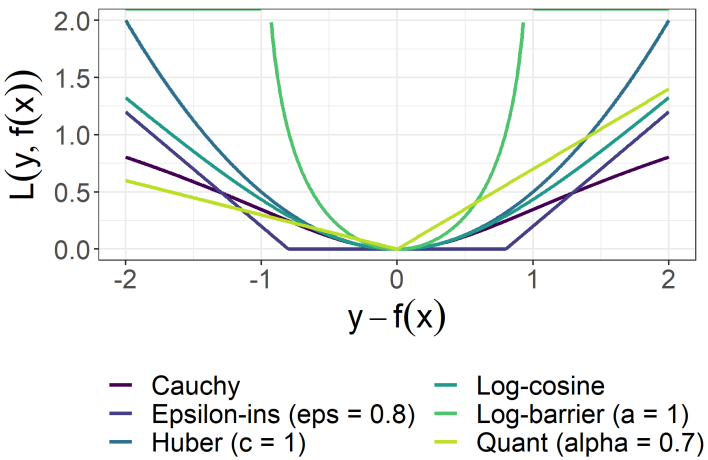
Introduction to Machine Learning

Advanced Regression Losses



Learning goals

- Know the Huber loss
- Know the log-barrier loss
- Know the ϵ-insensitive loss
- Know the quantile loss
- Know the Cauchy loss
- Know the log-cosh loss

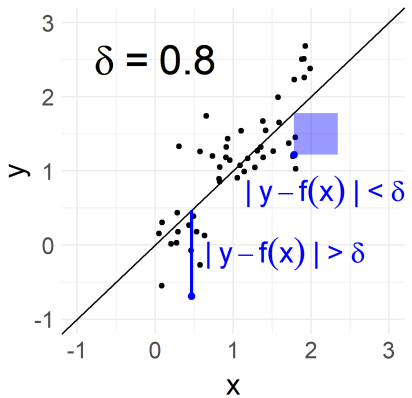
ADVANCED LOSS FUNCTIONS

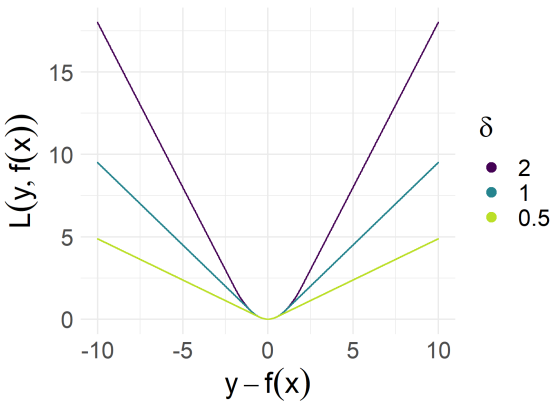
- Advanced loss functions are designed to achieve special properties (e.g., robustness and smoothness for the Huber or Cauchy loss).
- Furthermore, special loss functions are necessary in certain applications.
- Examples:
  - Quantile loss: Overestimating a clinical parameter might not be as bad as underestimating it.
  - Log-barrier loss: Extremely under- or overestimating demand in production would put company profit at risk.
  - ϵ-insensitive loss: A certain amount of deviation in production does no harm, larger deviations do.
- Sometimes a custom loss must be designed specifically for the given application.
- Some learning algorithms use specific loss functions, e.g., the hinge loss for SVMs.

HUBER LOSS

$$L(y, f(\mathbf{x})) = \begin{cases} \frac{1}{2}(y - f(\mathbf{x}))^2 & \text{if } |y - f(\mathbf{x})| \leq \delta \\ \delta |y - f(\mathbf{x})| - \frac{1}{2}\delta^2 & \text{otherwise} \end{cases}, \quad \delta > 0$$

- Piece-wise combination of $L1/L2$ to have robustness/smoothness
- Analytic properties: convex, differentiable, robust





- Risk minimizer and optimal constant do not have a closed-form solution. To fit a model numerical optimization is necessary.
- The solution is a **trimmed mean**: a (conditional) mean between two (conditional) quantiles.

