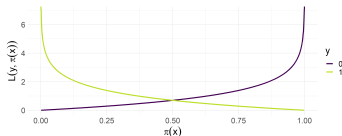


Introduction to Machine Learning

Bernoulli Loss



Learning goals

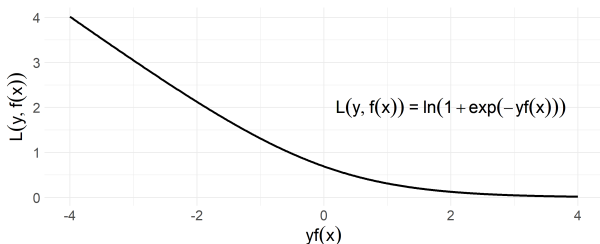
- Know the Bernoulli loss and related losses (log-loss, logistic loss, Binomial loss)
- Derive the risk minimizer
- Derive the optimal constant model
- Understand the connection between log-loss and entropy splitting

BERNOULLI LOSS

$$L(y, f(\mathbf{x})) = \ln(1 + \exp(-y \cdot f(\mathbf{x}))) \quad \text{for } y \in \{-1, +1\}$$

$$L(y, f(\mathbf{x})) = -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) \quad \text{for } y \in \{0, 1\}$$

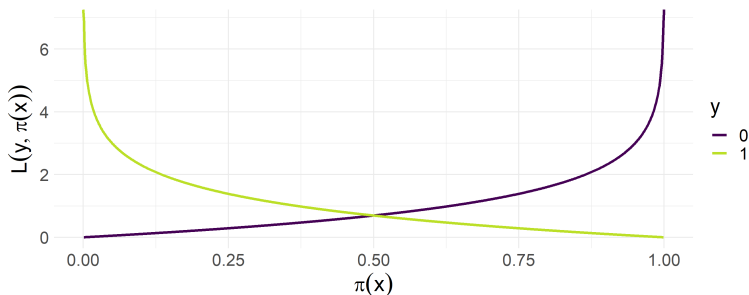
- Two equivalent formulations for different label encodings
- Negative log-likelihood of Bernoulli model, e.g., logistic regression
- Convex, differentiable
- Pseudo-residuals (0/1 case): $\tilde{r} = y - \frac{1}{1 + \exp(-f(\mathbf{x}))}$
Interpretation: $L1$ distance between 0/1-labels and posterior prob!



BERNOULLI LOSS ON PROBABILITIES

If scores are transformed into probabilities by the logistic function $\pi(\mathbf{x}) = (1 + \exp(-f(\mathbf{x})))^{-1}$, we arrive at another equivalent formulation of the loss, where y is again encoded as $\{0, 1\}$:

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



BERNOULLI LOSS: RISK MINIMIZER

The risk minimizer for the Bernoulli loss defined for probabilistic classifiers $\pi(\mathbf{x})$ and on $y \in \{0, 1\}$

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

is

$$\pi^*(\mathbf{x}) = \eta(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x}).$$

Proof: Again, we make use of the law of total expectation

$$\begin{aligned} \mathcal{R}(f) &= \mathbb{E}_{xy} [L(y, f(\mathbf{x}))] = \mathbb{E}_x [\mathbb{E}_{y|x} [L(y, f(\mathbf{x}))]] \\ &= \mathbb{E}_x \left[\sum_{k \in \mathcal{Y}} L(k, f(\mathbf{x})) \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}) \right]. \end{aligned}$$

BERNOULLI LOSS: RISK MINIMIZER

In the binary case this becomes

$$\mathcal{R}(f) = \mathbb{E}_{\mathbf{x}} [L(1, \pi(\mathbf{x})) \cdot \eta(\mathbf{x}) + L(0, \pi(\mathbf{x})) \cdot (1 - \eta(\mathbf{x}))],$$

with $\eta(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})$. We fix a specific \mathbf{x} and compute the point-wise optimal value c by setting the derivative to 0:

$$\begin{aligned} \frac{\partial}{\partial c} (-\log c \cdot \eta(\mathbf{x}) - \log(1 - c) \cdot (1 - \eta(\mathbf{x}))) &= 0 \\ -\frac{\eta(\mathbf{x})}{c} + \frac{1 - \eta(\mathbf{x})}{1 - c} &= 0 \\ -\frac{\eta(\mathbf{x})(1 - c)}{c(1 - c)} + \frac{c(1 - \eta(\mathbf{x}))}{c(1 - c)} &= 0 \\ \frac{-\eta(\mathbf{x}) + \eta(\mathbf{x})c + c - \eta(\mathbf{x})c}{c(1 - c)} &= 0 \\ c &= \eta(\mathbf{x}). \end{aligned}$$

BERNOULLI LOSS: RISK MINIMIZER

The risk minimizer for the Bernoulli loss defined on $y \in \{0, 1\}$ and scores $f(\mathbf{x})$ is the point-wise log-odds:

$$f^*(\mathbf{x}) = \ln \left(\frac{\mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})}{1 - \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})} \right).$$

The function is undefined when $P(y = 1 \mid \mathbf{x} = \mathbf{x}) = 1$ or $P(y = 1 \mid \mathbf{x} = \mathbf{x}) = 0$, but predicts a smooth curve which grows when $P(y = 1 \mid \mathbf{x} = \mathbf{x})$ increases and equals 0 when $P(y = 1 \mid \mathbf{x} = \mathbf{x}) = 0.5$.

