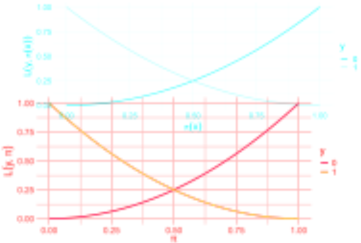
Introduction to Machine Learning

Advanced Risk Minimization

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

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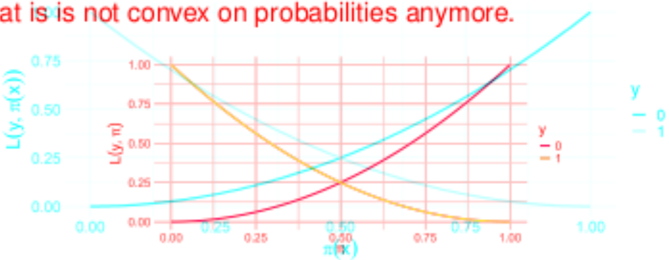
BRIER SCORE

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

$$L(y, \pi) = (\pi - y)^2$$

As the Brier score is a proper scoring rule, it can be used for calibration. Note that is is not convex on probabilities anymore.



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

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

BRIER SCORE: RISK MINIMIZER / 2

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

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

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

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

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

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

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

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

$$= \sum_{k=1}^{g} n_{\mathcal{N},k} \left(1 - \frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}}\right)^2 + (n_{\mathcal{N}} - n_{\mathcal{N},k}) \left(\frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}}\right)^2,$$

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

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