

Statistical Learning

Jordi Villà i Freixa

Universitat de Vic - Universitat Central de Catalunya
Study Abroad

jordi.villa@uvic.cat

course 2023-2024

1 Introduction

2 Bibliography

Preliminary note

The material in these slides is strongly based on [1]. When other materials are used, they are cited accordingly.

Mathematical notation follows as good as it can a [good practices proposal](<https://ctan.math.utah.edu/ctan/tex-archive/macros/latex/contrib/mlmath/mlmath.pdf>) from the Beijing Academy of Artificial Intelligence.

How is data analyzed and used?

Statistical learning interpret the model and quantify the uncertainty of the data.

Machine learning (or *data mining* making predictions using large scale data.

The goals of modelling data are:

- to predict data, based on existing one;
- to discover unusual or interesting patterns in data.

Tools to model data

Function approximation Model data with approximate and simple functions or maps.

Optimization Given a set of feasible mathematical models to the data, we may need to find the optimal one by fitting or calibrating a function to observed data.

Probability and Statistics Probability theory and statistical inference provides ways to quantify the uncertainty inherent in making predictions based on observed data.

Some basic notation I

Given an input or *feature* vector \mathbf{x} , ML aims at predicting an output or *response* variable vector \mathbf{y} . In particular, we search for a mathematical *prediction function* g such that we can *guess* an approximation to \mathbf{y} , $\hat{\mathbf{y}}$:

$$\begin{aligned} g: \mathcal{X} &\rightarrow \mathcal{Y} \\ \mathbf{x} &\mapsto \hat{\mathbf{y}} = g(\mathbf{x}) \end{aligned}$$

Definition

Dataset $S = \{\mathbf{z}_i\}_{i=1}^n = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ is sampled from a distribution \mathcal{D} over a domain $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$.

\mathcal{X} is the instance domain (a set), \mathcal{Y} is the label domain (a set), and $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ is the example domain (a set).

Some basic notation II

Usually, \mathcal{X} is a subset of \mathbb{R}^d and \mathcal{Y} is a subset of \mathbb{R}^{d_o} , where d is the input dimension, d_o is the output dimension.

$n = \#S$ is the number of samples. Without specification, S and n are for the training set.

- In *regression* problems, \mathbf{y} is a vector of real values.
- In *classification* problems, \mathbf{y} values lie within a finite set of c categories: $y \in \{0, 1, \dots, c - 1\}$.

Definition

A hypothesis space is denoted by \mathcal{H} . A hypothesis function is denoted by $f_{\theta}(\mathbf{x}) \in \mathcal{H}$ or $f(\mathbf{x}; \theta) \in \mathcal{H}$ with $f_{\theta} : \mathcal{X} \rightarrow \mathcal{Y}$.

θ denotes the set of parameters of f_{θ} .

If there exists a target function, it is denoted by f^* or $f : \mathcal{X} \rightarrow \mathcal{Y}$ satisfying $\mathbf{y}_i = f^*(\mathbf{x}_i)$ for $i = 1, \dots, n$.

Some basic notation III

A loss function, denoted by $\ell : \mathcal{H} \times \mathcal{Z} \rightarrow \mathbb{R}_+ := [0, +\infty)$, measures the difference (or error) between a predicted label and a true label, e.g., L^2 loss:

$$\ell(f_\theta, \mathbf{z}) = \frac{1}{2}(f_\theta(\mathbf{x}) - \mathbf{y})^2,$$

where $\mathbf{z} = (\mathbf{x}, \mathbf{y})$. $\ell(f_\theta, \mathbf{z})$ can also be written as

$$\ell(f_\theta(\mathbf{x}), \mathbf{y})$$

for convenience.

(In the case of a classification, $\ell(f_\theta, \mathbf{y}) = \mathbb{1}\{y \neq \hat{\mathbf{y}}\}$)

We will see other useful loss functions (cross entropy) or *hinge* loss functions) later in this course.

It is unlikely that a mathematical function $g \equiv f_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ would be able to make accurate predictions of all possible pairs $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$.

Some basic notation IV

So, we use a probabilistic approach here to empirical risk or training loss for a set $S = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ is denoted by $L_S(\boldsymbol{\theta})$ or $L_n(\boldsymbol{\theta})$ or $R_n(\boldsymbol{\theta})$ or $R_S(\boldsymbol{\theta})$,

$$L_S(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n \ell(f_{\boldsymbol{\theta}}(\mathbf{x}_i), \mathbf{y}_i). \quad (1)$$

The population risk or expected loss is denoted by $L_{\mathcal{D}}(\boldsymbol{\theta})$ or $R_{\mathcal{D}}(\boldsymbol{\theta})$

$$L_{\mathcal{D}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathcal{D}} \ell(f_{\boldsymbol{\theta}}(\mathbf{z}), \mathbf{y}), \quad (2)$$

where $\mathbf{z} = (\mathbf{x}, \mathbf{y})$ follows the distribution \mathcal{D} .

(In the case of a classification, we denote $L_{\mathcal{D}}(g) \equiv L_{\mathcal{D}}(\boldsymbol{\theta}) = \mathbb{P}_{\mathcal{D}}[f_{\boldsymbol{\theta}}(\mathbf{x}) \neq \mathbf{y}]$ and we say that g is a classifier.)

Because we are interested in minimizing the risk in our prediction, we are looking for the best possible $g^* := \operatorname{argmin}_g \mathbb{E}_{\mathcal{D}} \ell(f_{\boldsymbol{\theta}}(\mathbf{x}), \mathbf{y})$

Some basic notation V

(In classification, we look for $g^*(\mathbf{x}) = \underset{y \in \{0,1,\dots,c-1\}}{\operatorname{argmax}} \mathbb{P}[Y = y | X = \mathbf{x}]$.)

Theorem

For the squared-error loss $\ell(y, \hat{y}) = (y - \hat{y})^2$, the optimal prediction function g^ is equal to the conditional expectation of Y given $\mathbf{X} = \mathbf{x}$.*

which leads to write the random response Y as:

$$Y = g^*(\mathbf{x}) + \varepsilon(\mathbf{x})$$

Note that such random deviation satisfies $\mathbb{E}\varepsilon(\mathbf{x}) = 0$



Dirk P. Kroese, Zdravko Botev, Thomas Taimre, and Radislav Vaisman.

Data Science and Machine Learning: Mathematical and Statistical Methods.

Machine Learning & Pattern Recognition. Chapman & Hall/CRC, 2020.