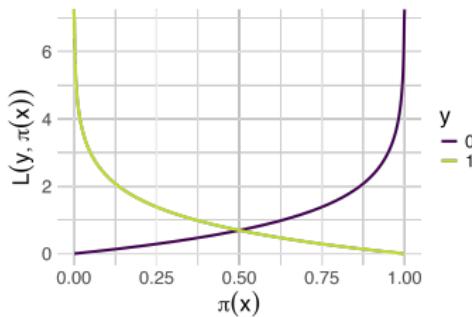


Introduction to Machine Learning

Advanced Risk Minimization Classification (Deep-Dive)



Learning goals

- Equivalence of different loss formulations
- Risk minimizer on scores
- Optimal constant model for the binary empirical log loss risk
- Optimal constant model for the empirical multiclass log loss risk

EQUIVALENCE OF LOSS FORMULATIONS

- Starting point Bernoulli loss on probs:

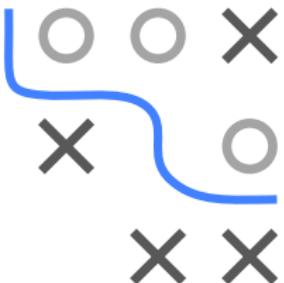
$$L(y, \pi(\mathbf{x})) = -y \log(\pi(\mathbf{x})) - (1-y) \log(1-\pi(\mathbf{x})), \quad y \in \{0, 1\}$$

- Loss on scores $f(\mathbf{x}) = \log\left(\frac{\pi(\mathbf{x})}{1-\pi(\mathbf{x})}\right) \Leftrightarrow \pi(\mathbf{x}) = (1 + \exp(-f(\mathbf{x})))^{-1}$:

$$\begin{aligned} L(y, \pi(\mathbf{x})) &= -y(\log(\pi(\mathbf{x})) - \log(1-\pi(\mathbf{x}))) - \log(1-\pi(\mathbf{x})) \\ &= -y \log\left(\frac{\pi(\mathbf{x})}{1-\pi(\mathbf{x})}\right) - \log\left(1 - \frac{1}{1 + \exp(-f(\mathbf{x}))}\right) \\ &= -yf(\mathbf{x}) - \log\left(\frac{\exp(-f(\mathbf{x}))}{1 + \exp(-f(\mathbf{x}))}\right) \\ &= -yf(\mathbf{x}) - \log\left(\frac{1}{1 + \exp(f(\mathbf{x}))}\right) \\ &= -yf(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) \end{aligned}$$

- Yields equivalent loss formulation

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



EQUIVALENCE OF LOSS FORMULATIONS

- For $y \in \{-1, +1\}$ convert labels using $y' = (y + 1)/2$

- Bernoulli loss on probs with $y \in \{-1, +1\}$:

$$L(y, \pi(\mathbf{x})) = -\frac{1+y}{2} \log(\pi(\mathbf{x})) - \frac{1-y}{2} \log(1-\pi(\mathbf{x})), \quad y \in \{-1, +1\}$$

- For $y \in \{-1, +1\}$ loss on scores becomes:

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

- For $y = -1$ plug $y' = 0$ in $L(y, f(\mathbf{x}))$ for $y \in \{0, 1\}$ loss:

$$L(0, f(\mathbf{x})) = \log(1 + \exp(f(\mathbf{x}))) \checkmark$$

- For $y = y' = 1$:

$$\begin{aligned} L(1, f(\mathbf{x})) &= -1 \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) \\ &= \log(1 + \exp(f(\mathbf{x}))) - \log(\exp(f(\mathbf{x}))) \\ &= \log(1 + \exp(-f(\mathbf{x}))) \quad \checkmark \end{aligned}$$



NAMING CONVENTIONS

We have seen several closely related loss functions:

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

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

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

$$L(y, \pi(\mathbf{x})) = -\frac{1+y}{2} \log(\pi(\mathbf{x})) - \frac{1-y}{2} \log(1 - \pi(\mathbf{x})) \quad \text{for } y \in \{-1, +1\}$$



