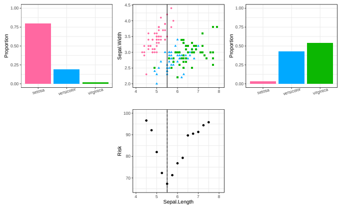
Introduction to Machine Learning

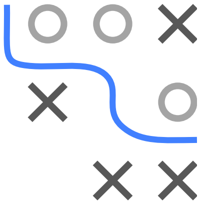
CART
Splitting Criteria for Classification



Learning goals

- Understand how to define split criteria via ERM
- Understand how to find splits in regression with L_2 loss

OPTIMAL CONSTANT MODELS



As losses in classification, we typically use:

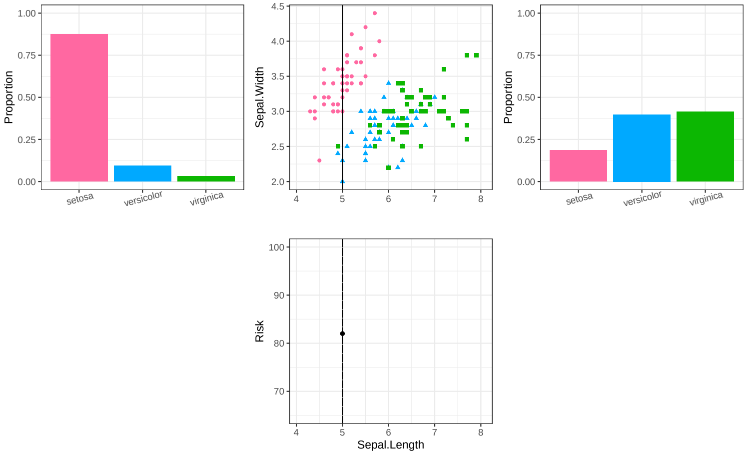
- (Multi-class) Brier score $L(y, \boldsymbol{\pi}) = \sum_{k=1}^{g} (\pi_k - o_k(y))^2$, a.k.a. L_2 loss on probabilities
- (Multi-class) Log loss $L(y, \boldsymbol{\pi}) = -\sum_{k=1}^{g} o_k(y) \log(\pi_k)$, as in logistic regression

Optimal constant predictions (in a node) for both losses are simply the proportions of the contained classes:

$$
\begin{aligned}
c_{\mathcal{N}} &= (\hat{\pi}_1^{(\mathcal{N})}, \dots, \hat{\pi}_g^{(\mathcal{N})}) \quad \text{with} \\
\hat{\pi}_k^{(\mathcal{N})} &= \frac{1}{|\mathcal{N}|} \sum_{(\mathbf{x}, y) \in \mathcal{N}} \mathbb{I}(y = k) \quad \forall k \in \{1, \dots, g\}
\end{aligned}
$$

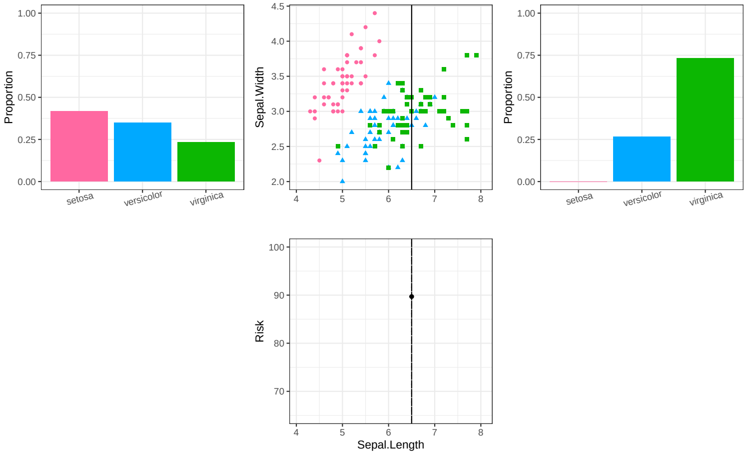
FINDING THE BEST SPLIT

Let's compute the Brier score for all splits, with optimal constant probability vectors in both children



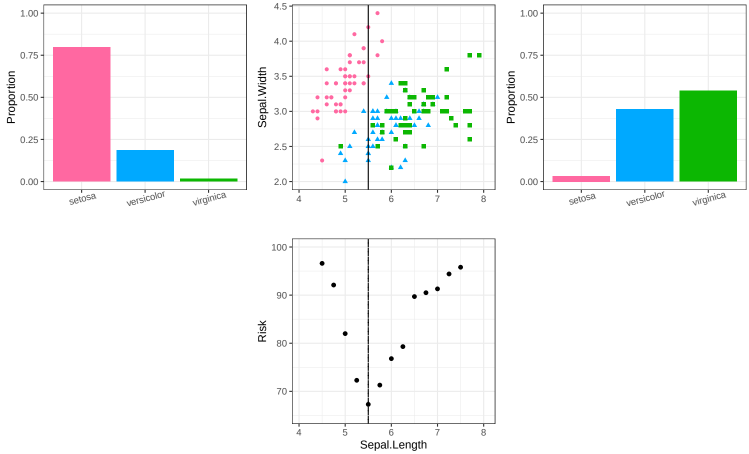
FINDING THE BEST SPLIT

Let’s compute the Brier score for all splits, with optimal constant probability vectors in both children

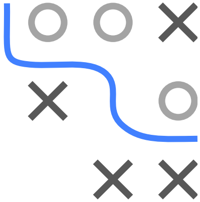


FINDING THE BEST SPLIT

The optimal split point typically creates greatest imbalance or purity of label distribution



RISK MINIMIZATION VS. IMPURITY



- Split crits are sometimes defined in terms of impurity reduction instead of ERM, where a measure of “impurity” is defined per node
- For regression trees, “impurity” is simply defined as variance of y, which is quite obviously L_2 loss
- Brier score is equivalent to Gini impurity

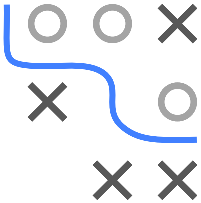
$$I(\mathcal{N}) = \sum_{k=1}^{g} \hat{\pi}_k^{(\mathcal{N})} \left(1 - \hat{\pi}_k^{(\mathcal{N})}\right)$$

- Log loss is equivalent to entropy

$$I(\mathcal{N}) = -\sum_{k=1}^{g} \hat{\pi}_k^{(\mathcal{N})} \log \hat{\pi}_k^{(\mathcal{N})}$$

- Trees can be understood completely through the lens of ERM, so this new terminology is unnecessary and perhaps confusing

SPLITTING WITH MISCLASSIFICATION LOSS



- Often, we want to minimize the MCE in classification
- Zero-One-Loss is not differentiable, but that is a non-issue in the tree-optimization based on loops
- Brier score and Log loss more sensitive to changes in the node probs, often produce purer nodes, and are still preferred

Split 1:

	class 0	class 1
$\mathcal{N}_1$	300	100
$\mathcal{N}_2$	100	300

Split 2:

	class 0	class 1
$\mathcal{N}_1$	400	200
$\mathcal{N}_2$	0	200

- Both splits are equivalent in MCE
- But: Split 2 results in purer nodes, both Brier score (Gini) and Log loss (Entropy) prefer 2nd split