

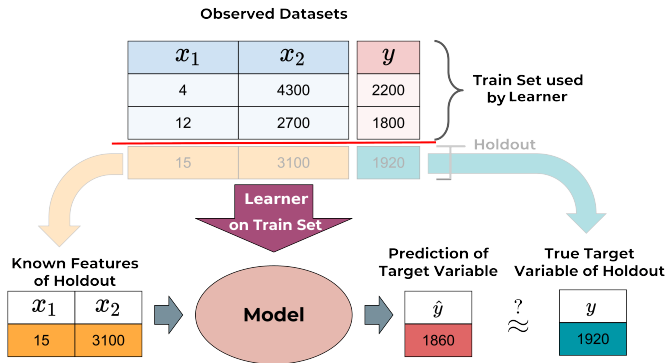
# **Introduction to Machine Learning**

## **Introduction: Losses & Risk Minimization**

[compstat-lmu.github.io/lecture\\_i2ml](https://compstat-lmu.github.io/lecture_i2ml)

# HOW TO EVALUATE MODELS

Compare predictions from a model with observed target values:



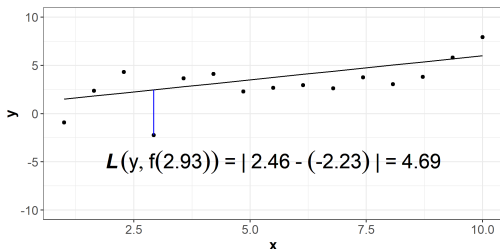
# MOTIVATION

- Assume we trained a model to predict flat rent based on some features (size, location, age, ...).
- The real rent of a flat is EUR 1600, our model predicts EUR 1300.
- How do we measure the performance of our model?
- Need to define a suitable criterion, e.g.:
  - Absolute error  $|1600 - 1300| = 300$
  - Squared error:  $(1600 - 1300)^2 = 90000$   
(puts more emphasis on predictions that are far off the mark)
- The choice of this metric has a major influence on the final model, because it determines what constitutes a *good* model: 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  $\mathbf{x}$ .

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

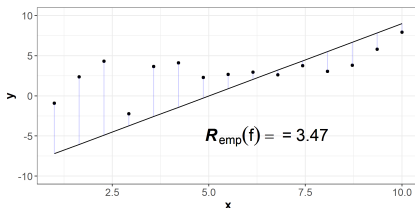
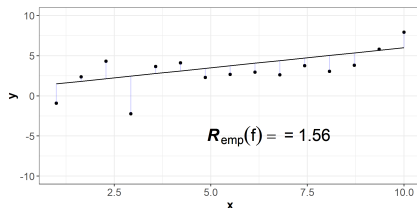


# RISK

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 **average loss**, also called "**empirical risk**":

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



????

The best model is the model with the smallest risk.

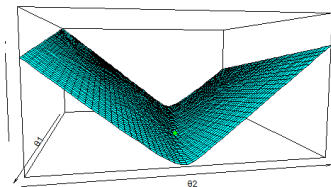
If we have a finite number of models  $f$ , we can compare the risk  $\mathcal{R}_{\text{emp}}(f)$  of all models:

| Model | $\theta_1$ | $\theta_2$ | $\mathcal{R}_{\text{emp}}(f)$ |
|-------|------------|------------|-------------------------------|
| $f_1$ | 10         | 10.0       | 61.92                         |
| $f_2$ | 2          | 0.5        | 1.95                          |
| $f_3$ | 4          | 1.0        | 6.42                          |
| $f_4$ | 3          | 2.0        | 10.92                         |
| $f_5$ | 1          | 0.5        | 1.56                          |

# ???

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

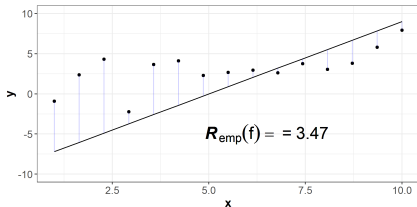
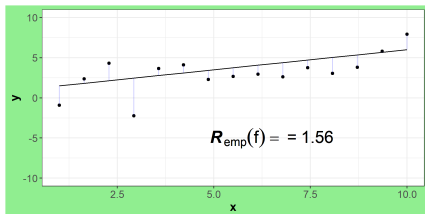
As the the mapping of the hypothesis space to its parameters is bijective, we can consider the error surface depending on the parameters:



# RISK MINIMIZATION

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

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





# RISK MINIMIZATION

Since the model  $f$  is usually defined by **parameters**  $\theta$  in a parameter space  $\Theta$ , this becomes:

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

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  $\mathcal{R}_{\text{emp}}(\theta)$  in  $\theta$ ?
  - Is  $\mathcal{R}_{\text{emp}}(\theta)$  differentiable so that we can use gradient-based methods?
  - Does  $\mathcal{R}_{\text{emp}}(\theta)$  have multiple local minima or saddlepoints over  $\Theta$ ?