \mathcal{T}^m with $m \ge m_{\mathcal{H}}^{\text{pac}}(\bar{\varepsilon}, \delta)$ then it returns $h_m = A(\mathcal{T}^m)$ such that

$$\mathbb{P}\Big(R(h_m) - R(h_{\mathcal{H}}) \le \overline{\varepsilon}\Big) \ge 1 - \delta .$$



Linear classifier minimizing classification error

- \mathcal{X} is a set of observations and $\mathcal{Y} = \{+1, -1\}$ a set of hidden labels
- $lacksymbol{\phi}: \mathcal{X} o \mathbb{R}^n$ is fixed feature map embedding \mathcal{X} to \mathbb{R}^n
- Task: find linear classification strategy $h\colon \mathcal{X} o \mathcal{Y}$, parametrized by a vector $m{w} \in \mathbb{R}^n$,

$$h(x; \boldsymbol{w}, b) = \operatorname{sign}(\langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b) = \begin{cases} +1 & \text{if } \langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b \ge 0\\ -1 & \text{if } \langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b < 0 \end{cases}$$

with minimal expected risk

$$R^{0/1}(h) = \mathbb{E}_{(x,y)\sim p}\Big(\ell^{0/1}(y,h(x))\Big) \quad \text{where} \quad \ell^{0/1}(y,y') = [y \neq y']$$

We are given a set of training examples

$$\mathcal{T}^m = \{ (x^i, y^i) \in (\mathcal{X} \times \mathcal{Y}) \mid i = 1, \dots, m \}$$

drawn from i.i.d. with the distribution p(x, y).



ERM learning for linear classifiers



• ERM for
$$\mathcal{H} = \{h(x; w, b) = \operatorname{sign}(\langle w, \phi(x) \rangle + b) \mid (w, b) \in \mathbb{R}^{n+1}\}$$
 leads to

$$(\boldsymbol{w}^*, b^*) \in \operatorname{Argmin}_{h \in \mathcal{H}} R^{0/1}_{\mathcal{T}^m}(h) = \operatorname{Argmin}_{(\boldsymbol{w}, b) \in (\mathbb{R}^n \times \mathbb{R})} R^{0/1}_{\mathcal{T}^m}(h(\cdot; \boldsymbol{w}, b))$$
(1)

where the empirical risk is

$$R_{\mathcal{T}^m}^{0/1}(h(\cdot;\boldsymbol{w},b)) = \frac{1}{m} \sum_{i=1}^m [y^i \neq h(x^i;\boldsymbol{w},b)]$$

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- Algorithmic issues (next lecture): in general, there is no known algorithm solving the task (1) in time polynomial in m.
- Does ULLN applies for the class of two-class linear classifiers?
 If yes then ERM is PAC successful learner.

Vapnik-Chervonenkis (VC) dimension



• VC dimension is a concept to measure complexity of an infinite hypothesis space $\mathcal{H} \subseteq \{-1, +1\}^{\mathcal{X}}$.

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Definition: Let $\mathcal{H} \subseteq \{-1, +1\}^{\mathcal{X}}$ and $\{x^1, \ldots, x^m\} \in \mathcal{X}^m$ be a set of m input observations. The set $\{x^1, \ldots, x^m\}$ is said to be shattered by \mathcal{H} if for all $y \in \{+1, -1\}^m$ there exists $h \in \mathcal{H}$ such that $h(x^i) = y^i$, $i \in \{1, \ldots, m\}$.

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Definition: Let $\mathcal{H} \subseteq \{-1, +1\}^{\mathcal{X}}$. The Vapnik-Chervonenkis dimension of \mathcal{H} is the cardinality of the largest set of points from \mathcal{X} which can be shattered by \mathcal{H} .

VC dimension of class of two-class linear classifiers



Theorem: The VC-dimension of the hypothesis class of all two-class linear classifiers operating in *n*-dimensional feature space $\mathcal{H} = \{h(x; \boldsymbol{w}, b) = \operatorname{sign}(\langle \boldsymbol{w}, \boldsymbol{\phi}(x) \rangle + b) \mid (\boldsymbol{w}, b) \in (\mathbb{R}^n \times \mathbb{R})\} \text{ is } n+1.$

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ULLN for two class predictors and 0/1-loss

Theorem: Let $\mathcal{H} \subset \{+1, -1\}^{\mathcal{X}}$ be a hypothesis class with VC dimension $d < \infty$ and $\mathcal{T}^m = \{(x^1, y^1), \dots, (x^m, y^m)\} \in (\mathcal{X} \times \mathcal{Y})^m$ a training set draw from i.i.d. rand vars with distribution p(x, y). Then for any $\varepsilon > 0$ it holds

$$\mathbb{P}\left(\sup_{h\in\mathcal{H}}\left|R^{0/1}(h) - R^{0/1}_{\mathcal{T}^m}(h)\right| \ge \varepsilon\right) \le 4\left(\frac{2\,e\,m}{d}\right)^d e^{-\frac{m\,\varepsilon^2}{8}}$$



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Corollary: Let $\mathcal{H} \subset \{+1, -1\}^{\mathcal{X}}$ be a hypothesis class with a finite VC dimension $d < \infty$. Then, ULLN applies for \mathcal{H} and there exists a constant C such that

$$m_{\mathcal{H}}^{\mathrm{pac}}(\varepsilon,\delta) \le C \frac{d - \log \delta}{\varepsilon^2}$$

that is, ERM is PAC successful learner.



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Remark: Recall that in case of finite hypothesis space $\mathcal{H} = \{h_1, \ldots, h_K\}$ and 0/1-loss we have the sample complexity $m_{\mathcal{H}}^{\text{pac}}(\varepsilon, \delta) = 2 \frac{\log 2|\mathcal{H}| - \log \delta}{\varepsilon^2}$.



Summary

Error decomposition: Generalization error = estimation error + approximation error + Bayes risk. 13/13

- Probably Approximately Correct (PAC) learning.
- ULLN implies that ERM is successful PAC learner.
- VC dimension: hypothesis space complexity of two-class classifier.
- VC dimension of linear hypothesis space.
- Finite VC dimension implies that ERM is a successful PAC learner.





























