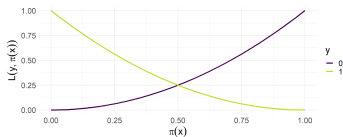


Introduction to Machine Learning

Brier Score



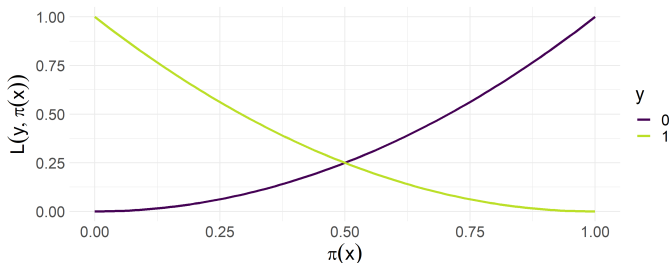
Learning goals

- Know the Brier score
- Derive the risk minimizer
- Derive the optimal constant model
- Understand the connection between Brier score and Gini splitting

BRIER SCORE

The binary Brier score is defined on probabilities $\pi(\mathbf{x}) \in [0, 1]$ and 0-1-encoded labels $y \in \{0, 1\}$ and measures their squared distance ($L2$ loss on probabilities).

$$L(y, \pi(\mathbf{x})) = (\pi(\mathbf{x}) - y)^2$$



BRIER SCORE: RISK MINIMIZER

The risk minimizer for the (binary) Brier score is

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

which means that the Brier score will reach its minimum if the prediction equals the “true” probability of the outcome.

The risk minimizer for the multiclass Brier score is

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

Proof: We only show the proof for the binary case. We need to minimize

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

BRIER SCORE: RISK MINIMIZER

which we do point-wise for every \mathbf{x} . We plug in the Brier score

$$\begin{aligned} & \arg \min_c L(1, c)\eta(\mathbf{x}) + L(0, c)(1 - \eta(\mathbf{x})) \\ &= \arg \min_c (c - 1)^2\eta(\mathbf{x}) + c^2(1 - \eta(\mathbf{x})) \\ &= \arg \min_c (c - \eta(\mathbf{x}))^2. \end{aligned}$$

The expression is minimal if $c = \eta(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})$.

BRIER SCORE: OPTIMAL CONSTANT MODEL

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

$$\begin{aligned}\min_{\theta} \mathcal{R}_{\text{emp}}(\theta) &= \min_{\theta} \sum_{i=1}^n \left(y^{(i)} - \theta\right)^2 \\ \Leftrightarrow \frac{\partial \mathcal{R}_{\text{emp}}(\theta)}{\partial \theta} &= -2 \cdot \sum_{i=1}^n (y^{(i)} - \theta) = 0 \\ \hat{\theta} &= \frac{1}{n} \sum_{i=1}^n y^{(i)}.\end{aligned}$$

This is the fraction of class-1 observations in the observed data. (This also directly follows from our $L2$ proof for regression).

Similarly, for the multiclass brier score the optimal constant is

$$\hat{\theta}_k = \frac{1}{n} \sum_{i=1}^n [y = k].$$

BRIER SCORE MINIMIZATION = GINI SPLITTING

When fitting a tree we minimize the risk within each node \mathcal{N} by risk minimization and predict the optimal constant. Another approach that is common in literature is to minimize the average node impurity $\text{Imp}(\mathcal{N})$.

Claim: Gini splitting $\text{Imp}(\mathcal{N}) = \sum_{k=1}^g \pi_k^{(\mathcal{N})} \left(1 - \pi_k^{(\mathcal{N})}\right)$ is equivalent to the Brier score minimization.

Note that $\pi_k^{(\mathcal{N})} := \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} [y = k]$

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

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

where Imp is the Gini impurity and $\mathcal{R}(\mathcal{N})$ is calculated w.r.t. the (multiclass) Brier score

$$L(y, \pi(\mathbf{x})) = \sum_{k=1}^g ([y = k] - \pi_k(\mathbf{x}))^2.$$

BRIER SCORE MINIMIZATION = GINI SPLITTING

$$\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x}, y) \in \mathcal{N}} \sum_{k=1}^g ([y = k] - \pi_k(\mathbf{x}))^2 = \sum_{k=1}^g \sum_{(\mathbf{x}, y) \in \mathcal{N}} \left([y = k] - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2,$$

by plugging in the optimal constant prediction w.r.t. the Brier score ($n_{\mathcal{N}, k}$ is defined as the number of class k observations in node \mathcal{N}):

$$\hat{\pi}_k(\mathbf{x}) = \pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} [y = k] = \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}}.$$

We split the inner sum and further simplify the expression

$$\begin{aligned} &= \sum_{k=1}^g \left(\sum_{(\mathbf{x}, y) \in \mathcal{N}: y=k} \left(1 - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2 + \sum_{(\mathbf{x}, y) \in \mathcal{N}: y \neq k} \left(0 - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2 \right) \\ &= \sum_{k=1}^g n_{\mathcal{N}, k} \left(1 - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2 + (n_{\mathcal{N}} - n_{\mathcal{N}, k}) \left(\frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2, \end{aligned}$$

since for $n_{\mathcal{N}, k}$ observations the condition $y = k$ is met, and for the remaining $(n_{\mathcal{N}} - n_{\mathcal{N}, k})$ observations it is not.

BRIER SCORE MINIMIZATION = GINI SPLITTING

We further simplify the expression to

$$\begin{aligned}\mathcal{R}(\mathcal{N}) &= \sum_{k=1}^g n_{\mathcal{N},k} \left(\frac{n_{\mathcal{N}} - n_{\mathcal{N},k}}{n_{\mathcal{N}}} \right)^2 + (n_{\mathcal{N}} - n_{\mathcal{N},k}) \left(\frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}} \right)^2 \\&= \sum_{k=1}^g \frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}} \frac{n_{\mathcal{N}} - n_{\mathcal{N},k}}{n_{\mathcal{N}}} (n_{\mathcal{N}} - n_{\mathcal{N},k} + n_{\mathcal{N},k}) \\&= n_{\mathcal{N}} \sum_{k=1}^g \pi_k^{(\mathcal{N})} \cdot (1 - \pi_k^{(\mathcal{N})}) = n_{\mathcal{N}} \text{Imp}(\mathcal{N}).\end{aligned}$$