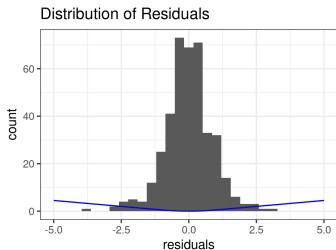


Introduction to Machine Learning

Maximum Likelihood Estimation vs. Empirical Risk Minimization



Learning goals

- Understand the connection between maximum likelihood and risk minimization
- Learn the correspondence of between a Gaussian error distribution and the L2 loss

MAXIMUM LIKELIHOOD

Let us approach regression from a maximum likelihood perspective. In the following we assume that

$$y \mid \mathbf{x} \sim p(y \mid \mathbf{x}, \boldsymbol{\theta}),$$

For example, we commonly consider a true underlying relationship f_{true} with additive noise:

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

where f_{true} is a function that is parameterized by $\boldsymbol{\theta}$ and ϵ being a RV that follows some distribution \mathbb{P}_{ϵ} , with $\mathbb{E}[\epsilon] = 0$. Further, we assume ϵ to be independent of \mathbf{x} .

MAXIMUM LIKELIHOOD

From a statistics / maximum-likelihood perspective, we assume (or we pretend) we know the underlying distribution $p(y \mid \mathbf{x}, \theta)$.

- Then, given data

$$\mathcal{D} = \left(\left(\mathbf{x}^{(1)}, y^{(1)} \right), \dots, \left(\mathbf{x}^{(n)}, y^{(n)} \right) \right)$$

the maximum-likelihood principle is to maximize the **likelihood**

$$\mathcal{L}(\theta) = \prod_{i=1}^n p \left(y^{(i)} \mid \mathbf{x}^{(i)}, \theta \right)$$

or to minimize the **negative log-likelihood**

$$-\ell(\theta) = - \sum_{i=1}^n \log p \left(y^{(i)} \mid \mathbf{x}^{(i)}, \theta \right).$$

MAXIMUM LIKELIHOOD

Let us take a machine learning perspective and assume our hypothesis space corresponds to the space of the (parameterized) f_{true} .

- Let us now simply define the negative log-likelihood as **loss function**

$$L(y, f(\mathbf{x} \mid \theta)) := -\log p(y \mid \mathbf{x}, \theta)$$

- Maximum-likelihood optimization can be formulated as an empirical risk minimization problem

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

- We can even disregard multiplicative or additive constants in the loss as they do not change the minimizer.

MAXIMUM LIKELIHOOD

- For every error distribution \mathbb{P}_ϵ we can derive an equivalent loss function, which leads to the same point estimator for the parameter vector θ as maximum-likelihood.
- **NB:** The other way around does not always work: We cannot derive a probability density function or error distribution corresponding to every loss function – the Hinge loss is a prominent example.

GAUSSIAN ERRORS - L2-LOSS

Let us assume $y = f_{\text{true}}(\mathbf{x}) + \epsilon$ with additive Gaussian errors are Gaussian, i.e. $\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$. Then

$$y \mid \mathbf{x} \sim N(f_{\text{true}}(\mathbf{x}), \sigma^2) .$$

The likelihood is then

$$\begin{aligned} \mathcal{L}(\theta) &= \prod_{i=1}^n p\left(y^{(i)} \mid f\left(\mathbf{x}^{(i)} \mid \theta\right), \sigma^2\right) \\ &\propto \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \theta\right)\right)^2\right) . \end{aligned}$$

GAUSSIAN ERRORS - L2-LOSS

It is easy to see that minimizing the negative log-likelihood is equivalent to the L_2 -loss minimization approach since

$$\begin{aligned} -\ell(\boldsymbol{\theta}) &= -\log(\mathcal{L}(\boldsymbol{\theta})) \\ &= -\log\left(\exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^n\left(y^{(i)} - f(\mathbf{x}^{(i)} | \boldsymbol{\theta})\right)^2\right)\right) \\ &\propto \sum_{i=1}^n\left(y^{(i)} - f(\mathbf{x}^{(i)} | \boldsymbol{\theta})\right)^2. \end{aligned}$$

Note: We use \propto as “proportional to ... up to multiplicative and additive constants”.

GAUSSIAN ERRORS - L2-LOSS

- We simulate data $y \mid \mathbf{x} \sim \mathcal{N}(f_{\text{true}}(\mathbf{x}), 1)$ 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. L_2 -loss.
- With the help of a Q-Q-plot we can compare the empirical residuals vs. the theoretical quantiles of a Gaussian distribution.

