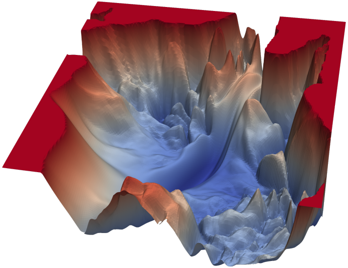
Introduction to Machine Learning

Properties of Loss Functions



Learning goals

- Know the concept of robustness
- Learn about analytical and computational properties of loss functions
- Understand that the loss function may influence convergence of the optimizer

THE ROLE OF LOSS FUNCTIONS

Why should we care about how to choose the loss function $L\left(y, f(\mathbf{x})\right)$?

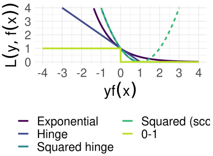
- **Statistical** properties: choice of loss implies statistical assumptions on the distribution of $y \mid \mathbf{x} = \mathbf{x}$ (see *maximum likelihood estimation vs. empirical risk minimization*).
- **Robustness** properties: some loss functions are more robust towards outliers than others.
- **Analytical** properties: the computational / optimization complexity of the problem

$$\arg\min_{\boldsymbol{\theta} \in \Theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$$

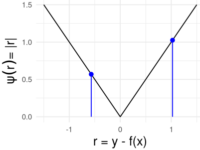
  is influenced by the choice of the loss function.

BASIC TYPES OF REGRESSION LOSSES

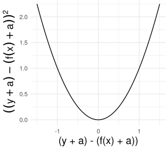
- Regression losses usually only depend on the **residuals** $r := y - f(\mathbf{x})$.
- Classification losses are usually expressed in terms of the **margin** $\nu := y \cdot f(\mathbf{x})$.
- A loss is called **distance-based** if
  - it can be written in terms of the residual, i.e., $L\left(y, f(\mathbf{x})\right) = \psi(r)$ for some $\psi : \mathbb{R} \to \mathbb{R}$, and
  - $\psi(r) = 0 \Leftrightarrow r = 0$.
- A loss is **translation-invariant** if $L(y + a, f(\mathbf{x}) + a) = L\left(y, f(\mathbf{x})\right)$, $a \in \mathbb{R}$.
- Losses are called **symmetric** if $L\left(y, f(\mathbf{x})\right) = L\left(f(\mathbf{x}), y\right)$.



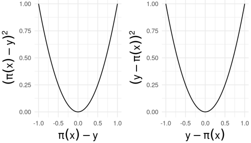
Margin-based losses



Distance-based: $L1$



Translation-invariant: $L2$



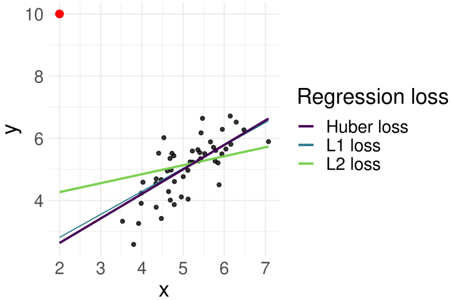
Symmetric: Brier score

ROBUSTNESS

Outliers (in y) have large residuals $r = y - f(\mathbf{x})$. Some losses are more strongly affected by large residuals than others.

$y - \hat{f}(\mathbf{x})$	$L1$	$L2$	Huber ($\epsilon = 5$)
1	1	1	0.5
5	5	25	12.5
10	10	100	37.5
50	50	2500	237.5

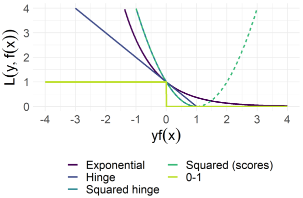
As a consequence, a model is less influenced by outliers than by inliers if the loss is **robust**.



$L2$ is an example for a loss function that is not very robust towards outliers. It penalizes large residuals more than $L1$ or Huber loss, which are considered robust.

ANALYTICAL PROPERTIES: SMOOTHNESS

- **Smoothness** of a function is a property measured by the number of continuous derivatives.
- A function is said to be $\mathcal{C}^k$ if it is k times continuously differentiable. A function is $\mathcal{C}^\infty$ if it is continuously differently for all orders k.
- Derivative-based methods require a certain level of smoothness of the risk function $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$.
  - If the loss function is not smooth, the risk minimization problem will generally not be smooth either.
  - This may require the use of derivative-free optimization (which might not be desirable).



Squared loss, exponential loss and squared hinge loss are continuously differentiable. Hinge loss is continuous but not differentiable. 0-1 loss is not even continuous.

ANALYTICAL PROPERTIES: SMOOTHNESS

Example: Lasso regression

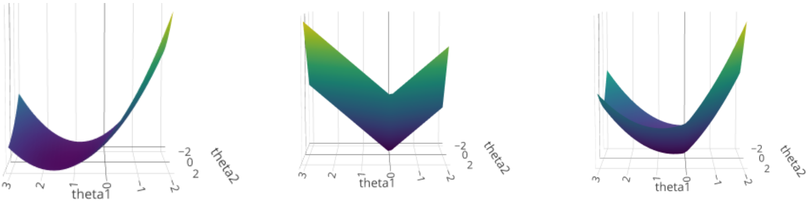
- Problem: Lasso has a non-differentiable objective function

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \lambda\|\boldsymbol{\theta}\|_1 \;\in \mathcal{C}^0,$$

  but many optimization methods are derivative-based, e.g.,

  - Gradient descent: requires existence of gradient $\nabla\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$,
  - Newton-Raphson: requires existence of Hessian $\nabla^2\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$.