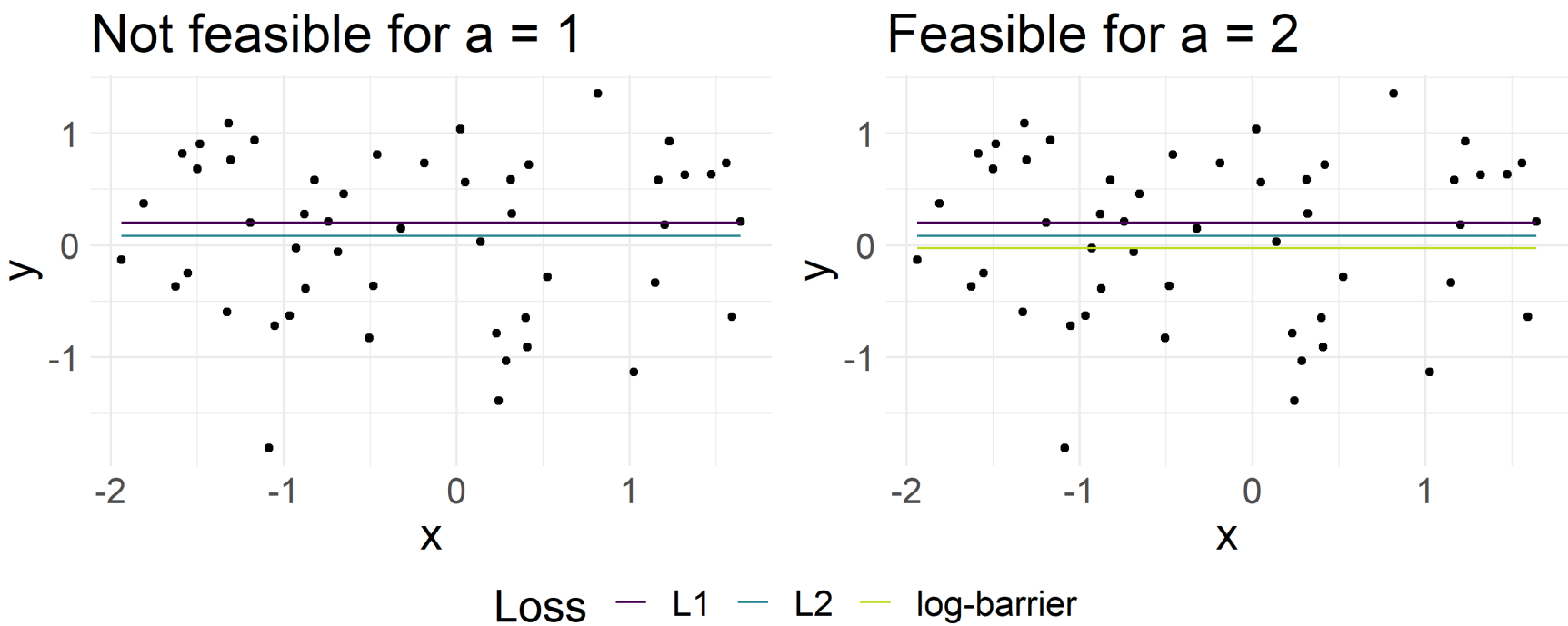
LOG-BARRIER LOSS

$$L(y, f(\mathbf{x})) = \begin{cases} -a^2 \cdot \log\left(1 - \left(\frac{|y - f(\mathbf{x})|}{a}\right)^2\right) & \text{if } |y - f(\mathbf{x})| \leq a \\ \infty & \text{if } |y - f(\mathbf{x})| > a \end{cases}$$

- Behaves like *L2* loss for small residuals.
- We use this if we don't want residuals larger than a at all.
- No guarantee that the risk minimization problem has a solution.
- Plot shows log-barrier loss for $a = 2$:

