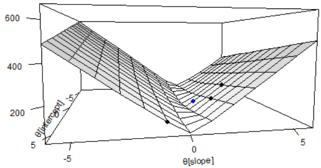
Introduction to Machine Learning

ML-Basics: Losses & Risk Minimization



Learning goals

- Know the concept of loss
- Understand the relationship between loss and risk
- Understand the relationship between risk minimization and finding the best model

HOW TO EVALUATE MODELS

- When training a learner, we optimize over our hypothesis space, to find the function which matches our training data best.
- This means, we are looking for a function, where the predicted output per training point is as close as possible to the observed label.

Features x		Target y		Prediction $\hat{y}$
People in Office (Feature 1) x_1	Salary (Feature 2) x_2	Worked Minutes Week (Target Variable)		Worked Minutes Week (Target Variable)
4	4300 €	2220	$\stackrel{?}{\approx}$	2588
12	2700 €	1800		1644
5	3100 €	1920		1870

$\mathcal{D}_{\text{train}}$

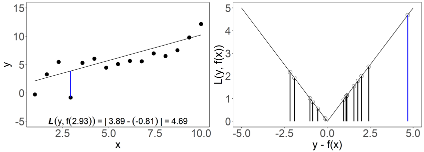
- To make this precise, we need to define now how we measure the difference between a prediction and a ground truth label pointwise.

LOSS

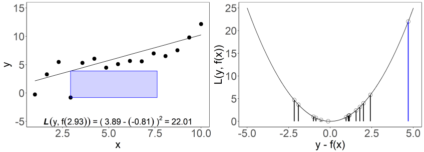
The **loss function** $L(y, f(\mathbf{x}))$ quantifies the "quality" of the prediction $f(\mathbf{x})$ of a single observation $\mathbf{x}$:

$$L : \mathcal{Y} \times \mathbb{R}^g \to \mathbb{R}.$$

In regression, we could use the absolute loss $L(y, f(\mathbf{x})) = |f(\mathbf{x}) - y|$;



or the L2-loss $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$:



RISK OF A MODEL

- The (theoretical) **risk** associated with a certain hypothesis $f(\mathbf{x})$ measured by a loss function $L(y, f(\mathbf{x}))$ is the **expected loss**

$$\mathcal{R}(f) := \mathbb{E}_{xy}[L(y, f(\mathbf{x}))] = \int L(y, f(\mathbf{x}))\, d\mathbb{P}_{xy}.$$

- This is the average error we incur when we use f on data from $\mathbb{P}_{xy}$.
- Goal in ML: Find a hypothesis $f(\mathbf{x}) \in \mathcal{H}$ that **minimizes** risk.

RISK OF A MODEL

Problem: Minimizing $\mathcal{R}(f)$ over f is not feasible:

- $\mathbb{P}_{xy}$ is unknown (otherwise we could use it to construct optimal predictions).
- We could estimate $\mathbb{P}_{xy}$ in non-parametric fashion from the data $\mathcal{D}$, e.g., by kernel density estimation, but this really does not scale to higher dimensions (see "curse of dimensionality").
- We can efficiently estimate $\mathbb{P}_{xy}$, if we place rigorous assumptions on its distributional form, and methods like discriminant analysis work exactly this way.

But as we have n i.i.d. data points from $\mathbb{P}_{xy}$ available we can simply approximate the expected risk by computing it on $\mathcal{D}$.

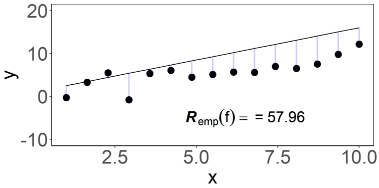
EMPIRICAL RISK

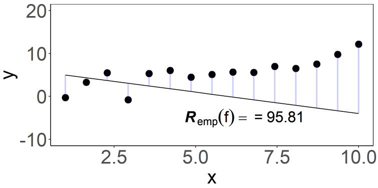
To evaluate, how well a given function f matches our training data, we now simply sum-up all f's pointwise losses.

$$\mathcal{R}_{\text{emp}}(f) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

This gives rise to the **empirical risk function** which allows us to associate one quality score with each of our models, which encodes how well our model fits our training data.

$$\mathcal{R}_{\text{emp}} : \mathcal{H} \rightarrow \mathbb{R}$$





EMPIRICAL RISK

- The risk can also be defined as an average loss

$$\bar{\mathcal{R}}_{\text{emp}}(f) = \frac{1}{n}\sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right).$$

  The factor $\frac{1}{n}$ does not make a difference in optimization, so we will consider $\mathcal{R}_{\text{emp}}(f)$ most of the time.

- Since f is usually defined by **parameters $\boldsymbol{\theta}$**, this becomes:

$$\mathcal{R} : \mathbb{R}^d \to \mathbb{R}$$

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)$$

EMPIRICAL RISK MINIMIZATION

The best model is the model with the smallest risk.

If we have a finite number of models f, we could simply tabulate them and select the best.

Model	$\boldsymbol{\theta}_{intercept}$	$\boldsymbol{\theta}_{slope}$	$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$
f_1	2	3	194.62
f_2	3	2	127.12
f_3	6	-1	95.81
f_4	1	1.5	57.96

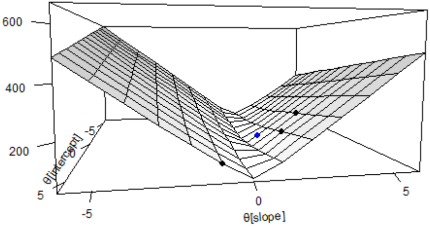
EMPIRICAL RISK MINIMIZATION

But usually $\mathcal{H}$ is infinitely large.

Instead we can consider the risk surface w.r.t. the parameters $\boldsymbol{\theta}$.
(By this I simply mean the visualization of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$)

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) : \mathbb{R}^d \to \mathbb{R}.$$

Model	$\boldsymbol{\theta}_{intercept}$	$\boldsymbol{\theta}_{slope}$	$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$
f_1	2	3	194.62
f_2	3	2	127.12
f_3	6	-1	95.81
f_4	1	1.5	57.96



EMPIRICAL RISK MINIMIZATION

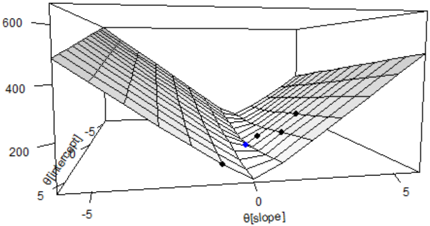
Minimizing this surface is called **empirical risk minimization** (ERM).

$$\hat{\theta} = \arg\min_{\boldsymbol{\theta} \in \Theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}).$$

Usually we do this by numerical optimization.

$$\mathcal{R} : \mathbb{R}^d \to \mathbb{R}.$$

Model	$\boldsymbol{\theta}_{intercept}$	$\boldsymbol{\theta}_{slope}$	$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$
f_1	2	3	194.62
f_2	3	2	127.12
f_3	6	-1	95.81
f_4	1	1.5	57.96
f_5	1.25	0.90	23.40



In a certain sense, we have now reduced the problem of learning to **numerical parameter optimization**.