- We must therefore resort to alternative optimization techniques – for instance, coordinate descent with subgradients.



Example: $y = x_1 + 1.2x_2 + \epsilon$. *Left:* unpenalized objective, *middle:* $L1$ penalty, *right:* penalized objective (all as functions of $\boldsymbol{\theta}$). We see how the $L1$ penalty nudges the optimum towards (0, 0) and compromises the original objective's smoothness.

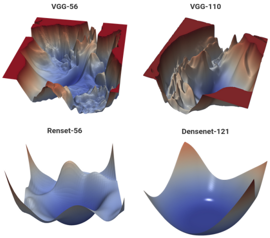
ANALYTICAL PROPERTIES: CONVEXITY

- A function $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is convex if

$$\mathcal{R}_{\text{emp}}\left(t \cdot \boldsymbol{\theta} + (1-t) \cdot \tilde{\boldsymbol{\theta}}\right) \leq t \cdot \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + (1-t) \cdot \mathcal{R}_{\text{emp}}\left(\tilde{\boldsymbol{\theta}}\right)$$

  $\forall\ t \in [0,1],\ \boldsymbol{\theta}, \tilde{\boldsymbol{\theta}} \in \Theta$ (strictly convex if the above holds with equality).
- In optimization, convex optimization problems are desirable because they have a number of conventient properties.
- In particular, it holds for convex problems that local optima are global optima
  $\rightarrow$ a strictly convex function has at most **one** global minimum (uniqueness).
- Note, however, that convexity of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ depends both on convexity of
  - $L(\cdot)$ – given in most cases – and
  - $f(\mathbf{x} \mid \boldsymbol{\theta})$ – often problematic.

Li et al., 2018: *Visualizing the Loss Landscape of Neural Nets*. The problem on the bottom right is convex, the others are not (note that very high-dimensional surfaces are coerced into 3D here).



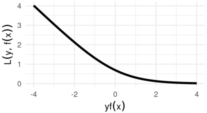
ANALYTICAL PROPERTIES: CONVERGENCE

The choice of the loss function may also impact convergence behavior.

In the extreme case of **complete separation** optimization might even fail entirely. Consider the following scenario:

- Margin-based loss that is antitonic in $y \cdot f$ – for example, **Bernoulli loss**:

$$L(y, f(\mathbf{x})) = \log(1 + \exp(-yf(\mathbf{x})))$$



- Data perfectly separable by our learner

$$\Rightarrow \; y^{(i)} f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right) > 0 \;\; \forall \mathbf{x}^{(i)} \neq \mathbf{0}$$

as every $\mathbf{x}^{(i)}$ is correctly classified: $f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right) < 0$ for $y^{(i)} = -1$, > 0 for $y^{(i)} = 1$

$$\Rightarrow \; yf(\mathbf{x} \mid \boldsymbol{\theta}) = |f(\mathbf{x} \mid \boldsymbol{\theta})|$$

- f linear in $\boldsymbol{\theta}$ – for example, **logistic regression** with $f(\mathbf{x} \mid \boldsymbol{\theta}) = s(\boldsymbol{\theta}^T \mathbf{x})$

ANALYTICAL PROPERTIES: CONVERGENCE

- In optimization, e.g., with gradient descent, we can always find a set of parameters $\boldsymbol{\theta}'$ that classifies all samples perfectly.
- But taking a closer look at $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$, we find that the same can be achieved with $2 \cdot \boldsymbol{\theta}'$ – and at lower risk:

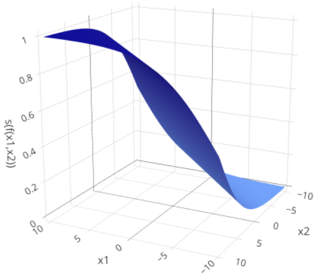
$$\mathcal{R}_{\text{emp}}(2 \cdot \boldsymbol{\theta}) = \sum_{i=1}^{n} L\left(\left| f\left(\mathbf{x}^{(i)} \mid 2 \cdot \boldsymbol{\theta}\right)\right|\right) = \sum_{i=1}^{n} L\left(2 \cdot \left| f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right|\right)$$
$$< \sum_{i=1}^{n} L\left(\left| f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right|\right) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$$

- This actually holds true for every $a \cdot \boldsymbol{\theta}$ with $a > 1$.

  $\Rightarrow$ By increasing $\|\boldsymbol{\theta}\|$, our loss becomes smaller and smaller, and optimization runs infinitely.

ANALYTICAL PROPERTIES: CONVERGENCE

- Geometrically, this translates to an ever steeper slope of the logistic/softmax function, i.e., increasingly sharp discrimination:



- In practice, data are seldom linearly separable and misclassified examples act as counterweights to increasing parameter values.
- Besides, we can apply **regularization** to encourage convergence to robust solutions.