LOG-BARRIER: OPTIMAL CONSTANT MODEL

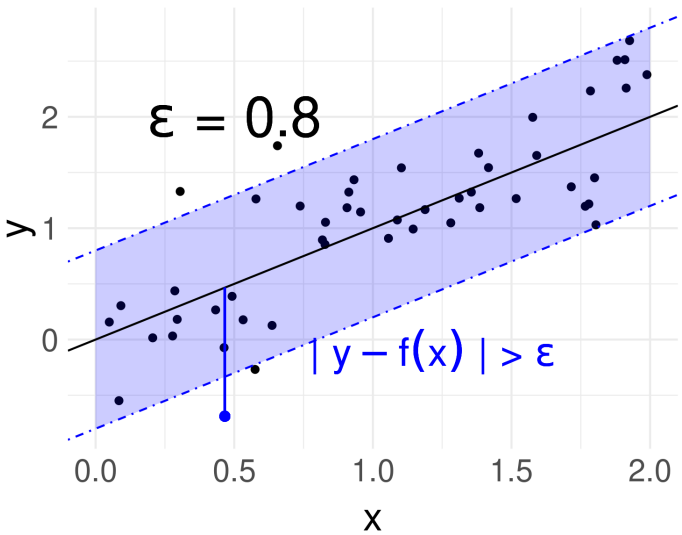
- Similarly to the Huber loss, there is no closed-form solution for the optimal constant model $f(\mathbf{x}) = \theta$ w.r.t. the log-barrier loss. Numerical optimization is necessary.
- Note that the optimization problem has no (finite) solution if there is no way to fit a constant where all residuals are smaller than a.

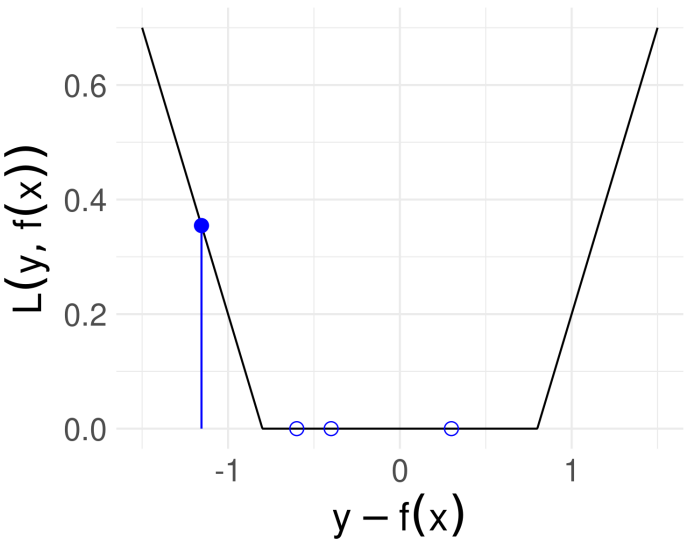


ϵ-INSENSITIVE LOSS

$$L(y, f(\mathbf{x})) = \begin{cases} 0 & \text{if } |y - f(\mathbf{x})| \leq \epsilon \\ |y - f(\mathbf{x})| - \epsilon & \text{otherwise} \end{cases}, \quad \epsilon \in \mathbb{R}_+$$

- Modification of $L1$ loss, errors below ϵ accepted without penalty.
- Properties: convex and not differentiable for $y - f(\mathbf{x}) \in \{-\epsilon, \epsilon\}$.





ϵ-INSENSITIVE LOSS: OPTIMAL CONSTANT

What is the optimal constant model $f(\mathbf{x}) = \theta$ w.r.t. the ϵ-insensitive loss $L(y, f(\mathbf{x})) = |y - f(\mathbf{x})| \, \mathbb{1}_{\{|y-f(\mathbf{x})|>\epsilon\}}$?