Proof: We consider the case $\mathcal{Y} = \{-1, +1\}$. We have seen that the (theoretical) optimal prediction c for an arbitrary loss function at fixed point \mathbf{x} is

$$\arg \min_c \sum_{k \in \mathcal{Y}} L(y, c) \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}).$$

BERNOULLI LOSS: RISK MINIMIZER

We plug in the Bernoulli loss

$$\begin{aligned} & \arg \min_c L(1, c) \underbrace{\mathbb{P}(y = 1 | \mathbf{x} = \mathbf{x})}_{\eta(\mathbf{x})} + L(-1, c) \underbrace{\mathbb{P}(y = -1 | \mathbf{x} = \mathbf{x})}_{1 - \eta(\mathbf{x})} \\ &= \arg \min_c \ln(1 + \exp(-c))\eta(\mathbf{x}) + \ln(1 + \exp(c))(1 - \eta(\mathbf{x})). \end{aligned}$$

Setting the derivative w.r.t. c to zero yields

$$\begin{aligned} 0 &= -\frac{\exp(-c)}{1 + \exp(-c)}\eta(\mathbf{x}) + \frac{\exp(c)}{1 + \exp(c)}(1 - \eta(\mathbf{x})) \\ &= -\frac{\exp(-c)}{1 + \exp(-c)}\eta(\mathbf{x}) + \frac{1}{1 + \exp(-c)}(1 - \eta(\mathbf{x})) \\ &= -\eta(\mathbf{x}) + \frac{1}{1 + \exp(-c)} \\ \Leftrightarrow \eta(\mathbf{x}) &= \frac{1}{1 + \exp(-c)} \\ \Leftrightarrow c &= \ln\left(\frac{\eta(\mathbf{x})}{1 - \eta(\mathbf{x})}\right) \end{aligned}$$

BERNOULLI: OPTIMAL CONSTANT MODEL

The optimal constant probability model $\pi(\mathbf{x}) = \theta$ w.r.t. the Bernoulli loss for labels from $\mathcal{Y} = \{0, 1\}$ is:

$$\hat{\theta} = \arg \min_{\theta} \mathcal{R}_{\text{emp}}(\theta) = \frac{1}{n} \sum_{i=1}^n y^{(i)}$$

Again, this is the fraction of class-1 observations in the observed data. We can simply prove this again by setting the derivative of the risk to 0 and solving for θ .

BERNOULLI: OPTIMAL CONSTANT MODEL

The optimal constant score model $f(\mathbf{x}) = \theta$ w.r.t. the Bernoulli loss labels from $\mathcal{Y} = \{-1, +1\}$ or $\mathcal{Y} = \{0, 1\}$ is:

$$\hat{\theta} = \arg \min_{\theta} \mathcal{R}_{\text{emp}}(\theta) = \ln \frac{n_+}{n_-} = \ln \frac{n_+/n}{n_-/n}$$

where n_- and n_+ are the numbers of negative and positive observations, respectively.

This again shows a tight (and unsurprising) connection of this loss to log-odds.

Proving this is also a (quite simple) exercise.

BERNOULLI-LOSS: NAMING CONVENTION

We have seen three loss functions that are closely related. In the literature, there are different names for the losses:

$$L(y, f(\mathbf{x})) = \ln(1 + \exp(-yf(\mathbf{x}))) \quad \text{for } y \in \{-1, +1\}$$

$$L(y, f(\mathbf{x})) = -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) \quad \text{for } y \in \{0, 1\}$$

are referred to as Bernoulli, Binomial or logistic loss.

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

is referred to as cross-entropy or log-loss.

For simplicity, we will call all of them **Bernoulli loss**, and rather make clear whether they are defined on labels $y \in \{0, 1\}$ or $y \in \{-1, +1\}$ and on scores $f(\mathbf{x})$ or probabilities $\pi(\mathbf{x})$.

LOG LOSS MINIMIZATION = ENTROPY SPLITTING

When fitting a tree we find splits that minimize node impurity (measured by a criterion). In each node $\mathcal{N} \subseteq \mathcal{D}$ we predict the optimal constant.

Claim: Entropy splitting is equivalent to the log loss minimization.

Proof: To prove this we show that the risk related to a subset of observations $\mathcal{N} \subseteq \mathcal{D}$ fulfills

$$\mathcal{R}(\mathcal{N}) = n_{\mathcal{N}} I(\mathcal{N}),$$

where I is the entropy criterion $I(\mathcal{N}) = -\sum_{k=1}^g \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})}$, and $\mathcal{R}(\mathcal{N})$ is calculated w.r.t. the log loss

$$L(y, \pi_k(\mathbf{x})) = \sum_{k=1}^g \mathbb{I}(y = k) \log(\pi_k(\mathbf{x})).$$

LOG LOSS MINIMIZATION = ENTROPY SPLITTING

$$\begin{aligned}\mathcal{R}(\mathcal{N}) &= \sum_{(\mathbf{x}, y) \in \mathcal{N}} \sum_{k=1}^g \mathbb{I}(y = k) \log \pi_k(\mathbf{x}) \stackrel{(*)}{=} \sum_{k=1}^g \sum_{(\mathbf{x}, y) \in \mathcal{N}} \mathbb{I}(y = k) \log \pi_k^{(\mathcal{N})} \\&= \sum_{k=1}^g \log \pi_k^{(\mathcal{N})} \underbrace{\sum_{(\mathbf{x}, y) \in \mathcal{N}} \mathbb{I}(y = k)}_{n_{\mathcal{N}} \cdot \pi_k^{(\mathcal{N})}} \\&= n_{\mathcal{N}} \sum_{k=1}^g \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})} = n_{\mathcal{N}} l(\mathcal{N}),\end{aligned}$$

where in $(*)$ the optimal constant $\hat{\pi}_k(\mathbf{x}) = \pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} \mathbb{I}(y = k)$ was plugged in.