Statistical Learning II

Lecture 3 - Supervised learning (continued)

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Supervised learning

Empirical risk

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Given a loss function $\ell : \mathscr{Y} \times \mathscr{Y} \to \mathbb{R}_+$, and a predictor $f : \mathscr{X} \to \mathscr{Y}$ define the empirical risk:

$$\hat{\mathscr{R}}_n(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i))$$

Also known as the training loss.

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Also known as the training loss. This quantifies how well we fit the data. But is this a good notion of learning?

$$f(x) = \begin{cases} y_i & \text{if } x \in \mathscr{D} \\ 0 & \text{otherwise} \end{cases} \quad \Rightarrow \quad \hat{\mathscr{R}}_n = 0$$

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- The “i.i.d.” assumption might not always hold. (Sampling bias, distribution shift, etc.)

- Under this assumption, $\hat{\mathcal{R}}_n$ is a random function.

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Define the notion of population risk of a predictor $f : \mathcal{X} \to \mathcal{Y}$:

$$\mathscr{R}(f) = \mathbb{E}\left[\ell(y, f(x))\right]$$

Also known as the generalisation or test error.

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$\mathscr{R}$ is a deterministic function of the predictor f

Validation set

In practice, the statistician almost never has access to the data distribution.

A common procedure to estimate $\mathscr{R}$ consists of splitting the training data in training and validation set $\mathscr{D} = \mathscr{D}_{\mathrm{T}} \cup \mathscr{D}_{\mathrm{V}}$.

Train on $\mathscr{D}_{\mathrm{T}}$, test on $\mathscr{D}_{\mathrm{V}}$.

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To reduce error, often one repeats this procedure k times, averaging over the result. This is known as k fold cross-validation.

Conditional risk

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$$= \mathbb{E}_{X\sim p_x}\left[\mathbb{E}[\mathscr{l}(Y, f(x)) \,|\, X = x]\right]$$

The internal expectation is over the conditional distribution $Y \,|\, X = x$

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Where we have defined:

$$r(z \mid x) = \mathbb{E}[\mathscr{l}(Y, z) \mid X = x]$$

"Conditional risk"

Bayes risk

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$$f_\star(x) \in \operatorname*{argmin}_{z \in \mathcal{Y}} r(z \mid x)$$

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- The Bayes predictor $f_\star$ might not be unique.
- Typically we have $\mathscr{R}_\star \neq 0$.

 Examples in the TD

Learning algorithm

Let $\mathscr{D}_p = \{(x_i, y_i) \in \mathscr{X} \times \mathscr{Y} : i = 1, \ldots, n\}$ denote training data sampled i.i.d. from p.

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You have seen many examples in *"Statistical Learning I"*:

- K-nearest neighbours
- Decision trees
- Random Forests
- Least-squares regression

No free lunch

Consider a binary classification task with $\mathcal{Y} = \{0,1\}$ and 0/1 loss $\ell(y,z) = \delta_{yz}$. Let $\mathcal{P}$ denote the set of probability distributions over $\mathcal{X} \times \{0,1\}$.

Theorem

For any $n \in \mathbb{N}$ and algorithm $\mathcal{A}$ over $(\mathcal{X} \times \{0,1\})^{\otimes n}$, there exists $p \in \mathcal{P}$ such that

$$\sup_{p \in \mathcal{P}} \left\{ \mathbb{E}\left[\mathcal{R}(\mathcal{A}(\mathcal{D}_p)) \right] - \mathcal{R}_\star \right\} \geq \frac{1}{2}$$

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In words: For any algorithm you choose, one can always construct a data distribution such that your error is at best equal than random guessing.

Empirical risk minimisation

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Empirical risk minimisation (ERM) is a class of learning algorithms that consist of minimising the empirical risk:

$$\min_f \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i)) \quad (= \hat{\mathscr{R}}_n(f))$$

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By the law of large numbers, for a given f

$$\hat{\mathscr{R}}_n(f) \xrightarrow{P} \mathscr{R}(f) \qquad \text{as} \qquad n \to \infty$$

However, at fixed n, $\hat{\mathscr{R}}_n$ can be very different from $\mathscr{R}$

Empirical risk minimisation

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ERM maps supervised learning to an optimisation problem.

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But optimising on the space of functions is computationally intractable....

Empirical risk minimisation

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i)) \quad (= \hat{\mathcal{R}}_n(f))$$

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But optimising on the space of functions is computationally intractable....

