Introduction to Machine Learning

Introduction: Models & Parameters

compstat-lmu.github.io/lecture_i2ml

WHAT IS A MODEL?

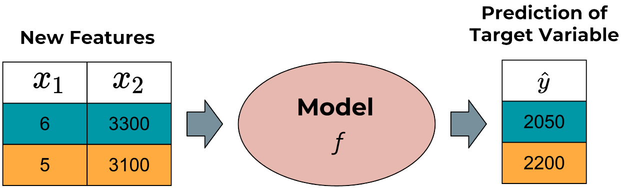
- A **model** (or **hypothesis**)

$$f : \mathcal{X} \to \mathbb{R}^g$$

  is a function that maps feature vectors to predicted target values.
- f is meant to capture intrinsic patterns of the data, the underlying assumption being that these patterns hold true for *all* data drawn from $\mathbb{P}_{xy}$.
- Loosely speaking: if f is fed a set of features, it will output the target corresponding to these feature values under our hypothesis.

In conventional regression we will have $g = 1$; for classification g equals the number of classes, and output vectors are scores or class probabilities (details later).

WHAT IS A MODEL?



- It is easily conceivable how models can range from super simple (e.g., tree stumps) to reasonably complex (e.g., variational autoencoders), and how there is an infinite number of them.
- In fact, machine learning requires **constraining** f to a certain type of functions.

HYPOTHESIS SPACES

- Without restrictions on the functional family, the task of finding a "good" model among all the available ones is impossible to solve.
- This means: we have to determine the class of our model *a priori*, thereby narrowing down our options considerably.
- The set of functions defining a specific model class is called a **hypothesis space** $\mathcal{H}$:

$$\mathcal{H} = \{f : f \text{ belongs to a certain functional family}\}$$

HYPOTHESIS SPACES

- **Example 1:** Hypothesis space of univariate linear functions

$$\mathcal{H} = \{f : f(\mathbf{x}) = \boldsymbol{\theta}^T\mathbf{x} = \theta_0 + \theta_1 x, \boldsymbol{\theta} \in \mathbb{R}^2\}$$

FIGURE

HYPOTHESIS SPACES

- **Example 2:** Hypothesis space of bivariate quadratic functions

$$\mathcal{H} = \{f : f(\mathbf{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2, \boldsymbol{\theta} \in \mathbb{R}^6\}$$

FIGURE

HYPOTHESIS SPACES

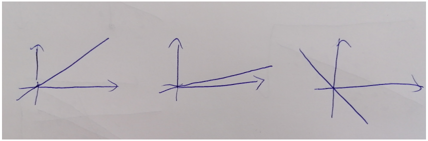
- **Example 3:** Hypothesis space of radial basis function networks

$$\mathcal{H} = \{f : f(\mathbf{x}) = ...\}$$

FIGURE

PARAMETERS OF A MODEL

- Considering the above examples, we see that all models within a hypothesis space share a common functional structure.
- In fact, the only aspect in which they differ is the values of **parameters**.
  $\rightarrow$ They are our means of configuration: once set, our model is fully determined.
- Revisiting the space of linear functions, tweaking θ_0 and θ_1 is what hands us arbitrary straight lines.



PARAMETERS OF A MODEL

- This means: finding the optimal model is perfectly equivalent to finding the optimal set of parameter values.
- We usually subsume all parameters in **parameter vector** $\boldsymbol{\theta} = (\theta_1, \theta_2, ...)$ from **parameter space** Θ.
- The bijective relation between optimization over $f \in \mathcal{H}$ and optimization over $\boldsymbol{\theta} \in \Theta$ allows us to operationalize our search for the best model via the search for the optimal value on a p-dimensional parameter surface.
- $\boldsymbol{\theta}$ might be scalar or comprise thousands of parameters, depending on the complexity of our model.

PARAMETERS, STATISTICS AND SUPERVISED ML

- Statistics, too, studies how to learn functions (or, rather: their parameters) from example data and how to perform inference on them and interpret the results.
- For historical reasons, though, statistics is mostly focused on fairly simple classes of mappings, like (generalized) linear models.
- Supervised ML also includes more complex kinds of mappings that can typically deal with more complicated and high-dimensional inputs.