They are equally referred to as Bernoulli-, Binomial-, logistic-, log-, or cross-entropy loss

PROOF RISK MINIMIZER ON SCORES

For $y \in \{0, 1\}$ the pointwise RM on scores is

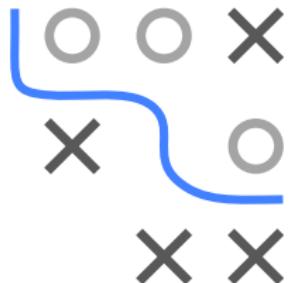
$$f^*(\mathbf{x}) = \log(\eta(\mathbf{x}) / (1 - \eta(\mathbf{x})))$$

Proof: As before we minimize

$$\begin{aligned}\mathcal{R}(f) &= \mathbb{E}_{\mathbf{x}} [L(1, f(\mathbf{x})) \cdot \eta(\mathbf{x}) + L(-1, f(\mathbf{x})) \cdot (1 - \eta(\mathbf{x}))] \\ &= \mathbb{E}_{\mathbf{x}} [\log(1 + \exp(-f(\mathbf{x})))\eta(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) (1 - \eta(\mathbf{x}))]\end{aligned}$$

For a fixed \mathbf{x} we compute the point-wise optimal value c by setting the derivative to 0:

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



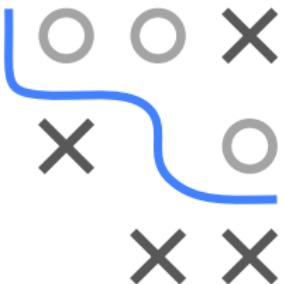
BINARY LOG LOSS: EMP. RISK MINIMIZER

Given $n \in \mathbb{N}$ observations $y^{(1)}, \dots, y^{(n)} \in \mathcal{Y} = \{0, 1\}$ we want to determine the optimal constant model for the empirical log loss risk.

$$\arg \min_{\theta \in (0,1)} \mathcal{R}_{\text{emp}} = \arg \min_{\theta \in (0,1)} - \sum_{i=1}^n y^{(i)} \log(\theta) + (1 - y^{(i)}) \log(1 - \theta).$$

The minimizer can be found by setting the derivative to zero, i.e.,

$$\begin{aligned} \frac{d}{d\theta} \mathcal{R}_{\text{emp}} &= - \sum_{i=1}^n \frac{y^{(i)}}{\theta} - \frac{1 - y^{(i)}}{1 - \theta} \stackrel{!}{=} 0 \\ \iff - \sum_{i=1}^n y^{(i)}(1 - \theta) - \theta(1 - y^{(i)}) &\stackrel{!}{=} 0 \\ \iff - \sum_{i=1}^n (y^{(i)} - \theta) &\stackrel{!}{=} 0 \\ \Rightarrow \hat{\theta} = \frac{1}{n} \sum_{i=1}^n y^{(i)} &\in (0, 1) \checkmark (\text{assuming both labels occur}) \end{aligned}$$



MULTICLASS LOG LOSS: EMP. RISK MINIMIZER

Given $n \in \mathbb{N}$ observations $y^{(1)}, \dots, y^{(n)} \in \mathcal{Y} = \{1, \dots, g\}$ with $g \in \mathbb{N}_{>1}$ we want to determine the optimal constant model $\theta \in (0, 1)^g$ for the empirical log loss risk



$$\begin{aligned} \arg \min_{\theta \in (0,1)^g} \mathcal{R}_{\text{emp}} &= \arg \min_{\theta \in (0,1)^g} - \sum_{i=1}^n \sum_{j=1}^g \mathbb{1}_{\{y^{(i)}=j\}} \log(\theta_j) \\ \text{s.t. } \sum_{j=1}^g \theta_j &= 1 \end{aligned}$$

We can solve this constrained optimization problem by plugging the constraint into the risk (we could also use Lagrange multipliers), i.e., we replace θ_g (this is an arbitrary choice) such that $\theta_g = 1 - \sum_{j=1}^{g-1} \theta_j$.