Therefore, we restrict to classes of mathematically and computationally amenable functions:

$$f \in \mathcal{H}$$

Also known as the hypothesis class.

Hypothesis class

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The choice of hypothesis (or architecture) induces an inductive bias in the learning.

e.g. linear functions can only learn linear relationships

Risk decomposition

For any $\theta \in \Theta$, we can decompose the excess risk:

$$\mathscr{R}(\theta) - \mathscr{R}_\star = \left(\mathscr{R}(\theta) - \inf_{\theta' \in \Theta} \mathscr{R}(\theta') \right) + \left(\inf_{\theta' \in \Theta} \mathscr{R}(\theta') - \mathscr{R}_\star \right)$$

Estimation error

Approximation error

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- Approximation error $\inf_{\theta' \in \Theta} \mathscr{R}(\theta') - \mathscr{R}_\star$
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  - Deterministic
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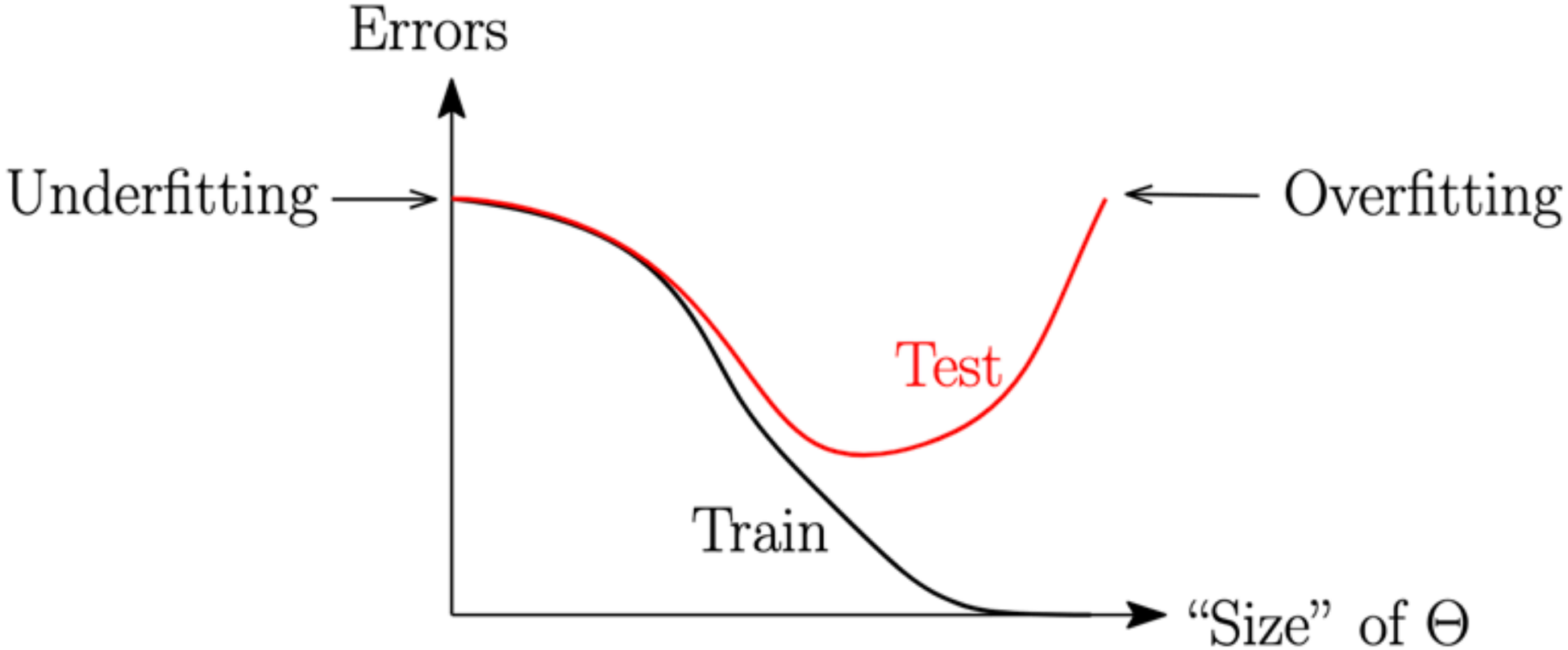

Figure from "Learning Theory from First Principles", F. Bach 2024

Summary of ERM

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- What properties of the data distribution p makes the problem easier / harder?