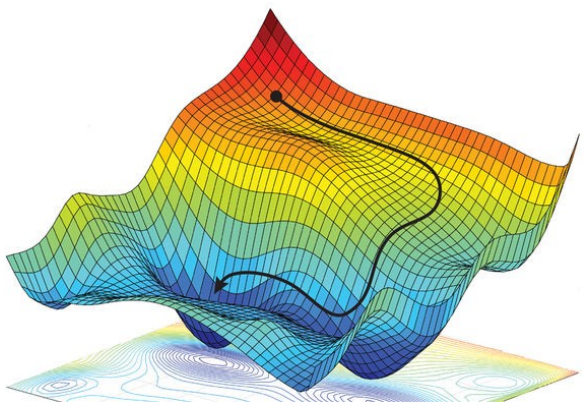
Introduction to Machine Learning

Bernoulli Loss



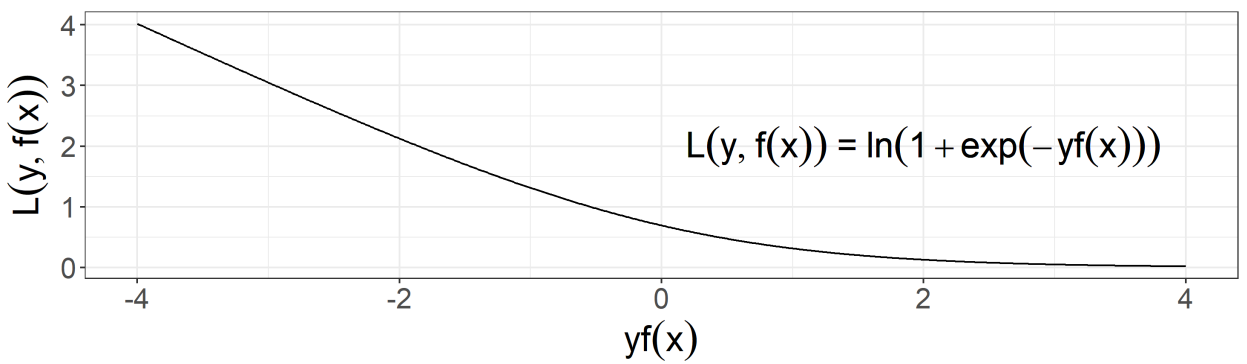
Learning goals

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

BERNOULLI LOSS

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

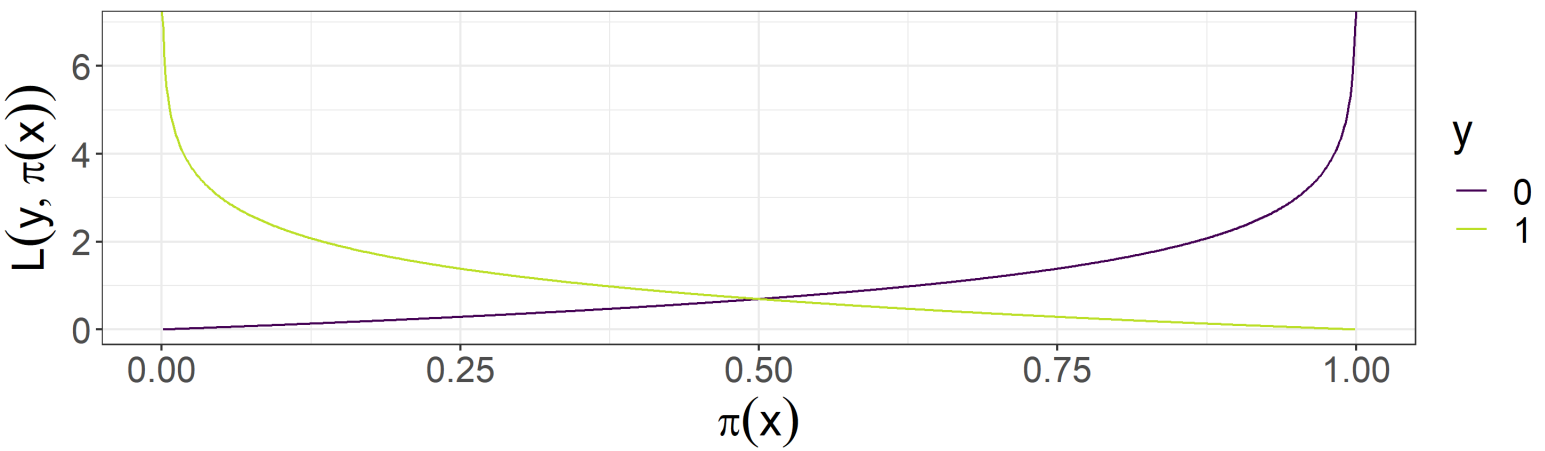
- Two equivalent formulations for different label encodings
- Negative log-likelihood of Bernoulli model, e.g., logistic regression
- Convex, differentiable
- Pseudo-residuals (0/1 case): $\tilde{r} = y - \frac{1}{1+\exp(-f(\mathbf{x}))}$
  Interpretation: $L1$ distance between 0/1-labels and posterior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

To derive the risk minimizer for the Bernoulli loss for the formulation

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

we again make use of the law of total expectation

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

In the binary case this becomes

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

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

BERNOULLI LOSS: RISK MINIMIZER

We fix a specific $\mathbf{x}$ and compute the point-wise optimal value c by setting the derivative to 0:

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

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

BERNOULLI LOSS: RISK MINIMIZER

To derive the risk minimizer for the Bernoulli loss we again compute the point-wise optimum for a fixed $\mathbf{x}$. The point-wise log-odds:

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

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

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

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

BERNOULLI LOSS: RISK MINIMIZER

We plug in the Bernoulli loss

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

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:

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

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:

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

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:

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

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

Entropy splitting in trees is equivalent to minimizing the log-loss of a node. The logarithmic loss for multiple classes $y \in \{1, 2, ..., g\}$ is defined as

$$L(y, \pi_k(\mathbf{x})) = \sum_{k=1}^{g} [y = k] \log \left(\pi_k(\mathbf{x})\right).$$

$$\begin{aligned}
\mathcal{R}(\mathcal{N}) &= \sum_{(\mathbf{x},y)\in\mathcal{N}} \sum_{k=1}^{g} [y = k] \log \pi_k(\mathbf{x}) \\
&= \sum_{k=1}^{g} \sum_{(\mathbf{x},y)\in\mathcal{N}} [y = k] \log \pi_k^{(\mathcal{N})} \\
&= \sum_{k=1}^{g} n_{\mathcal{N}k} \log \pi_k^{(\mathcal{N})} = n_{\mathcal{N}} \sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})} = n_{\mathcal{N}} I(\mathcal{N}),
\end{aligned}$$

plugging in the optimal constant $\pi_k(\mathbf{x}) = \pi_k^{(\mathcal{N})}$.