Empirical Risk Minimization

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Prediction task and its solution by learning from data

Empirical risk minimization

Statistical consistency

Uniform Law of Large Numbers

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Structured Output Prediction: the statistical model

The setting

- \bullet \mathcal{X} set of input observations
- \mathcal{Y} finite set of hidden states, e.g.
 - Flat classification: $\mathcal{Y} = \{1, \dots, K\}$
 - Structured classif.: $\mathcal{Y} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_{|\mathcal{V}|}$ is a labeling of parts \mathcal{V} .
- $(x,y) \in \mathcal{X} \times \mathcal{Y}$ randomly drawn from r.v. with p.d.f. p(x,y)
- $\ell \colon \mathcal{Y} \times \mathcal{Y} \to [0,\infty)$ loss function



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The task: find a strategy $h \colon \mathcal{X} \to \mathcal{Y}$ with the minimal expected risk

$$R^* = \min_{h \colon \mathcal{X} \to \mathcal{Y}} R(h) \quad \text{where} \quad R(h) = \mathbb{E}_{(x,y) \sim p}[\ell(y, h(x))]$$



Solving the prediction problem from examples

• Assumption: we have an access to examples

$$\{(x^1, y^1), (x^2, y^2), \ldots\}$$

drawn from i.i.d. r.v. distributed according to unknown p(x, y).



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

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b) Learning: find $h: \mathcal{X} \to \mathcal{Y}$ with small R(h) using training set

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

drawn i.i.d. from p(x, y).

Estimation of the expected risk from examples

Given a predictor $h \colon \mathcal{X} \to \mathcal{Y}$, compute the empirical risk

$$R_{\mathcal{S}^l}(h) = \frac{1}{l} \sum_{i=1}^l \ell(y^i, h(x^i))$$

and use it as a proxy for $R(h) = \mathbb{E}_{(x,y)\sim p}(\ell(y,h(x))).$

- The value of the empirical risk $R_{S^l}(h)$ is a random number.
- Application of Hoeffding inequality: for any \varepsilon > 0 the probability of seeing a "bad test set" can be bound by

$$\mathbb{P}_{\mathcal{S}^{l} \sim p}\left(\left|R_{\mathcal{S}^{l}}(h) - R(h)\right| \ge \varepsilon\right) \le 2e^{-\frac{2l\varepsilon^{2}}{(\ell_{\min} - \ell_{\max})^{2}}}$$

Learning algorithm

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

drawn from i.i.d. according to unknown p(x, y).

Use prior knowledge to select hypothesis space

$$\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}} = \{h \colon \mathcal{X} \to \mathcal{Y}\}$$

The learning algorithm

$$A\colon \cup_{m=1}^{\infty} (\mathcal{X} \times \mathcal{Y})^m \to \mathcal{H}$$

selects strategy $h_m = A(\mathcal{T}^m)$ based on the training set \mathcal{T}^m .

Generative learning (to come later)

1. Use the training set $\mathcal{T}^m = \{(x^i, y^i) \in \mathcal{X} \times \mathcal{Y} \mid i \in \{1, \dots, m\}\}$ to approximate p(x, y) by $\hat{p}(x, y)$.

For example, use the Maximum-Likelihood method:

(a) Guess the shape of the distribution, e.g.

$$\hat{p}_{\boldsymbol{w}}(x,y) = \frac{1}{Z(\boldsymbol{w})} \exp\langle \boldsymbol{w}, \boldsymbol{\phi}(x,y) \rangle, \qquad \boldsymbol{w} \in \mathcal{W}$$

(b) Find the ML estimate

$$\boldsymbol{w}_m \in \operatorname*{argmax}_{\boldsymbol{w} \in \mathcal{W}} \sum_{i=1}^m \log \hat{p}_{\boldsymbol{w}}(x^i, y^i)$$

2. Construct a plug-in classifier

$$h_m(x) \in \operatorname*{argmin}_{h: \mathcal{X} \to \mathcal{Y}} \mathbb{E}_{(x,y) \sim \hat{p}_{\boldsymbol{w}_m}}[\ell(y, h(x))]$$

