# Machine Learning

## Module 3.0 - Models: Introduction

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# Context

In ML, models are mainly used for **supervised learning**, the aim is

- Predict a response $y$: regression if numerical, classification if categorical.
- From features $x = \{x_1, \ldots, x_p\}$: available at the moment of prediction,
- With the best possible quality: built from the data in an optimal way.

The $n$ observed features and responses are denoted

$$(y_1, x_1), \ldots, (y_n, x_n).$$

# Elements

In ML, a model consists mainly of three elements:

- A prediction formula, taking the features $x$, returning a prediction $\hat{y} = f(x)$ for $y$,
- A loss function $\mathcal{L}(y, \hat{y})$ measuring how "wrong" a prediction $\hat{y}$ is for $y$.
- An algorithm which can optimize the prediction formula $f$ using the observed data.

# The prediction formula

The prediction formula is a mathematical formula (sometimes a more complex algorithm) using **parameters**[1] $\theta$, combining them with the feature $x$, returning a prediction

$$f(x;\theta).$$

Thus, $\theta$ must be chosen carefully to obtain good predictions of $y$.

[1] Also called **weights**, especially for Neural Networks.

# The loss function

The loss function indicates how wrong is a prediction $\hat{y}$ of the corresponding $y$.

A classical example for regression is the square of the error:

$$\mathcal{L}(y, \hat{y}) = (y - \hat{y})^2.$$

The larger $\mathcal{L}(y, \hat{y})$, the further $\hat{y}$ is from $y$.

# The optimal parameters

Good parameters $\theta$ must have a low loss. We want $\mathcal{L}(y, f(x;\theta))$ to be small for all $(y, x)$. To achieve an overall quality on the whole available data base, we want $\theta$ achieving a small

$$\bar{\mathcal{L}}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}\{y_i, f(x_i;\theta)\}.$$

Example: with the square of the error, this is

$$\bar{\mathcal{L}}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \{y_i, f(x_i;\theta)\}^2.$$

# The optimization algorithm

Finding the optimal $\hat{\theta}$ is done by applying an algorithm, i.e., a procedure that finds

$$\hat{\theta} = \arg\max_{\theta} \bar{\mathcal{L}}(\theta).$$

The algorithm is often a sequential procedure. It builds a sequence $\theta_1, \theta_2, \theta_3, \ldots$ such that

$$\bar{\mathcal{L}}(\theta_1) > \bar{\mathcal{L}}(\theta_2) > \bar{\mathcal{L}}(\theta_3) > \ldots$$

Ultimately, this should reach the minimum possible $\bar{\mathcal{L}}(\theta)$.

# Mathematical considerations

- More flexible model $f$ provides better opportunity to minimize $\bar{\mathcal{L}}$. Often, this is associated with the size of $\theta$ (number of parameters).
- The algorithm may not reach the global minimum of $\bar{\mathcal{L}}$. Most algorithms cannot guaranty such results except under theoretical assumptions.
- A probabilistic interpretation: the optimal $\theta$ is obtained by minimizing the expected loss on the population of $(Y, X)$

$$E\left[\mathcal{L}\{Y, f(X;\theta)\}\right].$$

The data base is used to estimate it with an empirical mean

$$\hat{E}\left[\mathcal{L}\{Y, f(X;\theta)\}\right] = \frac{1}{n}\sum_{i=1}^{n}\mathcal{L}\{y_i, f(x_i;\theta)\}.$$

This estimate is minimized in turn to find an estimate of the optimal $\theta$.