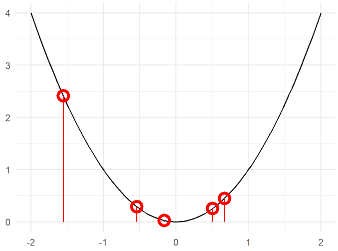
Introduction to Machine Learning

Advanced Risk Minimization
Regression Losses: L2 and L1 loss



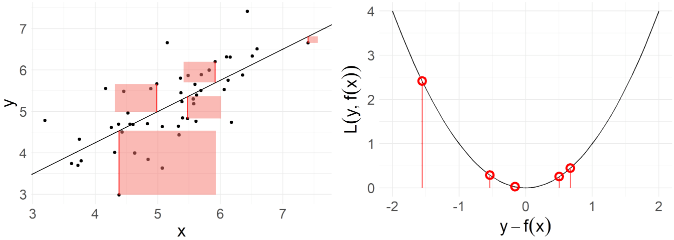
Learning goals

- Derive the risk minimizer of the L2-loss
- Derive the optimal constant model for the L2-loss
- Know risk minimizer and optimal constant model for L1-loss

L2-LOSS

$$L(y, f) = (y - f)^2 \quad \text{or} \quad L(y, f) = 0.5\,(y - f)^2$$

- Tries to reduce large residuals (if residual is twice as large, loss is 4 times as large), hence outliers in y can become problematic
- Analytic properties: convex, differentiable $\Rightarrow$ gradient no problem in loss minimization
  (**Warning**: $\mathcal{R}_{\text{emp}}(f)$ can still be non-smooth/non-convex due to $f(\mathbf{x})$)



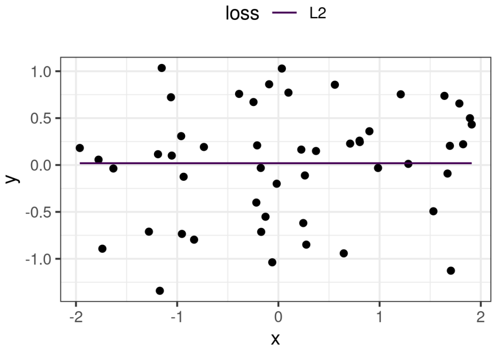
L2-LOSS: OPTIMAL CONSTANT MODEL

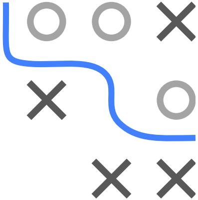
Let us consider the (true) risk for $\mathcal{Y} = \mathbb{R}$ and $L2$-Loss $L(y, f) = (y - f)^2$ with $\mathcal{H}$ restricted to constants. The optimal constant model f_c^* in terms of the theoretical risk is the expected value over y:

$$
\begin{aligned}
f_c^* &= \arg\min_{c \in \mathbb{R}} \mathbb{E}_{xy}\left[(y - c)^2\right] = \arg\min_{c \in \mathbb{R}} \mathbb{E}_y\left[(y - c)^2\right] \\
&= \arg\min_{c \in \mathbb{R}} \underbrace{\mathbb{E}_y\left[(y - c)^2\right] - (\mathbb{E}_y[y] - c)^2}_{= \mathrm{Var}_y[y - c] = \mathrm{Var}_y[y]} + (\mathbb{E}_y[y] - c)^2 \\
&= \arg\min_{c \in \mathbb{R}} \mathrm{Var}_y[y] + (\mathbb{E}_y[y] - c)^2 \\
&= \mathbb{E}_y[y]
\end{aligned}
$$

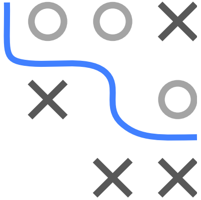
L2-LOSS: OPTIMAL CONSTANT MODEL / 2

The optimizer $\hat{f}_c$ of the empirical risk is $\bar{y}$ (the empirical mean over $y^{(i)}$), which is the empirical estimate for $\mathbb{E}_y[y]$.





L2-LOSS: OPTIMAL CONSTANT MODEL / 3



Proof:

For the optimal constant model f_c^* for the L2-loss $L(y, f) = (y - f)^2$ we solve the optimization problem

$$\operatorname*{arg\,min}_{f \in \mathcal{H}} \mathcal{R}_{\text{emp}}(f) = \operatorname*{arg\,min}_{\theta \in \mathbb{R}} \sum_{i=1}^{n} (y^{(i)} - \theta)^2.$$

We calculate the first derivative of $\mathcal{R}_{\text{emp}}$ w.r.t. θ and set it to 0:

$$\begin{aligned}
\frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \theta} = -2 \sum_{i=1}^{n} \left(y^{(i)} - \theta \right) &\overset{!}{=} 0 \\
\sum_{i=1}^{n} y^{(i)} - n\theta &= 0 \\
\hat{\theta} &= \frac{1}{n} \sum_{i=1}^{n} y^{(i)} =: \bar{y}.
\end{aligned}$$

L2-LOSS: RISK MINIMIZER

Let us consider the (true) risk for $\mathcal{Y} = \mathbb{R}$ and the $L2$-Loss $L(y, f) = (y - f)^2$ with unrestricted $\mathcal{H} = \{f : \mathcal{X} \to \mathbb{R}^g\}$.

