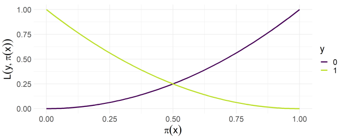
# Introduction to Machine Learning

# Brier Score



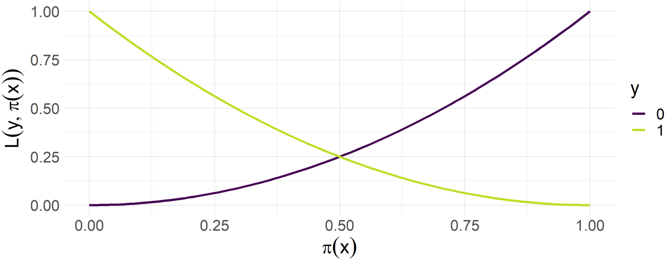

## Learning goals

- 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 Brier score is

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

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

**Proof:** We have seen that the (theoretical) optimal prediction $c$ for an arbitrary loss function at fixed point $\mathbf{x}$ is

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

# BRIER SCORE: RISK MINIMIZER

We plug in the Brier score

$$
\begin{aligned}
& \arg\min_c L(1, c) \underbrace{\mathbb{P}(y = 1|\mathbf{x} = \mathbf{x})}_{=\eta(\mathbf{x})} + L(0, c) \underbrace{\mathbb{P}(y = 0|\mathbf{x} = \mathbf{x})}_{=1-\eta(\mathbf{x})} \\
= \quad & \arg\min_c \quad (c - 1)^2 \eta(\mathbf{x}) + c^2 (1 - \eta(\mathbf{x})) \\
= \quad & \arg\min_c \quad (c - \eta(\mathbf{x}))^2.
\end{aligned}
$$

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).

# BRIER SCORE MINIMIZATION = GINI 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:** Gini splitting is equivalent to the Brier score 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 Gini impurity with $I(\mathcal{N}) = \sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \left(1 - \pi_k^{(\mathcal{N})}\right)$, and $\mathcal{R}(\mathcal{N})$ is calculated w.r.t. the Brier score

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

# BRIER SCORE MINIMIZATION = GINI SPLITTING

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

In the last step we plugged in the optimal prediction w.r.t. the Brier score (the fraction of class-$k$ observations):

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

# BRIER SCORE MINIMIZATION = GINI SPLITTING

We further simplify the expression to

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