Discriminative learning by Empirical Risk Minimization

• Use the training set $\mathcal{T}^m = \{(x^i, y^i) \in \mathcal{X} \times \mathcal{Y} \mid i \in \{1, \dots, m\}\}$ to approximate the expected risk R(h) by the empirical risk

$$R_{\mathcal{T}^m}(h) = \frac{1}{m} \sum_{i=1}^m \ell(y^i, h(x^i))$$

• The ERM learning algorithm returns h_m such that

$$h_m \in \operatorname{Argmin}_{h \in \mathcal{H}} R_{\mathcal{T}^m}(h) \tag{1}$$

Depending on the choice of *H*, *l* and algorithm solving (1) we get individual instances, e.g.: Structured-Output Perceptron, Structured-Output Support Vector Machines, Logistic regression, Neural Networks learned by back-propagation, AdaBoost,

Errors characterizing a learning algorithm

The characters of the play:

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- $R(h_m)$ risk of $h_m = A(\mathcal{T}_m)$ learned from \mathcal{T}^m

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Excess error: the quantity we want to minimize

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

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- The excess and the estimation error are random variables
- The estimation error depends on m and $\mathcal H$

• The approximation error depends on \mathcal{H} (so called inductive bias)

Statistically consistent learning algorithm

Definition 1. The algorithm $A: \cup_{m=1}^{\infty} (\mathcal{X} \times \mathcal{Y})^m \to \mathcal{H}$ is statistically consistent in $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ w.r.t. p(x, y) if for every $\varepsilon > 0$ and $\delta \in (0, 1)$ there exist $m_0 \in \mathcal{N}$ such that

$$\mathbb{P}_{\mathcal{T}^m \sim p} \left(R(A(\mathcal{T}^m)) - R(h_{\mathcal{H}}) \ge \varepsilon \right) \le 1 - \delta$$

holds for every $m \ge m_0$.

If A is consistent for any p(x, y) then A is universally consistent in \mathcal{H} .

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Question:

• Is the ERM learning algorithm statistically consistent ?

• Let $\mathcal{X} = [a, b] \subset \mathbb{R}$, $\mathcal{Y} = \{+1, -1\}$, $\ell(y, y') = [y \neq y']$, $p(x \mid y = +1)$ and $p(x \mid y = -1)$ be uniform distributions on \mathcal{X} and p(y = +1) = 0.8.

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- The optimal strategy is h(x) = +1 with the Bayes risk $R^* = 0.2$.
- Consider learning algorithm which for a given training set $\mathcal{T}^m = \{(x^1, y^1), \dots, (x^m, y^m)\}$ returns strategy

$$h_m(x) = \begin{cases} y^j & \text{if } x = x^j \text{ for some } j \in \{1, \dots, m\} \\ -1 & \text{otherwise} \end{cases}$$

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• The empirical risk is $R_{\mathcal{T}^m}(h_m) = 0$ with probability 1 for any m.

• The expected risk is $R(h_m) = 0.8$ for any m.

Uniform Law of Large Numbers

Definition 2. The hypothesis space $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ satisfies the uniform law of large numbers if for every distributon p(x, y), $\varepsilon > 0$ and $\delta \in (0, 1)$ there exists $m_0 \in \mathcal{N}$ such that

$$\mathbb{P}_{\mathcal{T}^m \sim p} \left(\sup_{h \in \mathcal{H}} \left| R(h) - R_{\mathcal{T}^m}(h) \right| \ge \varepsilon \right) \le 1 - \delta$$

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Theorem 1. If \mathcal{H} satisfies ULLN then ERM is statistically consistent in \mathcal{H} .

Proof: ULLN implies consistency of ERM

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

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

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Therefore $\varepsilon \leq R(h_m) - R(h_{\mathcal{H}})$ implies $\frac{\varepsilon}{2} \leq \sup_{h \in \mathcal{H}} \left| R(h) - R_{\mathcal{T}^m}(h) \right|$ and

$$\mathbb{P}\bigg(R(h_m) - R(h_{\mathcal{H}}) \ge \varepsilon\bigg) \le \mathbb{P}\bigg(\sup_{h \in \mathcal{H}} \left|R(h) - R_{\mathcal{T}^m}(h)\right| \ge \frac{\varepsilon}{2}\bigg)$$

Two examples of ${\mathcal H}$ which satisfy ULLN

1. \mathcal{H} is a finite set and $\ell \colon \mathcal{Y} \times \mathcal{Y} \to [\ell_{min}, \ell_{max}]$. Then,

$$\mathbb{P}_{\mathcal{T}\sim p^m}\left(\max_{h\in\mathcal{H}}\left|R(h)-R_{\mathcal{T}^m}(h)\right|\geq\varepsilon\right)\leq 2|\mathcal{H}|\exp\left(\frac{-2m\varepsilon^2}{(\ell_{max}-\ell_{min})^2}\right)$$