MULTICLASS LOG LOSS: EMP. RISK MINIMIZER

With this, we find the equivalent optimization problem

$$\begin{aligned} \arg \min_{\theta \in (0,1)^{g-1}} \mathcal{R}_{\text{emp}} &= \arg \min_{\theta \in (0,1)^{g-1}} - \sum_{i=1}^n \sum_{j=1}^{g-1} \mathbb{1}_{\{y^{(i)}=j\}} \log(\theta_j) \\ &\quad + \mathbb{1}_{\{y^{(i)}=g\}} \log(1 - \sum_{j=1}^{g-1} \theta_j) \\ \text{s.t. } &\sum_{j=1}^{g-1} \theta_j < 1. \end{aligned}$$

For $j \in \{1, \dots, g-1\}$, the j -th partial derivative of our objective

$$\begin{aligned} \frac{\partial}{\partial \theta_j} \mathcal{R}_{\text{emp}} &= - \sum_{i=1}^n \mathbb{1}_{\{y^{(i)}=j\}} \frac{1}{\theta_j} - \mathbb{1}_{\{y^{(i)}=g\}} \frac{1}{1 - \sum_{j=1}^{g-1} \theta_j} \\ &= - \frac{n_j}{\theta_j} + \frac{n_g}{\theta_g} \end{aligned}$$

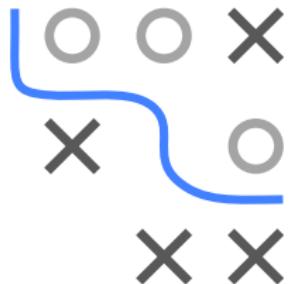
where n_k with $k \in \{1, \dots, g\}$ is the number of label k in y and we assume that $n_k > 0$



MULTICLASS LOG LOSS: EMP. RISK MINIMIZER

For the minimizer, it must hold for $j \in \{1, \dots, g - 1\}$ that

$$\begin{aligned} & \frac{\partial}{\partial \theta_j} \mathcal{R}_{\text{emp}} \stackrel{!}{=} 0 \\ \iff & -n_j \theta_g + n_g \theta_j \stackrel{!}{=} 0 \\ \Rightarrow & \sum_{j=1}^{g-1} (-n_j \theta_g + n_g \theta_j) \stackrel{!}{=} 0 \\ \iff & -(n - n_g) \theta_g + n_g (1 - \theta_g) \stackrel{!}{=} 0 \\ \iff & -n \theta_g + n_g \stackrel{!}{=} 0 \\ \Rightarrow & \hat{\theta}_g = \frac{n_g}{n} \in (0, 1) \checkmark \\ \Rightarrow \forall j \in \{1, \dots, g-1\} : & \hat{\theta}_j = \frac{\hat{\theta}_g n_j}{n_g} = \frac{n_j}{n} \in (0, 1) \checkmark \\ (\Rightarrow & \sum_{j=1}^{g-1} \hat{\theta}_j = 1 - \hat{\theta}_g = 1 - \frac{n_g}{n} < 1 \checkmark) \end{aligned}$$



CONVEXITY

Finally, we check that we indeed found a minimizer by showing that \mathcal{R}_{emp} is convex for the multiclass case (binary is a special case of this):

The Hessian of \mathcal{R}_{emp}

$$\nabla_{\theta}^2 \mathcal{R}_{\text{emp}} = \begin{pmatrix} \frac{n_1}{\theta_1^2} & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \frac{n_{g-1}}{\theta_{g-1}^2} \end{pmatrix}$$

is positive definite since all its eigenvalues

$$\lambda_j = \frac{n_j}{\theta_j^2} > 0 \quad \forall j \in \{1, \dots, g-1\}.$$

From this, it follows that \mathcal{R}_{emp} is (strictly) convex