- By the law of total expectation

$$\begin{aligned}
\mathcal{R}_L(f) &= \mathbb{E}_{xy}\left[L\left(y, f(\mathbf{x})\right)\right] = \mathbb{E}_x\left[\mathbb{E}_{y|x}\left[L\left(y, f(\mathbf{x})\right) \mid \mathbf{x} = \mathbf{x}\right]\right] \\
&= \mathbb{E}_x\left[\mathbb{E}_{y|x}\left[(y - f(\mathbf{x}))^2 \mid \mathbf{x} = \mathbf{x}\right]\right].
\end{aligned}$$

- Since $\mathcal{H}$ is unrestricted, at any point $\mathbf{x} = \mathbf{x}$, we can predict any value c we want. The best point-wise prediction is the cond. mean

$$f^*(\mathbf{x}) = \arg\min_c \mathbb{E}_{y|x}\left[(y - c)^2 \mid \mathbf{x} = \mathbf{x}\right] \overset{(*)}{=} \mathbb{E}_{y|x}\left[y \mid \mathbf{x}\right].$$

$^{(*)}$ follows from the drivation of f_c^*

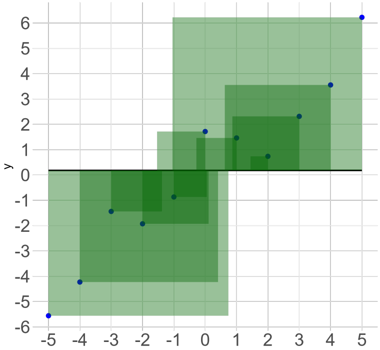
L2 LOSS MEANS MINIMIZING VARIANCE

Rethinking what we did in the opt. constant model: We optimized for a constant whose squared distance to all data points is minimal (in sum, or on average). This turned out to be the mean.

What if we calculate the loss of $\hat{\theta} = \bar{y}$? That's $\mathcal{R}_{\text{emp}} = \sum_{i=1}^{n} (y^{(i)} - \bar{y})^2$.

Average this by $\frac{1}{n}$ or $\frac{1}{n-1}$ to obtain variance.

Optimal constant model gives "unscaled" variance



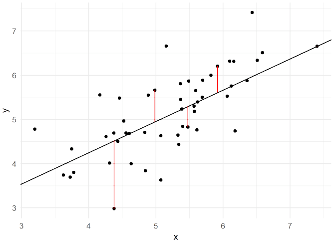
- Generally, if model yields unbiased predictions, $\mathbb{E}_{y \mid \mathbf{x}} [y - f(\mathbf{x}) \mid \mathbf{x}] = 0$, using $L2$-loss means minimizing variance of model residuals
- Same holds for the pointwise construction / conditional distribution considered before

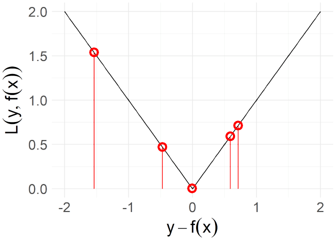
L1-LOSS

The L1 loss is defined as

$$L(y, f) = |y - f|$$

- More robust than $L2$, outliers in y are less problematic.
- Analytical properties: convex, not differentiable for $y = f(\mathbf{x})$ (optimization becomes harder).





L1-LOSS: RISK MINIMIZER

We calculate the (true) risk for the $L1$-Loss $L(y, f) = |y - f|$ with unrestricted $\mathcal{H} = \{f : \mathcal{X} \to \mathcal{Y}\}$.

- We use the law of total expectation

$$\mathcal{R}(f) = \mathbb{E}_x \left[\mathbb{E}_{y|x} \left[|y - f(\mathbf{x})| \mid \mathbf{x} = \mathbf{x} \right] \right].$$

- As the functional form of f is not restricted, we can just optimize point-wise at any point $\mathbf{x} = \mathbf{x}$. The best prediction at $\mathbf{x} = \mathbf{x}$ is then

$$f^*(\mathbf{x}) = \arg\min_c \mathbb{E}_{y|x} \left[|y - c| \right] = \text{med}_{y|x} \left[y \mid \mathbf{x} \right].$$

L1-LOSS: OPTIMAL CONSTANT MODEL

The optimal constant model in terms of the theoretical risk for the L1 loss is the median over y:

$$f_c^* \quad = \quad \text{med}_{y|x}\left[y \mid \mathbf{x}\right] \overset{\text{drop } \mathbf{x}}{=} \text{med}_y\left[y\right]$$

The optimizer $\hat{f}_c$ of the empirical risk is $\text{med}(y^{(i)})$ over $y^{(i)}$, which is the empirical estimate for $\text{med}_y\left[y\right]$.