

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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→ Need to define what we expect from that decision function.

Decision theory

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Abraham Wald (1939)

Decision theoretic framework

- \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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- $f(x)$ is the action that has the smallest possible cost when y occurs.

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Loss function

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

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 \hat{f} .

$$\begin{array}{ccc} \mathcal{A} : & \bigcup_{n \in \mathcal{N}} (\mathcal{X} \times \mathcal{Y})^n & \rightarrow \mathcal{A}^{\mathcal{X}} \\ & D_n & \mapsto \hat{f} \end{array}$$

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

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

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If there *exists* a *unique* function f^* such that $\mathcal{R}(f^*) = \inf_{f \in \mathcal{A}^X} \mathcal{R}(f)$, then f^* is called the *target function*, *oracle function* or *Bayes predictor*.

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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.

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

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

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Excess risk

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

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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What could be the target function ?

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

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

Ordinary least squares regression : summary

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- square loss :

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- mean square risk :

$$\begin{aligned}\mathcal{R}(f) &= \mathbb{E}[(f(X) - Y)^2] \\ &= \mathbb{E}[(f(X) - \mathbb{E}[Y|X])^2] + \mathbb{E}[(Y - \mathbb{E}[Y|X])^2] \\ &= \mathbb{E}[(f(X) - f^*(X))^2] + \mathcal{R}(f^*)\end{aligned}$$

$$\text{with } \mathcal{R}(f^*) = \mathbb{E}[(Y - \mathbb{E}[Y|X])^2] = \mathbb{E}[\text{Var}(Y|X)].$$

- target function :

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

Example 2 : classification

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

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$$\max_{a \in \mathcal{A}} \mathbb{P}(a = Y \mid X = x) = \max_{a \in \mathcal{A}} \mathbb{P}(Y = a \mid X = x)$$

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

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

Classification : summary

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

- 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

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

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- output variable : $Y \in \mathcal{Y} = \{-1, 1\}$
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- predictor $(X, X') \mapsto (f(X), f(X'))$

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Assume that given a pair of random variables $(X, X') \in \mathcal{X}^2$, a preference variable $Y \in \{-1, 1\}$ is defined.

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- No unique target function. No simple expression.

Example 4 : sequence decoding (OCR)

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

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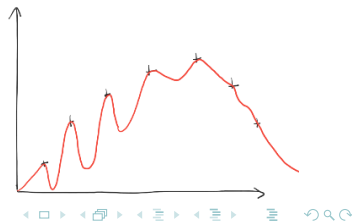
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It is necessary to add an *inductive bias* by restricting the **hypothesis space**, using **regularization** or using a **Bayesian prior**.

Hypothesis space

For both computational and statistical reasons, it is necessary to 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