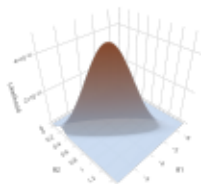


MAXIMUM LIKELIHOOD / 2

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

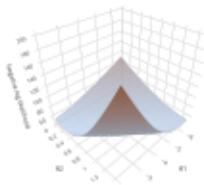
- Then, given i.i.d data $\mathcal{D} = ((\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)}))$ from \mathbb{P}_{xy} the maximum-likelihood principle is to maximize the **likelihood**

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



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

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



MAXIMUM LIKELIHOOD / 3

From an ML perspective we assume our hypothesis space corresponds to the space of the (parameterized) f_{true} .

- Simply define neg. log-likelihood as **loss function**

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

- Then, maximum-likelihood = ERM

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

- NB: When we are only interested in the minimizer, we can ignore multiplicative or additive constants.
- We use \propto as “proportional up to multiplicative and additive constants”



GAUSSIAN ERRORS - L2-LOSS / 2

Easy to see: minimizing neg. log-likelihood with Gaussian errors is the same as ERM with L_2 -loss:

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

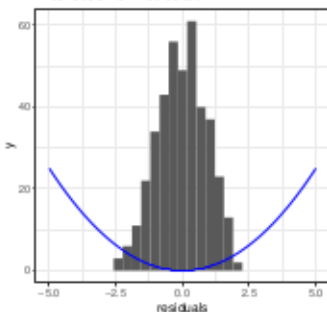


GAUSSIAN ERRORS - L2-LOSS / 3

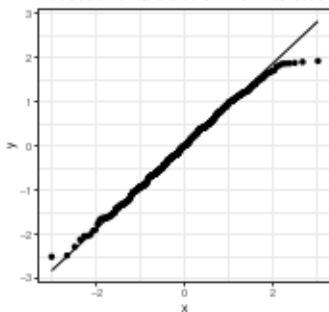
- We simulate data $y | \mathbf{x} \sim \mathcal{N}(f_{\text{true}}(\mathbf{x}), 1)$ with $f_{\text{true}} = 0.2 \cdot \mathbf{x}$
- Let's plot empirical errors as histogram, after fitting our model with L_2 -loss
- Q-Q-plot compares empirical residuals vs. theoretical quantiles of Gaussian



Distribution of Residuals



Residuals vs. Quantiles of Error Distribution



DISTRIBUTIONS AND LOSSES / 2

When does the reverse direction hold?

- If we can write the loss as $L(y, f(\mathbf{x})) = L(y - f(\mathbf{x})) = L(r)$ for $r \in \mathbb{R}$, then minimizing $L(y - f(\mathbf{x}))$ is equivalent to maximizing a conditional log-likelihood $\log(p(y - f(\mathbf{x}|\theta)))$ if
 - $\log(p(r))$ is affine trafo of L (undoing the \propto):

$$\log(p(r)) = a - bL(r), \quad a \in \mathbb{R}, b > 0$$

- p is a pdf (non-negative and integrates to one)

Thus, a loss L corresponds to MLE under *some* distribution if there exist $a \in \mathbb{R}$, $b > 0$ such that

$$\int_{\mathbb{R}} \exp(a - bL(r)) dr = 1$$