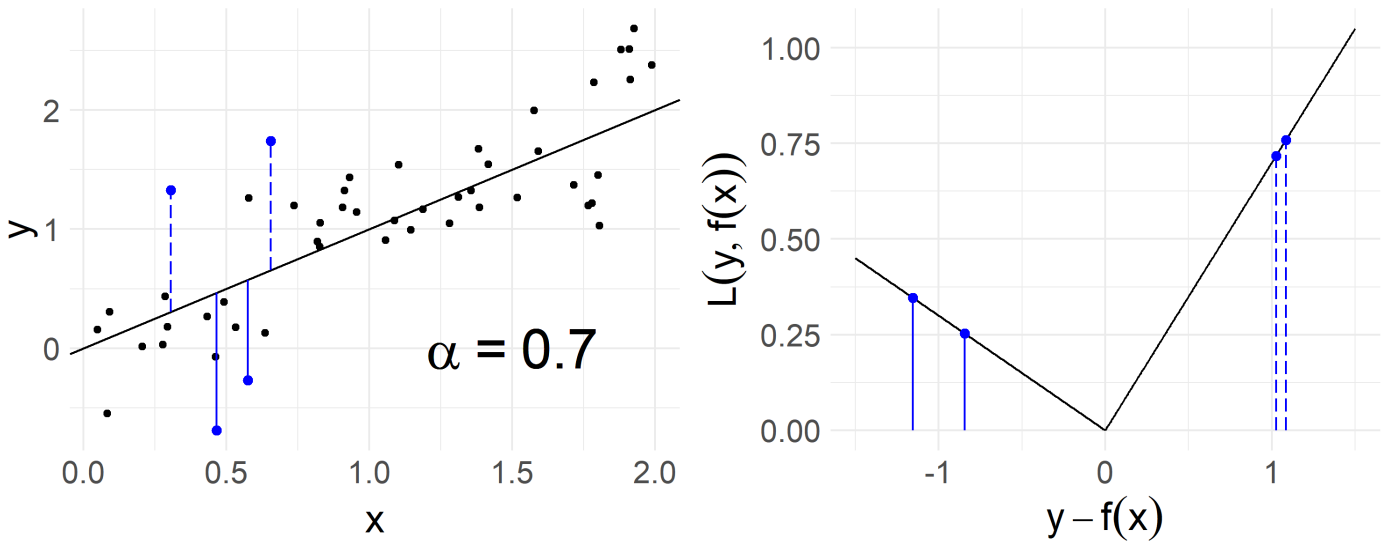
$$
\begin{aligned}
\hat{\theta} &= \arg\min_{\theta \in \mathbb{R}} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) \\
&= \arg\min_{\theta \in \mathbb{R}} \sum_{i \in I_\epsilon} \left|y^{(i)} - \theta\right| - \epsilon \\
&= \arg\min_{\theta \in \mathbb{R}} \sum_{i \in I_\epsilon} \left|y^{(i)} - \theta\right| - \sum_{i \in I_\epsilon} \epsilon \\
&= \text{median}\left(\left\{y^{(i)} \mid i \in I_\epsilon\right\}\right) - |I_\epsilon| \cdot \epsilon
\end{aligned}
$$

with $I_\epsilon := \left\{i : |y^{(i)} - f\left(\mathbf{x}^{(i)}\right)| \leq \epsilon\right\}$.

QUANTILE LOSS

$$L(y, f(\mathbf{x})) = \begin{cases} (1-\alpha)(f(\mathbf{x}) - y) & \text{if } y < f(\mathbf{x}) \\ \alpha(y - f(\mathbf{x})) & \text{if } y \geq f(\mathbf{x}) \end{cases}, \quad \alpha \in (0, 1)$$

- Extension of $L1$ loss (equal to $L1$ for $\alpha = 0.5$).
- Weights either positive or negative residuals more strongly.
- $\alpha < 0.5$ ($\alpha > 0.5$) penalty to over-estimation (under-estimation)
- Also known as **pinball loss**.



QUANTILE LOSS

What is the optimal constant model $f(\mathbf{x}) = \boldsymbol{\theta}$ w.r.t. the quantile loss?

