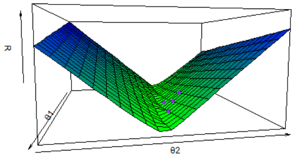
Introduction to Machine Learning

Introduction: 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

- In the training, we want to optimize $\boldsymbol{\theta}$. To score $\boldsymbol{\theta}$, we have to compare the actual output with the predicted output:

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	$\overset{?}{\approx}$	2588
12	2700 €	1800		1644
5	3100 €	1920		1870

$\underbrace{\text{Features } x \;\; \text{Target } y}_{\mathcal{D}_{\text{train}}}$

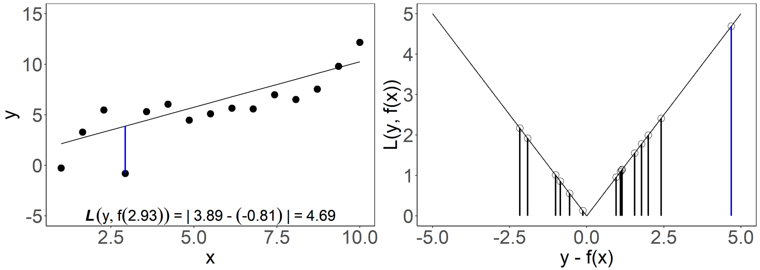
- We need to define a suitable criterion, e.g.:
  - Absolute error $|2588 - 2220| = 368$
  - Squared error: $(2588 - 2220)^2 = 135,424$
- The choice of this metric has a major influence on the final model, as it determines what a *good* model is.
- It will determine the ranking of the different models $f \in \mathcal{H}$.
- The metric we use is called the **loss function**.

LOSS

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

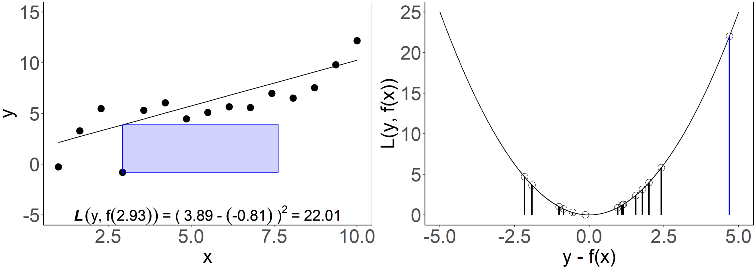
$$L : \mathcal{Y} \times \mathbb{R}^g \to \mathbb{R}.$$

How "close" $f(\mathbf{x})$ is to y can be quantified e. g. by the absolute loss $L(y, f(\mathbf{x})) = |f(\mathbf{x}) - y|$.



LOSS

Often, we use the L2-loss $L\left(y, f(\mathbf{x})\right) = (y - f(\mathbf{x}))^2$:



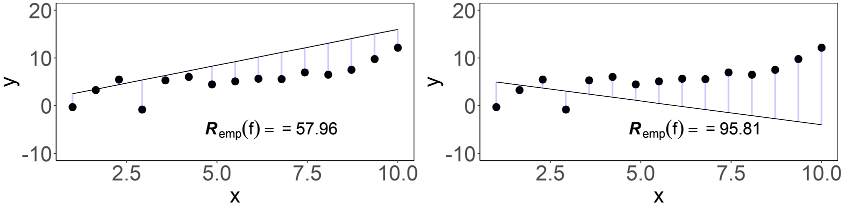
RISK

The **risk function** quantifies the "quality" of the whole model.

The ability of a model f to reproduce the association between $\mathbf{x}$ and y that is present in the data $\mathcal{D}$ can be measured by the **summed loss**, also called **"empirical risk"**:

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

$$\mathcal{R} : \mathcal{H} \to \mathbb{R}.$$



RISK

Notes:

- The risk is often denoted as empirical mean over $L(y, f(\mathbf{x}))$

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

  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 the model f is usually defined by **parameters** $\boldsymbol{\theta}$ in a parameter space Θ, this becomes:

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

$$\begin{aligned} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) \\ \hat{\boldsymbol{\theta}} &= \arg\min_{\boldsymbol{\theta} \in \Theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) \end{aligned}$$

RISK MINIMIZATION

The best model is the model with the smallest risk.

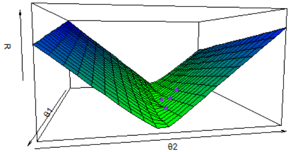
If we have a finite number of models f, we can compare the risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ of all models:

Model	$\boldsymbol{\theta}_{intercept}$	$\boldsymbol{\theta}_{slope}$	$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$
f_1	2.00	3.00	194.62
f_2	3.00	2.00	127.12
f_3	6.00	-1.00	95.81
f_4	1.00	1.50	57.96

RISK MINIMIZATION

But: Normally, the hypothesis space $\mathcal{H}$ is infinitely large.

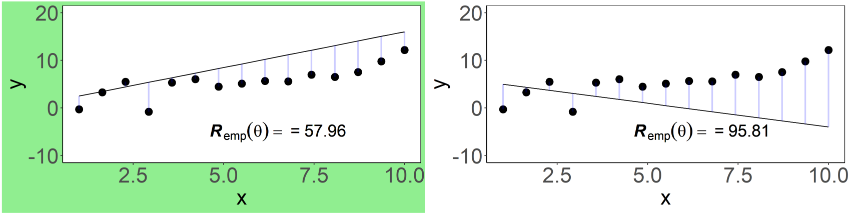
As the the mapping of the hypothesis space to its parameters is bijective, we can consider the error surface depending on the parameters:



RISK MINIMIZATION

The process of finding the best model is called **empirical risk minimization** (ERM).

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



Most learners in ML try to solve the above *optimization problem*, which implies a tight connection between ML and optimization.

FURTHER REMARKS

- For regression tasks, the loss often only depends on the residual $L(y, f(\mathbf{x})) = L(y - f(\mathbf{x})) = L(\epsilon)$.
- The choice of loss implies which kinds of errors are important or not – requires *domain knowledge*!
- For learners that correspond to probabilistic models, the loss determines / is equivalent to distributional assumptions.
- Since learning can be re-phrased as minimizing the loss, the choice of loss strongly affects the computational difficulty of learning:
  - How smooth is $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ in $\boldsymbol{\theta}$?
  - Is $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ differentiable so that we can use gradient-based methods?
  - Does $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ have multiple local minima or saddlepoints over Θ?