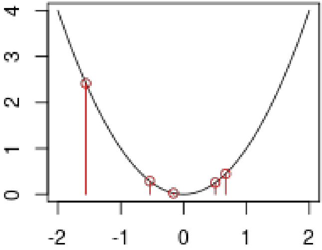
Introduction to Machine Learning

Regression Losses: L2-loss



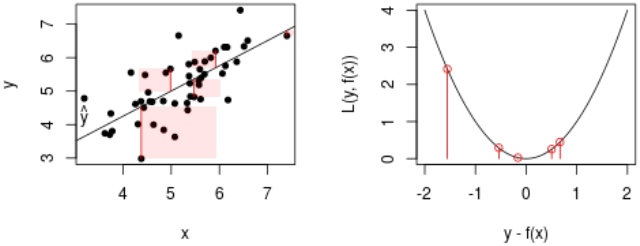
Learning goals

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

L2-LOSS

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

- 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 (gradient no problem in loss minimization)
- Residuals = Pseudo-residuals: $\tilde{r} = -\frac{\partial 0.5(y - f(\mathbf{x}))^2}{\partial f(\mathbf{x})} = y - f(\mathbf{x}) = r$



L2-LOSS: RISK MINIMIZER

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

- By the law of total expectation

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

- Since $\mathcal{H}$ is unrestricted we can choose f as we wish: At any point $\mathbf{x} = \mathbf{x}$ we can predict any value c we want. The best point-wise prediction is the conditional mean

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

L2-LOSS: RISK MINIMIZER

$^{(*)}$ follows from:

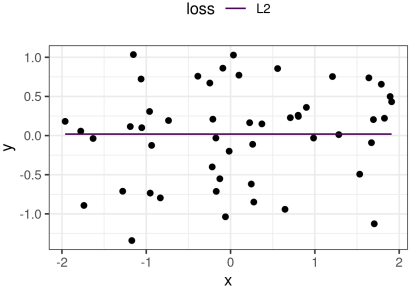
$$\begin{aligned} & \text{argmin}_c \mathbb{E}\left[(y-c)^2\right] = \text{argmin}_c \underbrace{\mathbb{E}\left[(y-c)^2\right] - (\mathbb{E}[y]-c)^2}_{=\text{Var}[y-c]=\text{Var}[y]} + (\mathbb{E}[y]-c)^2 \\ = \quad & \text{argmin}_c \text{Var}[y] + (\mathbb{E}[y]-c)^2 = \mathbb{E}[y]. \end{aligned}$$

L2-LOSS: OPTIMAL CONSTANT MODEL

The optimal constant model in terms of the (theoretical) risk for the L2 loss is the expected value over y:

$$f(\mathbf{x}) \quad = \quad \mathbb{E}_{y \mid \mathbf{x}}\left[y \mid \mathbf{x}\right] \overset{\text{drop } \mathbf{x}}{=} \mathbb{E}_{y}\left[y\right]$$

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



L2-LOSS: OPTIMAL CONSTANT MODEL

Proof:

For the optimal constant model $f(\mathbf{x}) = \boldsymbol{\theta}$ for the L2-loss $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ we solve the optimization problem

$$\operatorname*{arg\,min}_{f \in \mathcal{H}} \mathcal{R}_{\text{emp}}(f).$$

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

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