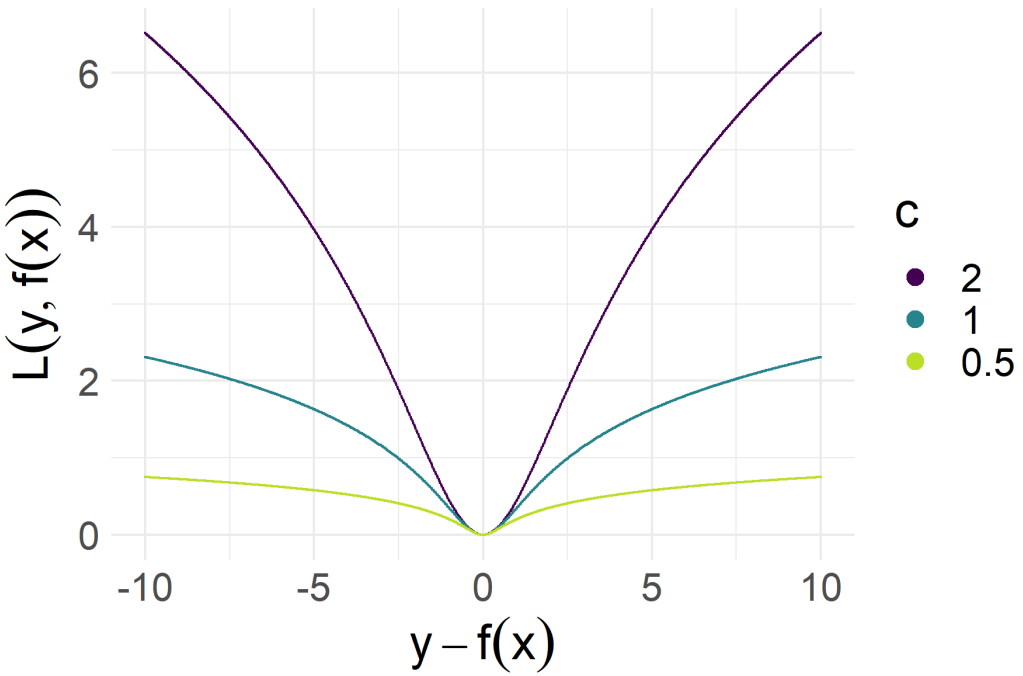
$$
\begin{aligned}
& \hat{\boldsymbol{\theta}} &=& \arg\min_{\boldsymbol{\theta} \in \mathbb{R}} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) \\
\Leftrightarrow \quad & \hat{\boldsymbol{\theta}} &=& \arg\min_{\boldsymbol{\theta} \in \mathbb{R}} \left\{ (1-\alpha) \sum_{y^{(i)} < \boldsymbol{\theta}} \left| y^{(i)} - \boldsymbol{\theta} \right| + \alpha \sum_{y^{(i)} \geq \boldsymbol{\theta}} \left| y^{(i)} - \boldsymbol{\theta} \right| \right\} \\
\Leftrightarrow \quad & \hat{\boldsymbol{\theta}} &=& Q_\alpha(\{y^{(i)}\})
\end{aligned}
$$

where $Q_\alpha(\cdot)$ computes the empirical α-quantile of $\{y^{(i)}\}$, $i = 1, ..., n$.

CAUCHY LOSS

$$L(y, f(\mathbf{x})) = \frac{c^2}{2} \log\left(1 + \left(\frac{|y - f(\mathbf{x})|}{c}\right)^2\right), \quad c \in \mathbb{R}$$

- Particularly robust toward outliers (controllable via c).
- Analytic properties: differentiable, robust, but not convex!



LOG-COSH LOSS

$$L(y, f(\mathbf{x})) = \log\left(\cosh(|y - f(\mathbf{x})|)\right)$$

- Logarithm of the hyperbolic cosine of the residual.
- Approximately equal to $0.5(|y - f(\mathbf{x})|)^2$ for small $\mathbf{x}$ and to $|y - f(\mathbf{x})| - \log 2$ for large $\mathbf{x}$, meaning it works mostly like *L2* loss but is less outlier-sensitive.
- Has all the advantages of Huber loss and is, moreover, twice differentiable everywhere.