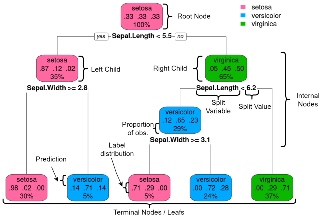
Introduction to Machine Learning

Advanced Risk Minimization

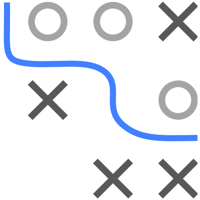
Loss functions and tree splitting



Learning goals

- Know how tree splitting is ’nothing new’ and related to loss functions
- Brier score minimization corresponds to gini splitting
- Bernoulli loss minimization corresponds to entropy splitting

BERNOULLI LOSS MIN = ENTROPY SPLITTING



For an introduction on trees and splitting criteria we refer our **I2ML** lecture (Chapter 6, ▸ Bischl et al. 2022)

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

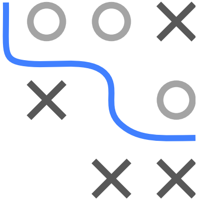
Claim: Entropy splitting $\text{Imp}(\mathcal{N}) = -\sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})}$ is equivalent to minimize risk measured by the Bernoulli loss.

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

Proof: To prove this we show that the risk related to a subset of observations $\mathcal{N} \subseteq \mathcal{D}$ fulfills $\mathcal{R}(\mathcal{N}) = n_{\mathcal{N}} \text{Imp}(\mathcal{N})$,
where $\mathcal{R}(\mathcal{N})$ is calculated w.r.t. the (multiclass) Bernoulli loss

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

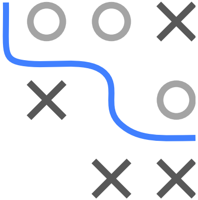
BERNOULLI LOSS MIN = ENTROPY SPLITTING / 2



$$
\begin{aligned}
\mathcal{R}(\mathcal{N}) &= \sum_{(\mathbf{x},y)\in\mathcal{N}} \left(-\sum_{k=1}^{g} [y = k] \log \pi_k(\mathbf{x}) \right) \\
&\overset{(*)}{=} -\sum_{k=1}^{g} \sum_{(\mathbf{x},y)\in\mathcal{N}} [y = k] \log \pi_k^{(\mathcal{N})} \\
&= -\sum_{k=1}^{g} \log \pi_k^{(\mathcal{N})} \underbrace{\sum_{(\mathbf{x},y)\in\mathcal{N}} [y = k]}_{n_{\mathcal{N}} \cdot \pi_k^{(\mathcal{N})}} \\
&= -n_{\mathcal{N}} \sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})} = n_{\mathcal{N}} \operatorname{Imp}(\mathcal{N}),
\end{aligned}
$$

where in $^{(*)}$ the optimal constant per node $\pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x},y)\in\mathcal{N}} [y = k]$ was plugged in.

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

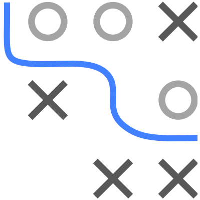
Proof: We show that the risk related to a subset of observations $\mathcal{N} \subseteq \mathcal{D}$ fulfills

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

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 / 2



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

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 $\mathcal{N}$):

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

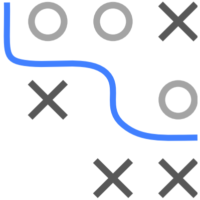
We split the inner sum and further simplify the expression

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

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

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 / 3



We further simplify the expression to

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