Supervised learning and Decision Theory

MATH-412 - Statistical Machine Learning

Supervised learning

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- A prediction task consists in predicting the y' associated to a new x'.
- A more general task consists in making a decision that would be determined from (x', y') except it needs to be made from x' alone.

Formalizing supervised learning

We will assume that we have some **training data**

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$\rightarrow$ Need to define what we expect from that decision function.

Decision theory

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Abraham Wald (1939)

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- $\mathcal{X}$ input data space
- $\mathcal{Y}$ output data space
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Produce a decision function such that given a new input x the action $f(x)$ is a "good" action when confronted to the unseen corresponding output y.

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Loss function

$$\begin{array}{rccc} \ell : & \mathcal{A} \times \mathcal{Y} & \to & \mathbb{R} \\ & (a, y) & \mapsto & \ell(a, y) \end{array}$$

measures the cost incurred when action a is taken and y has occurred.

Generalization and expected behavior

Eventually, we need to design a learning algorithm that produces a predictor or decision function $\widehat{f}$.

$$\begin{array}{rccc} \mathscr{A}: & \bigcup_{n\in\mathcal{N}} (\mathcal{X}\times\mathcal{Y})^n & \to & \mathcal{A}^{\mathcal{X}} \\ & D_n & \mapsto & \widehat{f} \end{array}$$

Goal ? Minimize worst future loss *vs* average future loss ?

- Given x there might be some intrinsic uncertainty about y.

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- by a stationary stochastic process, or more simply, and in the rest of this course :
- as independent and identically distributed random variables (X_i, Y_i)

Formalizing the goal of learning as minimizing the risk

Risk

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Conditional risk

The conditional risk is the expected loss conditionally on the input data value, viewed as a function of the action taken.

$$\mathcal{R}(a \,|\, x) = \mathbb{E}[\ell(a, Y) \mid X = x] \quad = \quad \int \ell(a, y)\, dP_{Y|X}(y|x)$$

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if $\inf_{a\in\mathcal{A}} \mathcal{R}(a \,|\, x)$ is attained and unique for almost all x then we can define

$$f^*(x) = \text{arg}\min_{a\in\mathcal{A}} \mathcal{R}(a \,|\, x)$$

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Excess risk

$$\mathcal{E}(f) = \mathcal{R}(f) - \mathcal{R}(f^*) = \mathbb{E}\big[\ell(f(X), Y) - \ell(f^*(X), Y)\big]$$

Examples of the decision theoretic framework of Wald

Example 1 : ordinary least squares regression

Case where $\mathcal{A} = \mathcal{Y} = \mathbb{R}$.

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$$\mathcal{R}(f(X)|X) = \mathcal{R}(\tilde{f}(X)|X) + (\tilde{f}(X) - f(X))^2 \qquad \text{with} \quad \mathcal{R}(\tilde{f}(X)|X) = \mathrm{Var}(Y|X)$$

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So $\boxed{f^* = \tilde{f}}$

Ordinary least squares regression : summary

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- mean square risk :

$$\begin{aligned} \mathcal{R}(f) &= \mathbb{E}\big[(f(X) - Y)^2\big] \\ &= \mathbb{E}\big[(f(X) - \mathbb{E}[Y|X])^2\big] + \mathbb{E}\big[(Y - \mathbb{E}[Y|X])^2\big] \\ &= \mathbb{E}\big[(f(X) - f^*(X))^2\big] + \mathcal{R}(f^*) \\ \text{with} \quad \mathcal{R}(f^*) &= \mathbb{E}\big[(Y - \mathbb{E}[Y|X])^2\big] = \mathbb{E}\big[\,\mathrm{Var}(Y|X)\,\big]. \end{aligned}$$

- target function :

$$f^*(X) = \mathbb{E}[Y|X]$$

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So $\min_a \mathcal{R}(a \mid X = x)$ is equivalent to

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$$\boxed{f^*(x) \; = \; \operatorname{arg} \max_{1 \leq k \leq K} \mathbb{P}(Y = k \mid X = x)}$$

f^* simply predicts the most probable value of Y given X.

Classification : summary

Case where $\mathcal{A} = \mathcal{Y} = \{0, \ldots, K-1\}$.

- 0-1 loss :

$$\ell(a, y) = 1_{\{a \neq y\}}$$

- the risk is the misclassification error

$$\mathcal{R}(f) = \mathbb{P}(f(X) \neq Y)$$

- the target function is the assignment to the most likely class

$$f^*(X) = \text{argmax}_{1 \leq k \leq K} \mathbb{P}(Y = k | X)$$

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- No unique target function. No simple expression.

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Given $X = (X_1, \ldots, X_m) \in \mathcal{X}$ predict $Y = (Y_1, \ldots, Y_m)$.

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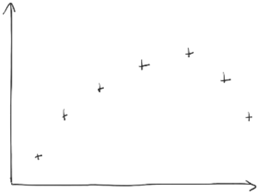

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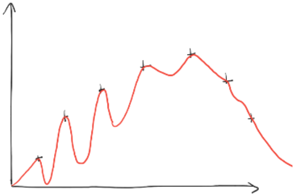

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It is necessary to add an *inductive bias* by restricting the **hypothesis space**, using **regularization** or using a **Bayesian prior**.

Hypothesis space

For both computational and statistical reasons, it is necessary
to to restrict the set of predictors or the set of hypotheses considered.
Given a hypothesis space $S \subset \mathcal{Y}^{\mathcal{X}}$ considered, the constrained ERM problem is of the form :

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- linear functions
- polynomial functions
- spline functions
- multiresolution approximation spaces (wavelet)
- functions defined by Mercer kernels
- neural network with a given architecture