Introduction to Machine Learning

Advanced Risk Minimization
Loss functions and tree splitting
(Deep-Dive)

Learning goals

- Tree splitting loss vs impurity:
- Bernoulli loss $\sim$ entropy splitting
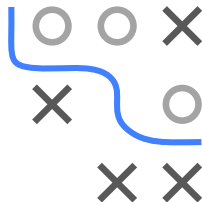- Brier score $\sim$ gini splitting

RISK MINIMIZATION AND IMPURITY

- Tree fitting: Find best way to split parent node $\mathcal{N}_0$ into child nodes $\mathcal{N}_1$ and $\mathcal{N}_2$ such that $\mathcal{N}_1 \cup \mathcal{N}_2 = \mathcal{N}_0$ and $\mathcal{N}_1 \cap \mathcal{N}_2 = \emptyset$
- Two options for evaluating how good a split is: Per node $\mathcal{N}$ compute the following:

  1. Compute impurity $\text{Imp}(\mathcal{N})$ directly from observations in $\mathcal{N}$
  2. Fit optimal constant using loss function, sum up losses for $\mathcal{N}$

- Summarize on split level:

  1. Weighted average ($n_0 = n_1 + n_2$ are number of obs in nodes)

$$\text{Imp(split)} = \frac{n_1}{n_0}\text{Imp}(\mathcal{N}_1) + \frac{n_2}{n_0}\text{Imp}(\mathcal{N}_2)$$

  2. Sum of individual losses

$$\mathcal{R}(\text{split}) = \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2)$$

BERNOULLI LOSS MIN = ENTROPY SPLITTING

Claim: Using entropy in (1) is equivalent to using Bernoulli loss in (2)

Proof: $\mathcal{N} \subseteq \mathcal{D}$ denotes subset of observations in that node.
Risk $\mathcal{R}(\mathcal{N})$ of node $\mathcal{N}$ w.r.t. (multiclass) Bernoulli loss

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

$\Rightarrow$ Optimal constant per node $\pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} \mathbb{I}[y = k]$.

Entropy of node $\mathcal{N}$:

$$\mathsf{Imp}(\mathcal{N}) = -\sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})}$$

RISK MINIMIZATION AND IMPURITY

$$\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x},y)\in\mathcal{N}} (-\sum_{k=1}^{g} \mathbb{I}[y=k]\log\pi_k(\mathbf{x}))$$

$$= -\sum_{k=1}^{g} \sum_{(\mathbf{x},y)\in\mathcal{N}} \mathbb{I}[y=k]\log\pi_k^{(\mathcal{N})}$$

$$= -\sum_{k=1}^{g} \log\pi_k^{(\mathcal{N})}$$

$$= -n_{\mathcal{N}} \sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \log\pi_k^{(\mathcal{N})} = n_{\mathcal{N}}\mathsf{Imp}(\mathcal{N})$$

$$\Rightarrow \mathcal{R}(\mathsf{split}) = \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2) = n_1\mathsf{Imp}(\mathcal{N}_1) + n_2\mathsf{Imp}(\mathcal{N}_2)$$

$$= n_0(\frac{n_1}{n_0}\mathsf{Imp}(\mathcal{N}_1) + \frac{n_2}{n_0}\mathsf{Imp}(\mathcal{N}_2)) = n_0\mathsf{Imp}(\mathsf{split})$$

Bernoulli-risk of the split $\mathcal{R}(\mathsf{split})$ is proportional to its entropy-impurity
$\mathsf{Imp}(\mathsf{split})$, i.e., $\arg\min_{\mathsf{split}} \mathcal{R}(\mathsf{split}) = \arg\min_{\mathsf{split}} \mathsf{Imp}(\mathsf{split})$

BRIER SCORE MINIMIZATION = GINI SPLITTING

Claim: Using Gini in (1) is equivalent to using Brier score in (2)
Proof:
Risk $\mathcal{R}(\mathcal{N})$ of node $\mathcal{N}$ w.r.t. (multiclass) Brier score
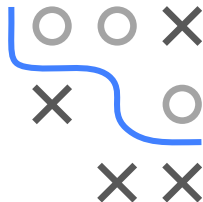
$$L\left(y, \pi(\mathbf{x})\right) = \sum_{k=1}^{g} (\mathbb{I}[y = k] - \pi_k(\mathbf{x}))^2$$

$\Rightarrow$ Optimal constant per node: $\pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x},y) \in \mathcal{N}} \mathbb{I}[y = k] = \frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}}$
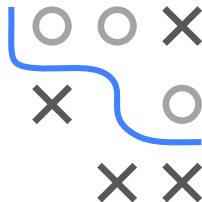
($n_{\mathcal{N},k}$ is the number of class k observations in node $\mathcal{N}$)

Gini index of node $\mathcal{N}$:

$$\text{Imp}(\mathcal{N}) = \sum_{k=1}^{g} \pi_k^{(\mathcal{N})} (1 - \pi_k^{(\mathcal{N})})$$

BRIER SCORE MINIMIZATION = GINI SPLITTING

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

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

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

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

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

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

$$= n_{\mathcal{N}} \sum_{k=1}^{g} \pi_k^{(\mathcal{N})} \cdot (1 - \pi_k^{(\mathcal{N})}) = n_{\mathcal{N}} \mathsf{Imp}(\mathcal{N})$$

$$\Rightarrow \mathcal{R}(\mathsf{split}) = \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2) = n_1 \mathsf{Imp}(\mathcal{N}_1) + n_2 \mathsf{Imp}(\mathcal{N}_2)$$

$$= n_0 \left(\frac{n_1}{n_0} \mathsf{Imp}(\mathcal{N}_1) + \frac{n_2}{n_0} \mathsf{Imp}(\mathcal{N}_2) \right) = n_0 \mathsf{Imp}(\mathsf{split})$$

Brier-risk of the split $\mathcal{R}(\mathsf{split})$ is proportional to its gini-impurity $\mathsf{Imp}(\mathsf{split})$, i.e.,
$\arg\min_{\mathsf{split}} \mathcal{R}(\mathsf{split}) = \arg\min_{\mathsf{split}} \mathsf{Imp}(\mathsf{split})$