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ℓ(y, y') = [y ≠ y'], 𝔅 = {+1, -1} and VC-dimension of 𝔅 is finite.
 VC-dimension d of 𝔅 is the maximal number of inputs which can be classified by strategies from 𝔅 in all possible (that is 2^d) ways. Then,

$$\mathbb{P}_{\mathcal{T}\sim p^m}\left(\sup_{h\in\mathcal{H}}\left|R(h)-R_{\mathcal{T}^m}(h)\right|\geq\varepsilon\right)\leq 4\left(\frac{2\,e\,m}{d}\right)^d e^{-\frac{m\,\varepsilon^2}{8}}$$

$$\bullet \text{ Let } z = (x,y) \in \mathcal{Z} = \mathcal{X} \times \mathcal{Y}, \ p(z) = p(x,y) \text{ and } g(z) = \ell(y,h(x)).$$

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Definition 3. Let $\mathcal{G} \subseteq [a, b]^{\mathcal{Z}}$ be a set of functions $g: \mathcal{Z} \to [a, b]$ where $a, b \in \mathbb{R}$ and a < b. Let $\mathcal{U}^m = \{z^1, \ldots, z^m\} \in \mathcal{Z}^m$ be drawn i.i.d. from p(z).

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The empirical Rademacher complexity of \mathcal{G} w.r.t. to the sample \mathcal{U}^m is

$$\hat{\mathfrak{R}}_m(\mathcal{G}, \mathcal{U}^m) = \mathbb{E}_{\sigma \sim \text{Unif}\{-1, +1\}} \left[\sup_{g \in \mathcal{G}} \frac{1}{m} \sum_{i=1}^m \sigma_i g(z_i) \right]$$

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The Rademacher complexity of \mathcal{G} w.r.t. distribution p(z) is

$$\mathfrak{R}_m(\mathcal{G}) = \mathbb{E}_{\mathcal{U}^m \sim p^m(z)} \left[\hat{\mathfrak{R}}_m(\mathcal{G}, \mathcal{U}^m) \right]$$

Rademacher-based uniform convergence

• Let $\mathcal{G} \subseteq [a, b]^{\mathcal{Z}}$ be a set of functions. Then, for every $\delta \in (0, 1)$

$$\sup_{g \in \mathcal{G}} \left| \mathbb{E}_{z \sim p}(g(z)) - \frac{1}{m} \sum_{i=1}^{m} g(z_i) \right| \le 2 \,\mathfrak{R}_m(\mathcal{G}) + (b-a) \sqrt{\frac{\log 2/\delta}{2m}}$$

holds with probability $1 - \delta$ at least, w.r.t. $\mathcal{U}^m = \{z^1, \ldots, z^m\} \sim p^m(z)$.

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$$\sup_{g \in \mathcal{G}} \left| \mathbb{E}_{z \sim p}(g(z)) - \frac{1}{m} \sum_{i=1}^{m} g(z_i) \right| \le 3 \,\hat{\Re}_m(\mathcal{G}, \mathcal{U}^m) + (b-a) \sqrt{\frac{\log 4/\delta}{2m}}$$

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Example: Rademacher complexity of linear functions

• Assume that $\mathcal{X} \subseteq \mathbb{R}^n$ and $p(m{x},y)$ is such that $\|m{x}\| \leq R$.

Assume that

$$\mathcal{G} = \left\{ \psi(\langle \boldsymbol{w}, \boldsymbol{x} \rangle, y) \mid \|\boldsymbol{w}\|_2 \leq B \right\}$$

where $\psi \colon \mathbb{R} \times \mathcal{Y} \to \mathbb{R}$ is such that $f(t) = \psi(t, y)$ is ρ -Lipschitz continuous for all $y \in \mathcal{Y}$.

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Then,

$$\hat{\mathfrak{R}}_m(\mathcal{G}) \le \frac{\rho \, B \, R}{\sqrt{m}}$$

We can also compute

$$b = \max_{t \in [-BR, BR]} \psi(t, y)$$
 and $a = \min_{t \in [-BR, BR]} \psi(t, y)$

