Introduction to Machine Learning

Maximum Likelihood Estimation vs. Empirical Risk Minimization

Distribution of Residuals
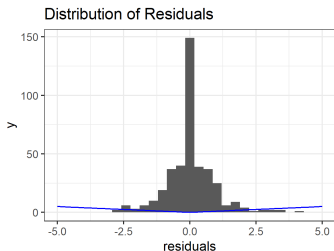
Learning goals

- Learn the correspondence between a Laplacian error distribution and the L1 loss

- Learn that there is no error distribution for the Huber loss

- Learn the correspondence between Bernoulli-distributed targets and the Bernoulli loss

LAPLACE ERRORS - L1-LOSS

Let us assume that errors are Laplacian, i.e. ϵ follows a Laplace distribution which has the density

$$\frac{1}{2\sigma} \exp\left(-\frac{|x|}{\sigma}\right), \sigma > 0.$$

Then

$$y = f_{\text{true}}(\mathbf{x}) + \epsilon$$

follows a Laplace distribution with mean $f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)$ and scale parameter σ.

LAPLACE ERRORS - L1-LOSS

The likelihood is then

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\theta}) &= \prod_{i=1}^{n} p\left(y^{(i)} \,\middle|\, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right), \sigma \right) \\
&\propto \exp\left(-\frac{1}{\sigma} \sum_{i=1}^{n} \left| y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right) \right| \right).
\end{aligned}
$$

The negative log-likelihood is

$$
-\ell(\boldsymbol{\theta}) \propto -\sum_{i=1}^{n} \left| y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right) \right|.
$$

Minimizing the negative log-likelihood for Laplacian error terms corresponds to empirical risk minimization with L1-loss.

LAPLACE ERRORS - L1-LOSS

- We simulate data $y \mid \mathbf{x} \sim \text{Laplacian}\left(f_{\text{true}}(\mathbf{x}), 1\right)$ with $f_{\text{true}} = 0.2 \cdot \mathbf{x}$.
- We can plot the empirical error distribution, i.e. the distribution of the residuals after fitting a regression model w.r.t. L1-loss.
- With the help of a Q-Q-plot we can compare the empirical residuals vs. the theoretical quantiles of a Laplacian distribution.
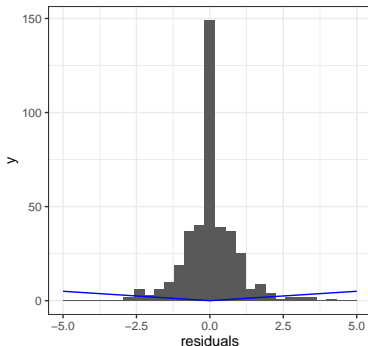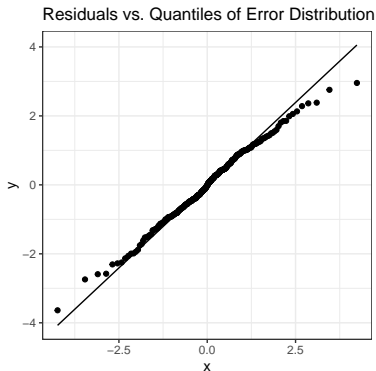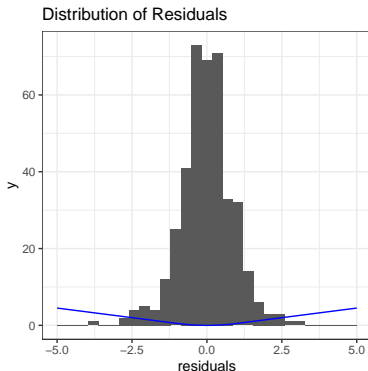

Distribution of Residuals | Residuals vs. Quantiles of Error Distribution
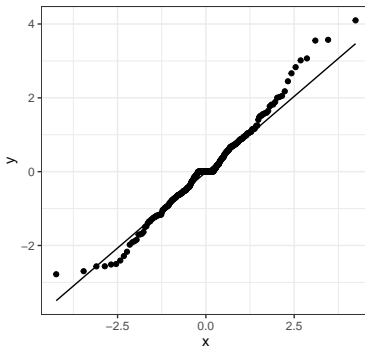
OTHER ERROR DISTRIBUTIONS

- There are losses that do not correspond to "real" error densities, like the Huber loss. (In the QQ-plot below we show residuals against quantiles of a normal.)

Distribution of Residuals

Residuals vs. Quantiles of Error Distribution

MAXIMUM LIKELIHOOD IN CLASSIFICATION

Let us assume the outputs y to be Bernoulli-distributed, i.e.

$$y \mid \mathbf{x} \sim \text{Ber}(\pi_{\text{true}}(\mathbf{x})).$$

The negative log likelihood is

$$
\begin{aligned}
-\ell(\boldsymbol{\theta}) &= -\sum_{i=1}^{n} \log p\left(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}\right) \\
&= -\sum_{i=1}^{n} \log \left[\pi\left(\mathbf{x}^{(i)}\right)^{y^{(i)}} \cdot \left(1 - \pi\left(\mathbf{x}^{(i)}\right)\right)^{\left(1 - y^{(i)}\right)} \right] \\
&= \sum_{i=1}^{n} -y^{(i)} \log[\pi\left(\mathbf{x}^{(i)}\right)] - \left(1 - y^{(i)}\right) \log[1 - \pi\left(\mathbf{x}^{(i)}\right)].
\end{aligned}
$$

MAXIMUM LIKELIHOOD IN CLASSIFICATION

This gives rise to the following loss function

$$L(y, \pi(\mathbf{x})) = -y \log(\pi(\mathbf{x})) - (1 - y) \log(1 - \pi(\mathbf{x})), \quad y \in \{0, 1\}$$

which we introduced as **Bernoulli** loss.