Introduction to Machine Learning

Introduction: Models & Parameters

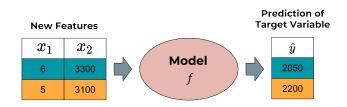
WHAT IS A MODEL?

A model (or hypothesis)

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

is a function that maps feature vectors to predicted target values.

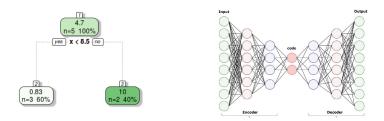
 Loosely speaking: if f is fed a set of features, it will output the target corresponding to these feature values under our hypothesis.



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?

- f is meant to capture intrinsic patterns of the data, the underlying assumption being that these hold true for all data drawn from \mathbb{P}_{xy} .
- 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 H:

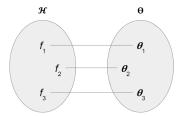
 $\mathcal{H} = \{f : f \text{ belongs to a certain functional family}\}$

PARAMETERS OF A MODEL

- All models within one hypothesis space share a common functional structure.
- In fact, the only aspect in which they differ is the values of parameters.
- We usually subsume all these parameters in a parameter vector $\theta = (\theta_1, \theta_2, ...)$ from a parameter space Θ .
- They are our means of configuration: once set, our model is fully determined.

PARAMETERS OF A MODEL

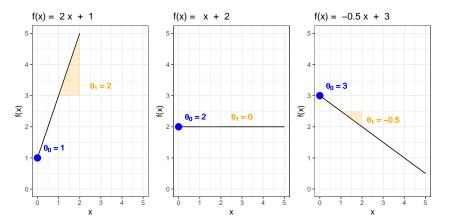
- This means: finding the optimal model is perfectly equivalent to finding the optimal set of parameter values.
- The bijective relation between optimization over $f \in \mathcal{H}$ and optimization over $\theta \in \Theta$ allows us to operationalize our search for the best model via the search for the optimal value on a p-dimensional parameter surface.



 $m{ heta}$ might be scalar or comprise thousands of parameters, depending on the complexity of our model.

Example 1: Hypothesis space of univariate linear functions

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



Example 2: Hypothesis space of bivariate quadratic functions

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

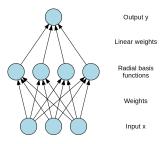
Example 3: Hypothesis space of radial basis function networks with Gaussian basis functions

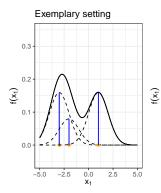
$$\mathcal{H} = \left\{ f : f(\mathbf{x}) = \sum_{i=1}^{n} a_{i} \rho(\|\mathbf{x} - \mathbf{c}_{i}\|) \right\},\,$$

where

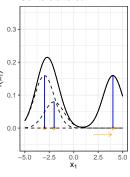
- a_i is the weight of the *i*-th neuron,
- c_i its center vector, and
- $\rho(\|\mathbf{x} \mathbf{c}_i\|) = \exp(-\beta \|\mathbf{x} \mathbf{c}_i\|^2)$ is the *i*-th radial basis function with bandwidth $\beta \in \mathbb{R}$.

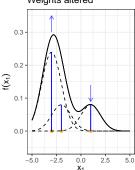
Usually, the number of centers, n, and the bandwidth β need to be set in advance (so-called *hyperparameters*).





Centers altered





$$a_1 = 0.4$$

 $a_2 = 0.2$
 $a_3 = 0.4$

$$c_1 = -3$$
 $c_2 = -2$
 $c_3 = 1$

$$a_1 = 0.4 a_2 = 0.2 a_1 = 0.4$$

•
$$c_1 = -3$$

 $c_2 = -2$
 $c_3 = 4$

$$a_1 = 0.6$$

 $a_2 = 0.2$
 $a_3 = 0.2$

•
$$c_1 = -3$$

 $c_2 = -2$
 $c_3 = 1$